

## ABSTRACT

NEEDHAM, CRAIG DANIEL. Crafting Detailed Kinetic Mechanisms for Gas- and Condensed-Phase Systems using Computational Quantum Chemistry. (Under the direction of Phillip R. Westmoreland).

Chemical mechanisms were created with computational quantum chemistry (CQC) for hypergolic bipropellant interactions, the combustion of an environmentally friendly refrigerant ( $\text{CH}_2=\text{CFCF}_3$ , HFO-1234yf),  $\text{H}_2/\text{O}_2$  combustion, and the interaction between trimethylaluminum (TMA) and a poly(methyl methacrylate) (PMMA) surface. Although the study of each system involved different methods, in all cases the general goal was to arrive at a quantitative understanding of the elementary reaction steps involved.

Two hypergolic bipropellant systems were studied: monomethylhydrazine/nitric acid ( $\text{MMH}/\text{HNO}_3$ ) and tetramethylethylenediamine/nitric acid ( $\text{TMEDA}/\text{HNO}_3$ ). A previously developed mechanism for  $\text{MMH}/\text{RFNA}$  was examined using reactor modeling. A missing element of the chemistry involving the reaction between the aerosolized fuel and oxidizer species was investigated using CQC and it was found to be integral to the ignition process. Reactive molecular dynamics was used to investigate the behavior of  $\text{TMEDA}$  and  $\text{HNO}_3$  at high temperatures.

A mechanism to describe  $\text{CH}_2=\text{CFCF}_3$  combustion was developed using CQC and tested using reactor modeling. A network of possible decomposition routes of the molecule was proposed by analyzing the molecule. Transition-state calculations were performed for each proposed reaction and calculation results were turned into rate-coefficient parameters for use in the kinetic mechanism. Reactor modeling of the new mechanism allowed its behavior to be compared to experimental data. In this way, simulations of the adiabatic flame speed of a

stoichiometric 1234yf/air flame were found to be fairly close to flame speeds found in experimental measurements, supporting the proposed mechanism.

The PrIME process informatics model was used to assess and optimize H<sub>2</sub>/O<sub>2</sub> combustion mechanisms against published experimental data. Mechanisms from the literature were combined and inputted into the PrIME database for use with the accompanying reactor-modeling and uncertainty-quantification (UQ) codes. Experimental data from shock tubes and flames were inputted as well. PrIME's reactor modeling capabilities were used to simulate the experimental results. Then PrIME's UQ tool was used to adjust the pre-exponential factors within their uncertainties to better predict the experimental results. The new, optimized mechanism was published in the PrIME database. The analysis also gave insight into the role of O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>) as a flame inhibitor.

For the TMA/PMMA interaction, CQC was used to investigate the previously unknown mechanism of reaction between the two species. Atomic layer deposition (ALD) experiments produced an IR spectrum that indicated the presence of an unknown species in the system, hypothesized to be the product of a reaction between TMA and PMMA. Possible products were proposed by physical/organic chemistry analysis of the molecules and simulated using CQC. The simulated spectra of these proposed products were then compared to the experimental spectra. The analysis found that the aluminum in TMA coordinates with a C=O bond in the PMMA. The prolonged proximity of the TMA allows it to undergo a six-centered, pericyclic reaction with the PMMA, bonding the aluminum to the PMMA side-group and producing ethane.

© Copyright 2016 Craig Daniel Needham  
All Rights Reserved

Crafting Detailed Kinetic Mechanisms for Gas- and Condensed-Phase Systems using  
Computational Quantum Chemistry

by  
Craig Daniel Needham

A dissertation submitted to the Graduate Faculty of  
North Carolina State University  
in partial fulfillment of the  
requirements for the degree of  
Doctor of Philosophy

Chemical Engineering

Raleigh, North Carolina

2016

APPROVED BY:

---

Prof. Phillip R. Westmoreland  
Committee Chair

---

Prof. Erik E. Santiso

---

Prof. Carol Hall

---

Prof. Don Brenner

## **DEDICATION**

To my parents, Mark and Judy. I have always sought to emulate the kindness and humility with which you have affected so many people's lives.

To my wife, Erinn. Every time I make a wish, I wish for a long, happy life with you.

## **BIOGRAPHY**

Craig Needham was born in Burlington, NJ to Mark Needham, at that time a Captain in the US Army, and Judy Needham, a classically trained city planner. Due to his father's job his childhood was spent moving around the country and the world. He attended Hickory High School in Chesapeake, VA for two years and graduated from Fort Knox High School, in Fort Knox, KY in 2007. He received the Singletary Scholarship to attend University of Kentucky and graduated with a Bachelor of Science in Chemical Engineering in 2011. He began his graduate career at NCSU the following fall and was accepted into Prof. Phil Westmoreland's group at the end of the year. He spent his graduate career studying reactive systems with computational tools, working on a variety of highly collaborative projects over the course of his studies. Most of his graduate work concerned investigating the chemistry of combustion and related processes.

## ACKNOWLEDGMENTS

The work presented in this thesis was funded by multiple sources:

- United States Army Research Office Multi-University Research Initiative (“Spray and Combustion of Gelled Hypergolic Propellants,” Grant W911NF-08-1-0171)
- Graduate Assistantships in Areas of National Need Fellowship (GAANN Grant P200A09008)
- National Science Foundation (“PrIME Database Support,” Supplement to Award 1340609; “Multiple-Scale Investigation of Chemical Looping with Oxygen Carrier Uncoupling,” Award 1510900)
- E. I. du Pont de Nemours and Company / Chemours (“Building a refrigerant combustion model”)
- Air Force Office of Scientific Research (“Stationary Mixed Metal-Oxide Acid Catalysts for Endothermic Fuel Decomposition and Enhanced Ignition/Flame Holding Characteristics,” Award GG11604-141694 with Dr. Chiping Li as the technical monitor).

Significant help was also provided to me by my group members. Dr. Nicole Labbe, while having a large hand in the hypergolic work presented below, also played a significant mentorship role during the end of her graduate career with the group when I was just starting. Many of the computational skills I gained in graduate school were started under her tutelage. Dr. Vikram Seshadri, with whom I shared an office for much of my studies, was equally helpful in both helping me develop and acting as a sounding board for ideas. The advice

both of them gave me about how to make my graduate school experience easier was indispensable, and I have tried to pass it on to the best of my ability. Sara Jo Taylor also deserves credit not only as a fellow group member but also as someone who was always willing to talk when I needed to.

My advisor, Dr. Phil Westmoreland, has showed me that a relentlessly good attitude can beat even the worst of days. I thank him for all his advice on work, the profession, and life that he has given me over the years. More than just computational techniques and chemical engineering principles, he taught me an intuition about chemical reactions that I will always count as the most useful scientific skill I learned during my graduate studies. Most of all, he taught me the joy in having your fingers in a lot of pies.

My family has been as supportive of me as anyone could be and has given me every advantage in life. I owe them everything I am and they all worked very hard to make me into the person I have become.

My wife, Erinn, who also finds herself among those I had the pleasure of collaborating with, deserves more credit than anyone (including probably myself) for my graduate career. Her hard work and determination inspire me to be better every day. Without her help I would probably never even wake up in the morning.

Much of the work presented in this thesis has been done in collaboration. I have attempted to acknowledge those who helped me with my work at the beginning of each chapter or during the course of each chapter where appropriate.



## TABLE OF CONTENTS

<b>TABLE OF CONTENTS .....</b>	<b>VI</b>
<b>LIST OF TABLES .....</b>	<b>XII</b>
<b>LIST OF FIGURES .....</b>	<b>XIII</b>
<b>CHAPTER 1. INTRODUCTION .....</b>	<b>1</b>
<b>CHAPTER 2. METHODS.....</b>	<b>4</b>
2.1 <i>Computational quantum chemistry .....</i>	4
2.2 <i>Calculating reaction rate data from CQC simulations using ChemRate .....</i>	4
2.3 <i>Reactor modeling with CHEMKIN-PRO .....</i>	5
2.4 <i>Reactive molecular dynamics.....</i>	6
2.4.1 <i>ReaxFF.....</i>	7
2.4.2 <i>RxnMD .....</i>	8
<b>CHAPTER 3. PREDICTIVE MODELING OF HYPERGOLIC BIROPELLANT PERFORMANCE:           REACTION-KINETICS           MODEL           FOR MONOMETHYLHYDRAZINE AND NITRIC ACID .....</b>	<b>9</b>
3.1 <i>Contributions of this author to the work in this chapter.....</i>	9
3.2 <i>Introduction.....</i>	10
3.3 <i>MMH/RFNA mechanism development.....</i>	11
3.3.1 <i>H<sub>2</sub>/O<sub>2</sub> set: forming a basis .....</i>	11

3.3.2	<i>H/N/O set: ammonia kinetics</i> .....	11
3.3.3	<i>H/C/N/O set: adding hydrocarbons</i> .....	14
3.3.4	<i>MMH and RFNA: developing a hypersonic model</i> .....	18
3.3.5	<i>Reduction of full mechanism</i> .....	19
3.4	<i>Performance evaluation</i> .....	20
3.5	<i>Aerosol mechanism</i> .....	25
3.6	<i>TMEDA/RFNA simulations</i> .....	31
3.7	<i>Conclusion</i> .....	36
 <b>CHAPTER 4. A COMBUSTION AND FLAMMABILITY REACTION MECHANISM FOR REFRIGERANT HFO-1234YF</b> .....		<b>37</b>
4.1	<i>Introduction</i> .....	37
4.2	<i>Methods for determining collisional-reaction rate coefficients</i> .....	37
4.3	<i>Mechanism development</i> .....	39
4.3.1	<i>Determining possible reaction pathways</i> .....	39
4.3.2	<i>Unimolecular decomposition reactions</i> .....	40
4.3.3	<i>Hydrogen abstraction reactions</i> .....	43
4.3.4	<i>Addition reactions</i> .....	46
4.3.5	<i>Mechanism summary</i> .....	51
4.4	<i>Computational evaluation and reaction path analysis</i> .....	54

4.4.1	<i>Mechanism evaluation by CHEMKIN-PRO</i> .....	54
4.4.2	<i>Reaction-path analysis</i> .....	56
4.5	<i>Conclusions</i> .....	59
<b>CHAPTER 5. DYNAMIC CHEMICAL MODEL FOR H<sub>2</sub>/O<sub>2</sub> COMBUSTION DEVELOPED THROUGH A COMMUNITY WORKFLOW .....</b>		<b>60</b>
5.1	<i>Contributions of this author to the work in this chapter</i> .....	60
5.2	<i>Introduction</i> .....	61
5.3	<i>Theory</i> .....	61
5.3.1	<i>The architecture and use of PrIMe</i> .....	61
5.3.2	<i>Towards a more careful preservation of rate constants</i> .....	64
5.4	<i>Data selection procedures</i> .....	65
5.4.1	<i>Reaction sets</i> .....	65
5.4.2	<i>Experimental data</i> .....	66
5.4.3	<i>Resolving data inconsistencies</i> .....	66
5.5	<i>Results and discussion</i> .....	67
5.5.1	<i>O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>)</i> .....	68
5.5.2	<i>Insights from data inconsistency</i> .....	69
5.6	<i>Conclusion</i> .....	70

<b>CHAPTER 6. TEMPERATURE-DEPENDENT REACTION BETWEEN TRIMETHYLALUMINUM AND POLY(METHYL METHACRYLATE) DURING SEQUENTIAL VAPOR INFILTRATION: EXPERIMENTAL AND <i>AB INITIO</i> ANALYSIS .....</b>	<b>71</b>
6.1 <i>Contributions of this author to the work in this chapter.....</i>	71
6.2 <i>Introduction.....</i>	72
6.3 <i>Experimental procedures .....</i>	74
6.3.1 <i>Chemicals and materials.....</i>	74
6.3.2 <i>Sequential vapor infiltration (SVI).....</i>	75
6.3.3 <i>Characterization .....</i>	76
6.3.4 <i>Quantum chemistry analysis.....</i>	77
6.4 <i>Results .....</i>	77
6.4.1 <i>In situ FTIR and QCM .....</i>	77
6.4.2 <i>Quantum chemical analysis .....</i>	84
6.4.3 <i>Observed chromatic shift.....</i>	88
6.5 <i>Discussion .....</i>	89
6.6 <i>Summary.....</i>	93
6.7 <i>Acknowledgements .....</i>	94
<b>CHAPTER 7. CONCLUSIONS AND RECOMMENDATIONS .....</b>	<b>95</b>

7.1	<i>Conclusions</i> .....	95
7.1.1	<i>Hypergolic Bipropellants</i> .....	95
7.1.2	<i>HFO-1234yf refrigerant combustion</i> .....	96
7.1.3	<i>PrIME investigation of H<sub>2</sub>/O<sub>2</sub> combustion</i> .....	97
7.1.4	<i>Interaction between TMA and PMMA</i> .....	99
7.2	<i>Recommendations for future work</i> .....	99
<b>REFERENCES</b> .....		<b>104</b>
<b>APPENDICES</b> .....		<b>114</b>
<b>APPENDIX A. CHEMKIN MECHANISMS</b> .....		<b>115</b>
A.1	<i>Labbe MMH/RFNA Sets</i> .....	115
A.1.1	<i>Full Labbe Model</i> .....	153
A.1.2	<i>RedLabbe Model</i> .....	287
A.2	<i>ARL MMH/RFNA Sets</i> .....	430
A.2.1	<i>Full ARL Model</i> .....	485
A.2.2	<i>Red ARL Model</i> .....	516
A.3	<i>HFO-1234yf</i> .....	543
<b>APPENDIX B. GAUSSIAN ARCHIVE FILES</b> .....		<b>621</b>
B.1	<i>Aerosols</i> .....	621
B.2	<i>HFO-1234yf sub-mechanism</i> .....	623

<i>B.3</i>	<i>PMMA/TMA</i> .....	639
<b>APPENDIX C. RELEVANT PRIME DATA</b> .....		<b>642</b>
<i>C.1</i>	<i>QoIs</i> .....	642

## LIST OF TABLES

Table 4.1: Active fractions for species used in collisional rate derivations.....	39
Table 4.2: Sub-mechanism for the combustion of HFO-1234yf into small species.....	52
Table 4.3: Thermochemistry data for new species .....	53
Table 6.1: Experimental, calculated and adjusted IR peak positions for methyl trimethylacetate as a model for PMMA. Experimental and calculated peak positions are also shown for the starting material after exposure to trimethylaluminum.....	87
Table B.1: Experimental shock-tube ignition-delay QOIs. ....	642
Table B.2: Experimental flame-speed QOIs. ....	645

## LIST OF FIGURES

Figure 3.1: Reactant profiles. Simulations are shown as lines and experiments are shown as points.....	12
Figure 3.2: Major product profiles.....	13
Figure 3.3: NO and N <sub>2</sub> O profiles. Left axis corresponds to N <sub>2</sub> O mole fraction and right axis corresponds to NO. ....	14
Figure 3.4: Sensitivity analysis for NO (top) and N <sub>2</sub> O (bottom). The five most sensitive reactions are shown for both species. ....	15
Figure 3.5: Fuel profiles.....	16
Figure 3.6: Oxidant O <sub>2</sub> and major product H <sub>2</sub> O profiles. ....	17
Figure 3.7: Product profiles. ....	17
Figure 3.8: Minor product and intermediate profiles.....	18
Figure 3.9: Temperature and reactant profiles for a fuel-lean ( $\phi = 0.5$ ) MMH–RFNA flame. Labbe mechanisms are shown in blue and ARL mechanisms are shown in orange. The thicker lines represent full sets and the thinner lines represent the reduced sets.....	21
Figure 3.10: Major product profiles for fuel-lean ( $\phi = 0.5$ ) MMH–RFNA flame.....	22
Figure 3.11: Temperature and reactant profiles for stoichiometric ( $\phi = 1$ ) MMH–RFNA flame. ....	23
Figure 3.12: Major product profiles for stoichiometric ( $\phi = 1$ ) MMH–RFNA flame. ....	24
Figure 3.13: Temperature and reactant profiles for fuel-rich ( $\phi = 2$ ) MMH–RFNA flame. ..	25
Figure 3.14: Major product profiles for fuel-rich ( $\phi = 2$ ) MMH–RFNA flame. ....	26
Figure 3.15: Simulation results showing the proton transferring from HNO <sub>3</sub> to MMH as more assisting molecules are added. Atoms of interest are highlighted in green and pink. HNO <sub>3</sub> in MMH is shown on top while MMH in HNO <sub>3</sub> is shown on bottom.....	28
Figure 3.16: Potential energy diagram of system as assisting molecules are added.....	30
Figure 3.17: H-abstraction routes for TMEDA.....	32
Figure 3.18: Concentration profiles for three species apposite for distinguishing the H-abstraction initiation channel of TMEDA/HNO <sub>3</sub> combustion.....	33



Figure 3.19: Major reactants, products, and abstractors in high temperature TMEDA/HNO <sub>3</sub> reaction.....	34
Figure 3.20: Major TMEDA decomposition pathway .....	35
Figure 4.1: Sub-mechanism describing the decomposition of HFO-1234yf into small fluorocarbon species. ....	41
Figure 4.2: Schematic of the electron transfer occurring during reaction $u_3$ .....	42
Figure 4.3: Energy diagram for unimolecular concerted reaction pathways $u_2$ and $u_3$ .....	43
Figure 4.4: Energy surfaces for H-abstraction from 1234yf.....	44
Figure 4.5: H addition to 1234yf and subsequent $\beta$ -scission of tetrafluoropropan-1-yl.....	47
Figure 4.6: Decomposition channels of tetrafluoropropoxyl radical produced by reaction $b_{12}$ .....	48
Figure 4.7: Decomposition of diradical product of reaction $c_2$ .....	50
Figure 4.8: Isomerization pathways after OH addition.....	51
Figure 4.9: Burning velocity of stoichiometric 1234yf in 35% O <sub>2</sub> /65% N <sub>2</sub> mixture [95]. Note: experimental data (solid squares) shown are from Takizawa's 800 torr case. Calculations (solid circles) were performed at atmospheric conditions because the experimental data shows little variation with pressure.....	55
Figure 4.10: Burning velocity of stoichiometric 1234yf/air mixture.....	56
Figure 4.11: Concentration profiles for reactants and major products from combustion of stoichiometric 1234yf/air mixture at 300K.....	57
Figure 4.12: Concentration profiles for main intermediate from combustion of stoichiometric 1234yf/air mixture at 300K.....	58
Figure 5.1: Step-by-step process for mechanism optimization using PrIME's UQ capabilities. Lead investigators (grouped by institution) for each step are listed under the area description. ....	63
Figure 5.2: Normalized dataset consistency sensitivity to ten data attributes (QoIs) with highest sensitivity. All are shock-tube QoIs except a00000483, which is a flame speed. Black bars represent upper-bound sensitivity; gray, lower-bound sensitivity.....	68
Figure 5.3: Impact factor and sensitivity of the prediction of flame speed QoI a00000484 to the top 20 reactions ranked by impact factor, where the impact factor is $0.5\log(U_e/L_e)$ multiplied by the absolute sensitivity. Note: For font reasons, O <sub>2</sub> ( <sup>1</sup> $\Delta_g$ ) is shown as O2( <sup>1</sup> D) in the PrIME database.....	69

Figure 6.1: *In situ* FTIR spectra collected after 150 TMA doses on 170 nm thick PMMA films on silicon. The spectra are shown in differential mode, relative to the starting PMMA. Two spectra collected after TMA + water at 70 and 150 °C are also included, and similarly referenced to the starting PMMA. .... 79

Figure 6.2: (a) Overall QCM mass response for 50 nm PMMA films exposed to 100 TMA doses at 70, 100 and 140 °C. (b) Magnified view of the mass response after 41-43 TMA doses..... 82

Figure 6.3: *In situ* FTIR data collected at 70 and 150 °C at several times during 150 TMA dose steps. Each differential spectrum is referenced to the preceding spectrum shown. The data shows different reaction trends at different temperatures, most noticeably in the region between 1500 and 1700  $\text{cm}^{-1}$ . .... 84

Figure 6.4: Relaxed chemical structures calculated using *ab initio* modeling, and their corresponding vibrational spectra referenced to spectra from structures calculated without TMA interaction. The bond models used for the calculations are also shown. The calculated spectrum for the PMMA model shows peaks at 1790  $\text{cm}^{-1}$  corresponding to C=O stretch, and features at 1307, 1212 and 1182  $\text{cm}^{-1}$  associated with =C-O- and -O-CH<sub>3</sub> coupled modes. For each structure, interaction with TMA leads to loss of the 1790  $\text{cm}^{-1}$  C=O mode and changes in the C-O vibrations. The peak at 1725  $\text{cm}^{-1}$  is TMA coordinated to the C=O in a physisorbed state, and is consistent with the IR and QCM results at lower temperature. Peaks between 1750 and 1500  $\text{cm}^{-1}$  in products **B** and **C** correspond to C=O coordinated with a neighboring covalently-bound Al-O, forming a resonant C=O $\cdots$ Al-O-C unit, consistent with the higher temperature product mode observed at 1568  $\text{cm}^{-1}$ . .... 86

Figure 6.5: Bulk PMMA powder, as received, was treated with 600 TMA doses at varying temperatures. At increased temperatures a color change was observed that was not seen at lower temperatures. A) PMMA powder as received. B) PMMA powder with 600 SVI TMA doses at 90 °C. C) PMMA powder with 600 SVI TMA doses at 150 °C immediately after removal from the reactor, after D) 1.5 hrs E) 24 hrs and F) 9 months. .... 89

Figure 6.6: Proposed pericyclic activation of ester to form metal acetate..... 93

## CHAPTER 1. INTRODUCTION

The creation of chemical kinetic mechanisms has long been a subject of inquiry, especially in the world of combustion [1–14] where even the simplest of reaction systems can contain hundreds of elementary reactions [9]. The development of more sophisticated tools has allowed mechanisms to transition from more lumped models [1,2] to more detailed groups of elementary reactions [4,9]. Particularly the development of computational quantum chemistry (CQC) [15–17] and sophisticated computational reactor modeling [18–21] have aided in the more targeted exploration of reacting systems, although other useful computational techniques continue to be developed. In this work, a variety of these computational tools is used to probe unexplored chemistry in a series of reactive systems.

At its most basic, a detailed chemical kinetic mechanism consists of a list of all the chemical reactions that may happen in a given system, along with parameters to describe the rate of each reaction. Generally, computation time will scale with number of species in a given mechanism. Reactions deemed unlikely or of negligible influence are neglected. The simplest description of a reaction rate coefficient comes from fitting a modified Arrhenius equation (equation 1) to measured or calculated data.

$$k(T) = AT^n e^{-E_A/RT} \quad (1.1)$$

The three parameters that are fitted are the pre-exponential factor,  $A$ , the temperature exponent,  $n$ , and the activation energy,  $E_A$ . In the absence of experimental data, these parameters can be fitted to rate coefficients calculated using transition-state theory [22]. This calculation requires knowledge of the energy of transition state, the molecular geometry that

exists at the maximum energy point along the lowest energy line connecting the reactants and products of a given reaction. CQC tools can be used to calculate this transition state.

In more complicated cases, it may be necessary to specify more than just the modified Arrhenius parameters to capture the rate of a reaction fully. A common way of accounting for more complicated reaction behavior is by expressing the rate as the sum of two modified Arrhenius expressions, although this is generally inadequate if a reaction is pressure-dependent. Pressure-dependent reactions, or collision-mediated reactions, can be said to occupy three different regimes of behavior: low P, high P, and a transition region. At low pressure, decomposition reactions are linearly dependent on the concentration of so-called third bodies, or species that give the reactant energy through collisions but do not undergo chemical changes upon reaction. At high enough pressure, this dependence disappears due to the reactant having more than adequate access to other species to collide with. The simplest way to describe pressure dependence is to assign a given reaction one set of rate parameters for the low-pressure, concentration-dependent region and one set of rate parameters for high-pressure, concentration-independent region. In many cases, the region between the low- and high-pressure regions is sufficiently large and different in behavior that some mathematical description of the transition is necessary. In these cases, it is common to use the Troe equation [23]. A sufficient description of the Troe equation form and its simpler analog, the Lindemann form, can be found in the CHEMKIN collection [18].

Simply creating a chemical mechanism is not sufficient to prove its veracity and worth. It is always necessary to use it to simulate experimental data and determine if the system of

interest has been sufficiently represented. For this purpose there is a variety of reactor modeling programs [19–21] that allow the user to produce simulated data that can be compared directly to experimental data. These techniques are almost always numerical solvers that attempt to satisfy the boundary conditions for a given reactor type by simultaneously solving the rate equations provided in the mechanism with the transport and/or governing equations of the reactor. Reactor modeling is the consistency check that allows reaction mechanisms to be proven conclusively to be useful for the system they claim to describe.

Armed with a sufficient knowledge of CQC techniques, transition-state theory, chemical kinetic theory, and provided with a few simple computational tools for mathematical rate derivation and reactor modeling, it is possible to propose and create detailed chemical kinetic mechanisms for a large variety of reactive systems.

## CHAPTER 2. METHODS

### 2.1 *Computational quantum chemistry*

Many of the studies within this dissertation require the use of quantum chemical calculations. Computational quantum chemistry (CQC) uses solutions of the Schrödinger equation [24] to describe chemical events on the atomic scale. The CQC field emerged out of the development of quantum mechanics during the late 19th to early 20th centuries. Once computation became possible, it began to be used to perform the calculations necessary to solve complicated systems [25,26]. Today, there exist many software packages that perform computational quantum-chemistry calculations, such as GAMESS [16], Gaussian [15], and GROMACS [17], to name a few. All CQC work reported in this thesis was conducted with Gaussian09 [15]. In most cases the CBS-QB3 method [27,28] was employed, although often preliminary exploratory calculations were done with the B3LYP/6-31G(d,p) method [29,30]. GaussView [31] was used to set up the molecular structures and to aid in the interpretations of results such as vibrational frequencies. Most transition-state calculations used the quadratic synchronous transit method (QST3) [32,33]. If there was any uncertainty about transition states being identified correctly, intrinsic reaction coordinate (IRC) calculations [34,35] were performed as a check.

### 2.2 *Calculating reaction rate data from CQC simulations using ChemRate*

ChemRate [36] was used to convert the results of QC geometry optimizations to ideal-gas thermochemistry in the NASA format [37] as well as to calculate rate parameters. Rate-

coefficient calculation for a given reaction was done by first inputting data for all involved species to the program from Gaussian geometry-optimization output files. For pressure-dependent kinetics, the collision model was assumed to be exponential-down with a constant energy transfer parameter  $\alpha$  of  $250 \text{ cm}^{-1}$  for each species. Barker [38] showed that while an energy-dependent  $\alpha$  is more accurate, a constant  $\alpha$  still produces reasonable results. Lennard-Jones parameters were either taken from the CHEMKIN Transport Manual [18] or estimated from similar species. The transition-state data were extracted from the corresponding output file in a similar manner to the reactant and product species. The reactants, products, and transition state were then linked together as a reaction. To compute the rate, tasks were created at temperatures varying from 300 – 2300 K, the temperature window of most interest. A ChemRate master-equation analysis was then carried out at each of these temperatures. After the calculation completed, rate coefficients were evaluated for the reaction.

### 2.3 *Reactor modeling with CHEMKIN-PRO*

Reactor modeling of reaction mechanisms was done with CHEMKIN-PRO [21]. Detailed descriptions of the different types of reactors that can be modeled and the method of running CHEMKIN simulations can be found in the CHEMKIN Collection [18]. The tightness of the solution convergence is generally controlled through the GRAD and CURV parameters, which control the maximum amount of gradient and curvature allowed between grid points in the solution. To help simulations with convergence, these parameters are left rather loose initially and then are tightened after a preliminary solution is reached, often multiple times

for each simulation. For all CHEMKIN simulations, the final GRAD and CURV parameters were set to 0.1 and 0.5, respectively. For flames, the final solution was also set to include the Soret thermophoresis effect.

#### 2.4 *Reactive molecular dynamics*

The method of molecular dynamics is a well-established one, dating back to Alder and Wainwright [39] in 1959, where it was originally conceived as a numerical solution to the many-body problem in physics. Using Hamilton's equations of motion and basic descriptions of the forces between atoms, molecular dynamics has long been used to simulate material properties [40] and protein folding [41]. More recently there has been a push in the field to be able to simulate chemical reactions using this method. This goal entails the creation of complex, "reactive" force fields with the goal of being able to simulate the reactions and physical properties accurately for any reactive system.

One key to a reactive force field is using bond order (BO). One approach is to say a simple sigma bond has a BO of one, a double bond has a BO of two, and so on with completely unbound atoms having a BO of zero. For a dynamic system, the BO will change for each bond depending on the configuration of the constituent and neighboring atoms. Each force field includes parameters to define the equilibrium bonding geometry and equations to describe how the BO will change as the geometry of the system changes. Where many force fields differ is the atom types and atomic/molecular forces they are able to describe.



### 2.4.1 *ReaxFF*

ReaxFF, as implemented in LAMMPS [42], is currently the most widely used reactive force field. It was developed by van Duin et al. in 2001 [43] and was originally parameterized for hydrocarbons. Unlike REBO, ReaxFF was developed to include intermolecular forces from the start and was fitted to reproduce reaction energy curves in a variety of hydrocarbon systems. For the most part, it was fitted against data acquired from density-functional theory calculations.

Since the original publication, many ReaxFF force fields have been created for more complex systems [44–51]. Each of these force fields performs well in the range of systems for which it was created but cannot be extended to systems with different species in them. For example, the reactive force field for gold can only simulate systems with gold, hydrogen, and oxygen [51]. Even force fields that have the same atoms in them are differently parameterized for their specific applications, as with the “Budzien” [49] and “RDX” [45,52] force fields. Each of these force fields contains C/H/O/N, but the Budzien force field is parameterized for shock-induced reactions in pentaerythritol tetranitrate crystals, while the RDX force field is parameterized for shock-induced reactions in RDX, a high-energy material. It is unclear without further investigation how easily these force fields translate to dissimilar systems. The lack of widespread applicability of any one ReaxFF force field, coupled with the difficulty of parameterizing a new force field, has hindered anyone wanting to work with ReaxFF on a new system.

### 2.4.2 *RxnMD*

RxnMD is a standalone reactive-molecular-dynamics simulation program [53] that started as MD\_REACT [54,55]. It is intended that atomic parameters from almost any equilibrium force field can be loaded into RxnMD and used to simulate reactive (i.e., non-equilibrium) systems. The advantage of using the parameters from equilibrium force fields is that they have already been developed to represent the physical properties of a system accurately. The latest version uses a set of force-field equations called RMDff, developed by Smith et al. [56]. Instead of relying on BO tracking, as with the other force fields discussed here, RMDff uses a valence-bond representation of the reaction coordinate (RC). The RC is a parameter that describes the position of a reacting species on the energy curve that spans from the reactants through the transition state to the products. At the reactant geometry/energy, the RC is zero, and at the products, the RC is one. Switching functions are used to transition the energy smoothly from reactants to products and to facilitate the change in atom type that occurs [57]. The advantage of the valence-bond technique is that reactions develop from the solutions of the equations of motion and not from costly on-the-fly quantum-chemistry calculations of total system bonding.

**CHAPTER 3. PREDICTIVE MODELING OF HYPERGOLIC BIROPELLANT  
PERFORMANCE: REACTION-KINETICS MODEL FOR  
MONOMETHYLHYDRAZINE AND NITRIC ACID**

Work in this chapter done in collaboration with Nicole Labbe<sup>1,2</sup>, Phillip R. Westmoreland<sup>3</sup>, Tyler G. Voskuilen<sup>4</sup>, and Timothée L. Pourpoint<sup>4</sup>.

<sup>1</sup>Chemical Sciences & Engineering Division, Argonne National Laboratory, Argonne, IL 60439

<sup>2</sup>Chemical Engineering Dept., University of Massachusetts Amherst, Amherst, MA 01003

<sup>3</sup>Chemical and Biomolecular Engineering Dept., North Carolina, State University, Raleigh, NC 27695

<sup>4</sup>School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907

*3.1 Contributions of this author to the work in this chapter*

The major role of this author in the following work was the study of aerosol chemistry and the study of TMEDA/RFNA interaction. Also, all simulation results for MMH/RFNA presented below were conducted by this author, although many of the simulations were done to mirror the simulations presented in the dissertation of Nicole Labbe [58] for the purposes of publishing the MMH/RFNA mechanism described in §3.3 that was developed by Dr. Labbe during her doctoral work. All work described in that section in reference to building and reducing the MMH/RFNA mechanism was done by Dr. Labbe, though the process is

described in the words of this author and presented here to give the scope of the work done on MMH/RFNA. Unlike elsewhere in this dissertation where a co-authored publication is reproduced, this chapter is written entirely in the words of this author.

### 3.2 *Introduction*

Hypergolic bipropellants, often shortened to “hypergols”, consist of a fuel and an oxidizer that ignite spontaneously when mixed. Their relatively foolproof mechanism of ignition has made them useful as rocket fuels and for aerospace applications. The most common hypergolic bipropellant pair is monomethylhydrazine (MMH) and red fuming nitric acid (RFNA). The interaction between the two compounds is heavily based on nitrogen chemistry, a part of the field that has seen considerable study [59–67]. The addition of the MMH/RFNA to this system has seen less study, though a recent publication by Anderson et al. [11] at the Army Research Labs (ARL) released a gas-phase mechanism for hypergolic combustion of MMH/RFNA based mostly on literature sources for nitrogen chemistry. This model was developed in an attempt to provide kinetics to a CFD model of an impinging stream vortex engine (ISVE). Although the model was created for hypergols, its significant basis in nitrogen chemistry should give it the versatility to simulate other nitrogenated systems. However, previous tests run by this group on comparing the ARL mechanism to experimental data [59,62,67,68] on nitrogen chemistry showed that its performance was unsatisfactory. This work focuses on the development of an improved nitrogen mechanism. The goal of this mechanism is to simulate hypergols with high accuracy, and the focus on a

strong basis will give the new mechanism versatility while also improving the performance for the target hypergolic system.

### 3.3 *MMH/RFNA mechanism development*

The chemical reaction sets described here are included in the supplementary material. Reverse-reaction rate coefficients are obtained by microscopic reversibility for gas-phase reactions.

#### 3.3.1 *H<sub>2</sub>/O<sub>2</sub> set: forming a basis*

The reaction system between molecular hydrogen and oxygen is a particularly well studied area in combustion kinetics [10,13,69–71], enabling us to use a previously developed mechanism with little modification. The model developed by Burke et al. [10] was used due to its consideration of many different experimental outcomes (e.g., ignition delay in shock tubes, laminar flame speed in premixed flames, mole fractions, rate constants, branching ratios), and the prevalence of falloff and third-body efficiency data.

#### 3.3.2 *H/N/O set: ammonia kinetics*

The addition of nitrogen chemistry to H/O mechanisms has seen considerable attention in the combustion community, and a number of models have been developed [9,11,61,63–66,72–74]. The nitrogen chemistry in the new model was developed by aggregating rate constants from these models and then filtering through the aggregated data—eliminating unrealistic rate constants and giving special attention to those rates with fall-off parameters. The first-pass set was iteratively reduced by comparing output to experimental data [59,60,62,67,68]

and then using sensitivity analysis to identify the most important reactions. Bias was also given to reactions from mechanisms that compared better to the experimental data.

To compare the performance of the nitrogen chemistry of the new model to ARL's, an ammonia flame study conducted by Bian et al. [59] was simulated for both models. This flame allows comparison of the models' performance in the absence of carbon. The new model predicts the profiles of the reactants and the major products ( $\text{H}_2\text{O}$  and  $\text{N}_2$ ) about as well as the ARL mechanism, with only slight differences in curve shape and magnitude. The profiles for the reactants and major products are shown in figures 3.1 and 3.2, respectively.

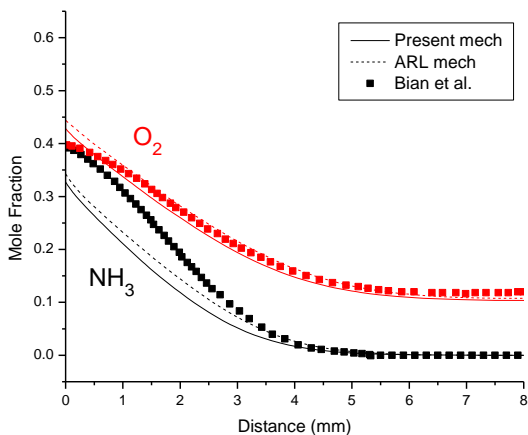


Figure 3.1: Reactant profiles. Simulations are shown as lines and experiments are shown as points.

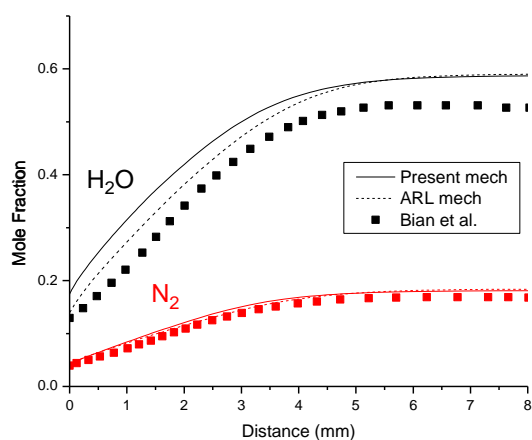


Figure 3.2: Major product profiles.

It is in the prediction of NO, a minor product, and N<sub>2</sub>O, an important intermediate, where the new model shows especially large improvements. These profiles are shown in figure 3.3. A sensitivity analysis on these two species, shown in figure 3.4, shows which reactions are most likely to be responsible for the improvements.

The only reaction that appears in both sensitivity plots is R2.1, which in the new model is taken from Burke et al. [10] and in the ARL mechanism is taken from Masten et al. [75,76]



The improvement here comes from Burke's consideration of many varied combustion schemes—using both shock tubes and flames and testing rates, ignition delay times, flames speeds, and more—while Masten was only comparing rates that had been reported in the literature at the time to his shock-tube experiments.

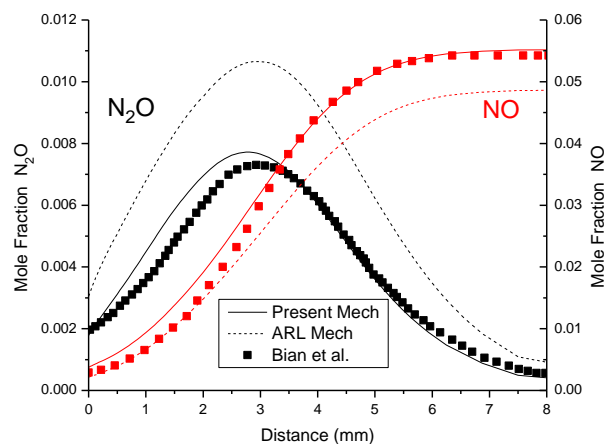


Figure 3.3: NO and N<sub>2</sub>O profiles. Left axis corresponds to N<sub>2</sub>O mole fraction and right axis corresponds to NO.

### 3.3.3 *H/C/N/O set: adding hydrocarbons*

Developing a model without carbon was desirable because of the importance of nitrogen chemistry in the MMH–HNO<sub>3</sub> system and because excluding carbon kept the mechanism small. The next step in making the full chemistry set was to add some of the more common carbon-containing molecules that would show up during combustion, namely hydrocarbons and related species, but in doing so it was important to add in chemistry for species containing both carbon and nitrogen. This expansion to the H/N/O set was developed in much the same way as the H/N/O set itself was, by pulling rate data from many published sources [9,11,61,63,65,73,74,77–79] and then eliminating different rate data depending on the criteria described above.



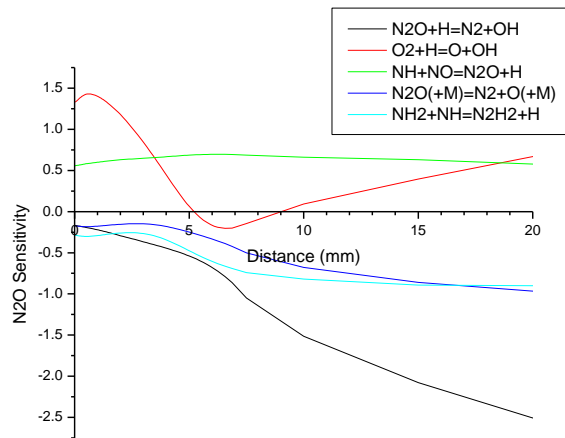
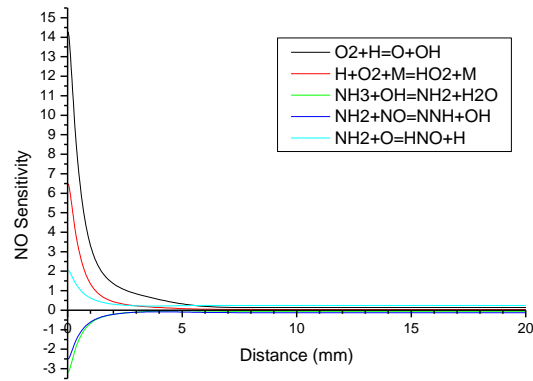


Figure 3.4: Sensitivity analysis for NO (top) and N<sub>2</sub>O (bottom). The five most sensitive reactions are shown for both species.

To compare the new set to reference [11], the two models were used to simulate the stoichiometric case of a methane/ammonia/oxygen MBMS flame study conducted by Tian et al. [65]. This study was chosen due to the simplicity of the reactants and the fact that both models contained all of the species in the reactant mixture. The reactant mixture that was

chosen for simulation is referred to by Tian et al. as  $R=0.5$ , implying that it was a stoichiometric flame with a molar ratio of 2:1  $\text{CH}_4:\text{NH}_3$ . Though not reported in the paper, the authors confirmed that the modeling work they did required shifting the temperature profile 4.5mm away from the burner [80]. To make up for this discrepancy in our modeling, all modeled profiles were shifted 4.5mm away from the burner for comparison with the data in the paper.

Profile for the reactants and major products are shown in figures 3.5-3.7. It can be seen that for the most part, the ARL model and the new model perform quite similarly with respect to these species, especially when taking into account any uncertainty that may be introduced by shifting the data. The biggest notable deviation here is that the ARL model fits the curve of the experimental CO profile a bit better than the new model, but both modeled profiles show agreement with the data.

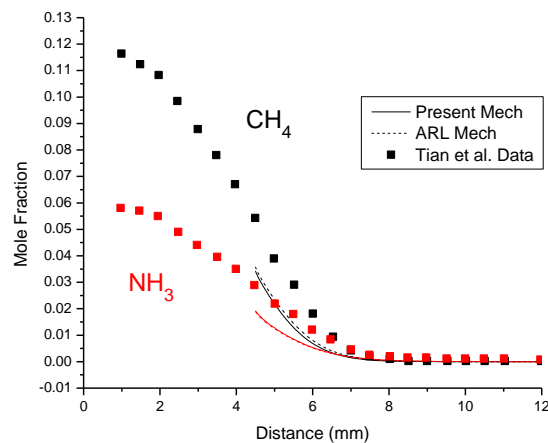


Figure 3.5: Fuel profiles.

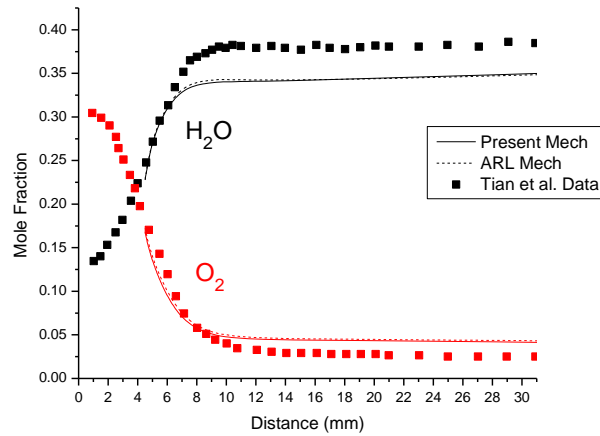


Figure 3.6: Oxidant  $O_2$  and major product  $H_2O$  profiles.

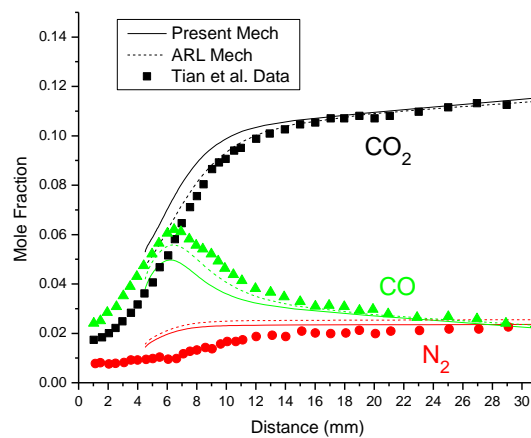


Figure 3.7: Product profiles.

Profiles for some of the minor products and intermediates are shown in figure 3.8. Here again the models perform similarly for all species except in this case  $NO$ , where the ARL model underpredicts the concentration while the new model overpredicts it. For  $NO_2$ , both models

predict almost no concentration ( $\sim 10^{-6}$  for both) while the data clearly show it as a minor product.

Although there are some minor differences in the predicted profiles, especially in the case of NO and slightly in the case of CO, the two models are comparable in their performance for the  $\text{CH}_4/\text{NH}_3/\text{O}_2$  flame. The new model has been able to improve upon the nitrogen chemistry of the ARL model and to replicate the ARL model's performance with regard to a flame containing nitrogen and carbon chemistry.

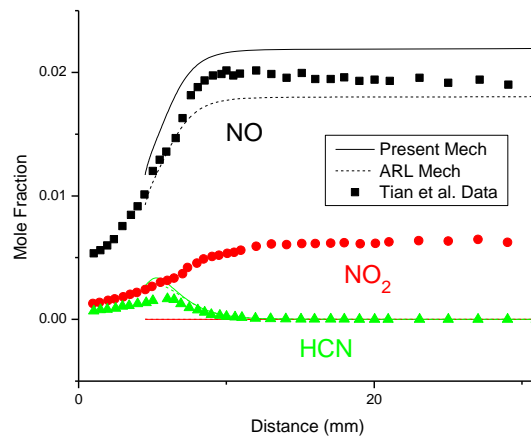


Figure 3.8: Minor product and intermediate profiles.

### 3.3.4 MMH and RFNA: developing a hypersonic model

Once the base set for carbon and nitrogen chemistry was established, it was necessary to add chemistry for the desired hypersonic bipropellants and related species. These kinetics were taken mostly from the ARL model [11] and from the shock-tube study conducted by Sun et al. [74]. Any abstraction routes not accounted for by Sun et al. [74] were estimated using

linear free-energy relationships. After adding the hypergolic chemistry, the full reaction set consisted of 177 species and 1620 reactions. The full model, hereafter referred to as the Labbe model, can be found in Appendix A.

### 3.3.5 *Reduction of full mechanism*

The Labbe set represents a rigorous, detailed model for the reactions of not only MMH with RFNA but also combustion of other nitrogen-containing fuels. However, this set is too large to be used in the CFD simulations. To remedy this, the full mechanism had to be stripped down to the essential species and reactions. For the purposes of comparison, the same techniques used to reduce the new model were used to reduce the ARL model.

Each model was iteratively reduced by first eliminating reactions that were found by sensitivity analysis to have little effect on the MMH–RFNA reaction system. Then, species were judged on their contribution to the system and eliminated. These procedures were done in an iterative fashion to eventually arrive at a set that was small enough to be used in the CFD calculations. Due to the computational limitations of CFD, the performance of these sets in CHEMKIN, when compared to the full sets, is expected to be significantly reduced. However, the resulting reduced model should give a good enough estimate of the chemistry to produce valid CFD results.

After the reduction procedure, two reduced sets were produced, one from each base model. The reduction of the Labbe model produced a set of 41 species and 200 reactions, this set will be referred to as the RedLabbe model for the rest of the paper. The reduction of the ARL

model produced a set of 25 species and 98 reactions, which will be hereafter referred to as the RedARL model. Both of these reduced sets can be found in the supplemental information section.

### 3.4 *Performance evaluation*

Because the MMH–RFNA chemistry was used as the criteria for the reduction of the base sets, it was necessary to model an MMH–RFNA system to compare the new reduced sets to the original sets. The new sets can be assessed by their ability to reproduce the chemistry of the full sets. For this comparison, three MMH–RFNA flames were modeled, at equivalence ratios of  $\phi = 0.5$ , 1, and 2, with all four chemistry sets so that the performance of the reduced sets could be evaluated at fuel-lean, stoichiometric, and fuel-rich conditions. To determine the inlet composition for these simulations, it was assumed that RFNA is composed of 85%  $\text{HNO}_3$  and 15%  $\text{NO}_2$ , the same proportion assumed in the CFD calculations, and that the sum of the moles of  $\text{HNO}_3$  and  $\text{NO}_2$  represents the moles of oxidizer in the system.

Figures 3.9 and 3.10 show the temperature profile and concentration profiles for the reactants

For the fuel-lean case, the RedLabbe set seems to suffer in some places, while the RedARL set seems to be performing very similarly to its full set except in a few cases. The RedLabbe set is especially problematic in regard to  $\text{NO}_2$  and to a lesser extent with the products, while the RedARL set has issues with  $\text{N}_2$  but seems fine otherwise. Overall, the RedLabbe set seems to not predict the chemistry of a fuel-lean mixture well, while the RedARL set seems to perform quite well.

and major products of a fuel-lean ( $\phi = 0.5$ ) MMH–RFNA flame.

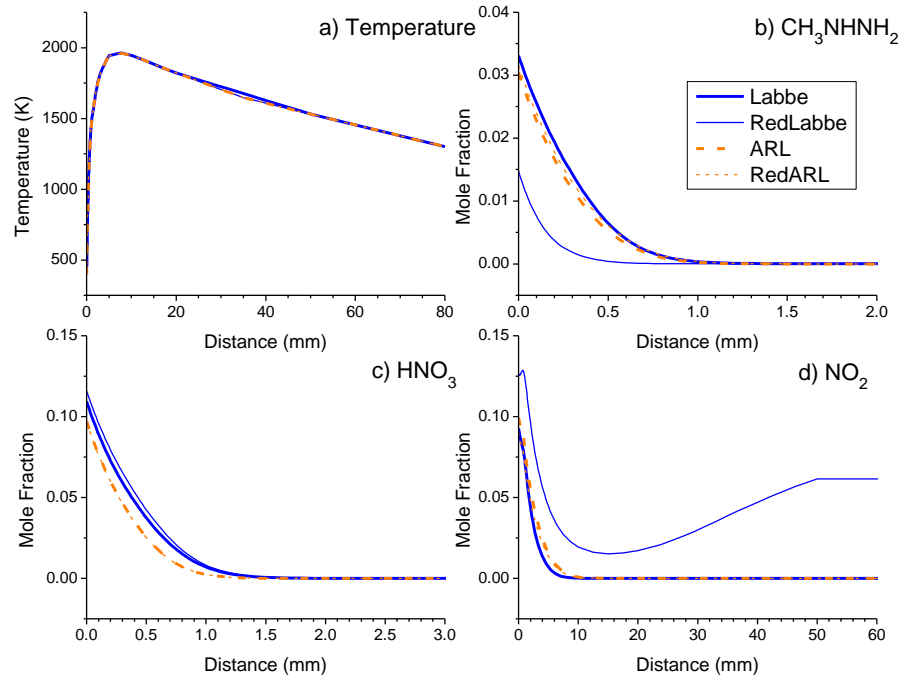


Figure 3.9: Temperature and reactant profiles for a fuel-lean ( $\phi = 0.5$ ) MMH–RFNA flame. Labbe mechanisms are shown in blue and ARL mechanisms are shown in orange. The thicker lines represent full sets and the thinner lines represent the reduced sets.

Figures 3.11 and 3.12 show the results from the simulation of a stoichiometric ( $\phi = 1$ ) MMH–RFNA flame.

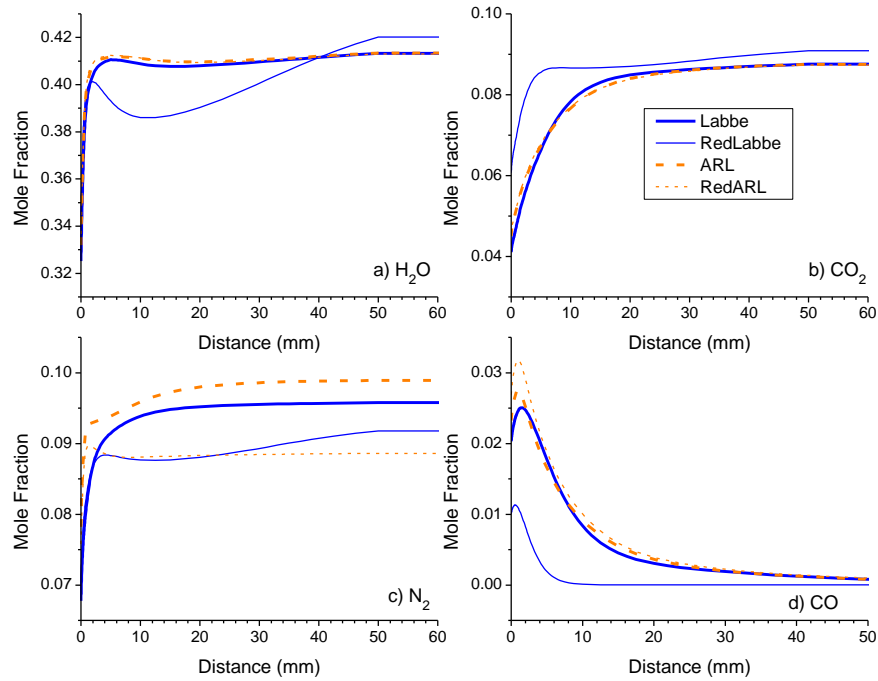


Figure 3.10: Major product profiles for fuel-lean ( $\phi = 0.5$ ) MMH-RFNA flame.

For the stoichiometric case, the RedLabbe set's performance looks very similar to the full model, with only minor deviations. RedARL on the other hand, starts to show rather large deviations in its prediction of the products, though the shapes of the curves seem still to match up well.

Figures 3.13 and 3.14 show the results of simulation of a fuel-rich ( $\phi = 2$ ) MMH-RFNA flame.



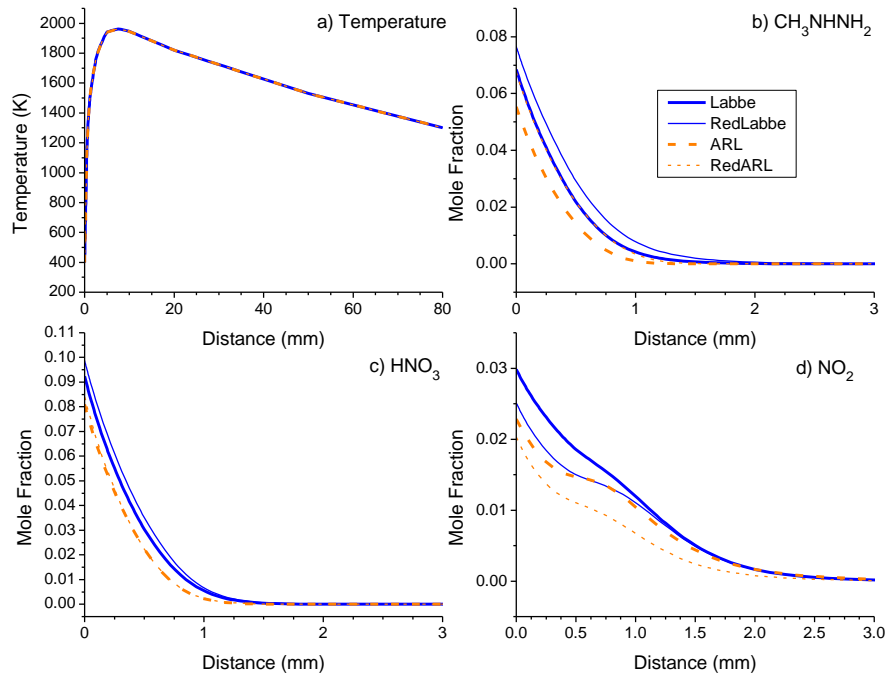


Figure 3.11: Temperature and reactant profiles for stoichiometric ( $\phi = 1$ ) MMH-RFNA flame.

The fuel-rich case looks similar to the stoichiometric case, with the RedARL model deviating largely from the product profiles, while this time the RedLabbe model shows a noticeable but by no means large deviation in its  $\text{N}_2$  profile. Interestingly, the full ARL set and the full Labbe set show some large differences in their predictions for the fuel-rich case, especially in  $\text{CO}_2$  and to a lesser extent  $\text{NO}_2$ , a phenomenon not seen in the other cases.

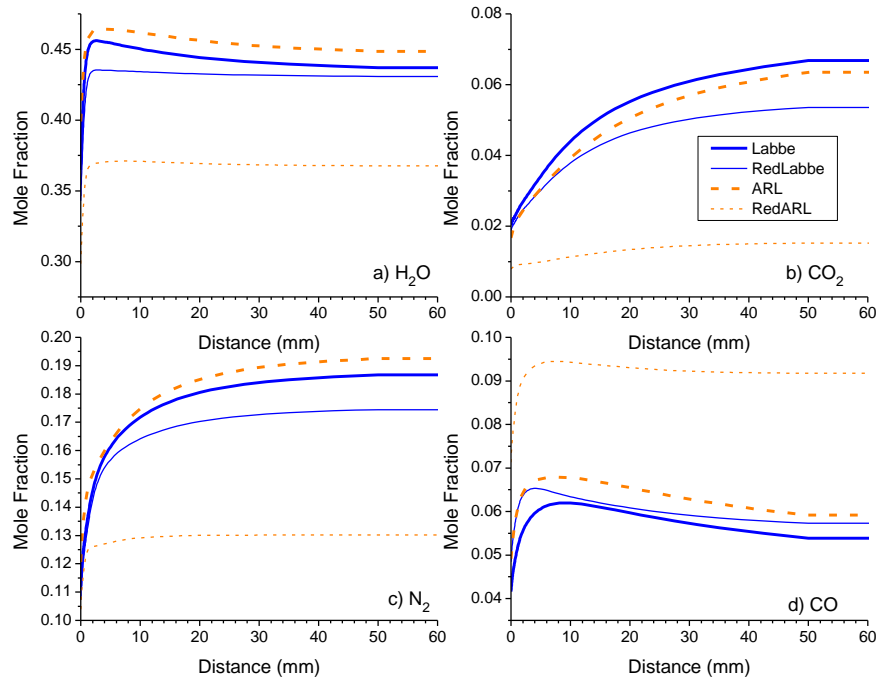


Figure 3.12: Major product profiles for stoichiometric ( $\phi = 1$ ) MMH-RFNA flame.

As expected, the reduced models both show at times a significant drop in performance from the full sets, but overall they are both good at giving good estimations of the chemistry of an MMH-RFNA flame. The RedLabbe model has issues with the fuel-lean case but performs well for stoichiometric and fuel-rich flames. The RedARL model is the opposite: performing well for the fuel-lean case and having issues for stoichiometric and fuel-rich flames. Both of these reduced models can be used in CFD simulations.

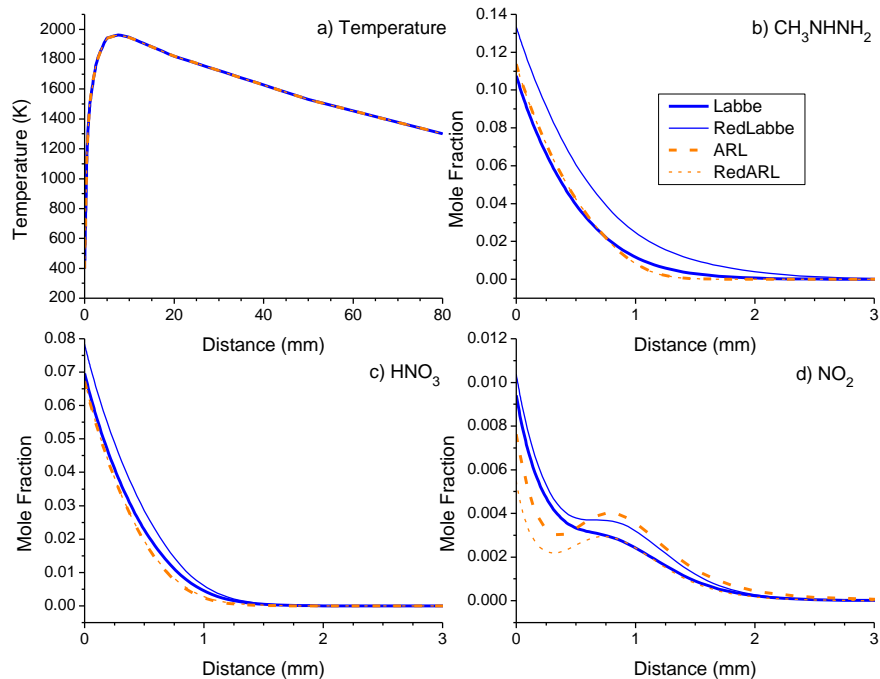


Figure 3.13: Temperature and reactant profiles for fuel-rich ( $\phi = 2$ ) MMH-RFNA flame.

### 3.5 Aerosol mechanism

A number of simulations using the reduced mechanisms were run by Tyler Voskuilen and Timothée Pourpoint at the School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN, 47907. All of these simulations used their CFD code that is an extension of the volume-of-fluid method [81,82] to include reactions. However, their simulations were unable to reach ignition with the current mechanisms. A literature search was undertaken to determine if there was any chemistry missing from the system. Wang and Thynell [83] showed that under certain experimental conditions, an aerosol cloud forms just prior to

ignition. They theorized that ability of the aerosol cloud to turn the gaseous fuel molecules into solvated ions gave the system enough energy to increase the temperature from the boiling point of the liquids to the ignition temperature.

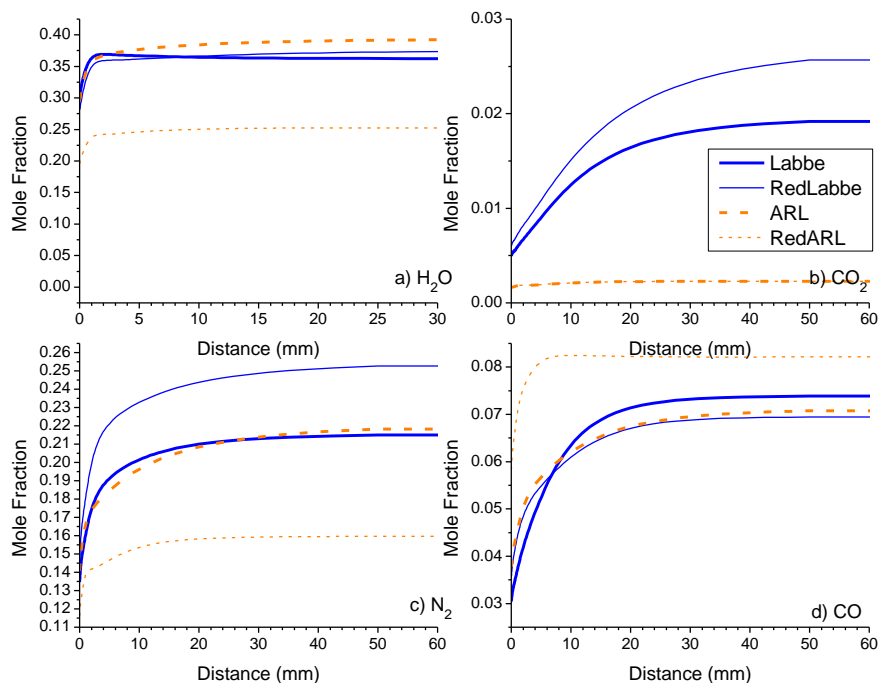


Figure 3.14: Major product profiles for fuel-rich ( $\phi = 2$ ) MMH-RFNA flame.

The new mechanism presented in this work includes reactions of the gas-phase propellants absorbing into aerosol droplets to form intermediate complexes, which then produce energy by solvating the propellants. Tao [84] determined that the presence of two assisting water molecules was necessary to facilitate proton transfer between nitric acid and ammonia. In the case of the hypergols, the assisting solvent molecules are the propellants themselves, which

form into small droplets dispersed among the gas phase. Thus, a small complex of one solute molecule surrounded by some number of solvent molecules is necessary to facilitate proton transfer between the solute and one solvent molecule.

For the bipropellant system, there are two systems requiring investigation: an MMH molecule reacting with an HNO<sub>3</sub> droplet and an HNO<sub>3</sub> molecule reacting with an MMH droplet. Gaussian 09 [15] simulations were used to evaluate the number of chaperone molecules necessary for proton transfer for these two systems. Figure 3.15 shows simulation snapshots that illustrate the change in the position of the solvating proton as more assisting molecules are added.

These results show that it takes 3 MMH molecules and 4 HNO<sub>3</sub> molecules to solvate a proton in their respective systems. In the case of MMH in HNO<sub>3</sub>, protons from two different HNO<sub>3</sub> molecules will attempt to transfer to the MMH. The simulation results show that the proton will transfer to the terminal carbon first, even though that ion is higher in energy than MMH<sup>+</sup> with the proton on the secondary carbon. This discrepancy is likely due to the terminal carbon being more accessible geometrically.

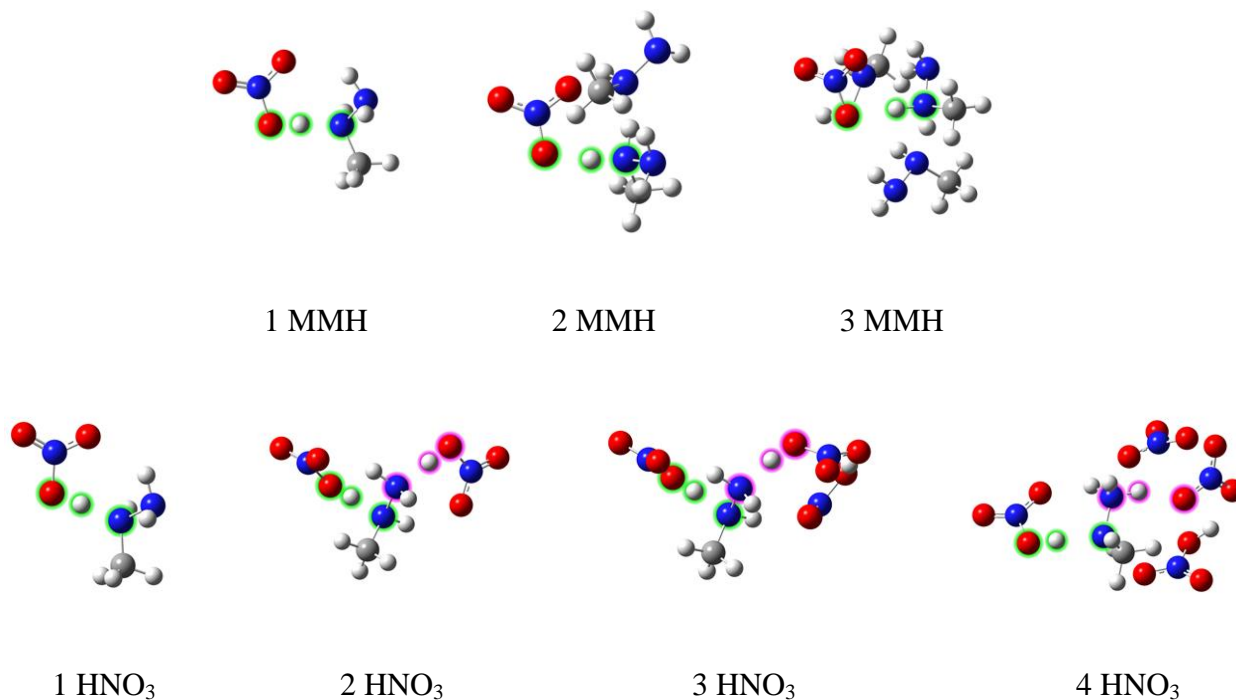


Figure 3.15: Simulation results showing the proton transferring from HNO<sub>3</sub> to MMH as more assisting molecules are added. Atoms of interest are highlighted in green and pink. HNO<sub>3</sub> in MMH is shown on top while MMH in HNO<sub>3</sub> is shown on bottom.

With these results, a chemical mechanism can be formulated for the systems:

#### MMH in HNO<sub>3</sub>

1.  $\text{MMH}_{(g)} + \text{HNO}_{3(l)} \rightarrow \text{MMH}\cdot\text{HNO}_{3(l)}$
2.  $\text{MMH}\cdot\text{HNO}_{3(l)} + \text{HNO}_{3(l)} \rightarrow \text{MMH}\cdot 2\text{HNO}_{3(l)}$
3.  $\text{MMH}\cdot 2\text{HNO}_{3(l)} + \text{HNO}_{3(l)} \rightarrow \text{MMH}\cdot 3\text{HNO}_{3(l)}$
4.  $\text{MMH}\cdot 3\text{HNO}_{3(l)} + \text{HNO}_{3(l)} \rightarrow (\text{MMH}\cdot\text{H}^+)(\text{NO}_3^-)\cdot 3\text{HNO}_3$

#### HNO<sub>3</sub> in MMH

1.  $\text{HNO}_{3(g)} + \text{MMH}_{(l)} \rightarrow \text{HNO}_3\cdot\text{MMH}_{(l)}$

2.  $\text{HNO}_3 \cdot \text{MMH}_{(l)} + \text{MMH}_{(l)} \rightarrow \text{HNO}_3 \cdot \text{MMH}_{(l)}$
3.  $\text{HNO}_3 \cdot 2\text{MMH}_{(l)} + \text{MMH}_{(l)} \rightarrow (\text{MMH} \cdot \text{H}^+)(\text{NO}_3^-) \cdot 2\text{MMH}$

These two mechanisms can be combined into two overall reactions that the system can undergo:



The quantum-chemistry calculations give the energy produced by these processes. Figure 3.16 shows the energy released as assisting molecules are added; e.g.,  $E(\text{HNO}_3 \cdot 2\text{MMH}) - E(\text{HNO}_3) - 2E(\text{MMH})$ . The initial interaction of MMH and  $\text{HNO}_3$  yields 13.4 kcal/mol.

For  $\text{HNO}_3$  in MMH, the interaction energy of the third MMH is sufficient to protonate MMH and to separate it from  $\text{NO}_3^-$ , providing an exothermicity of 20.2 kcal/mol. In contrast, protonating MMH with four  $\text{HNO}_3$  provides 40.7 kcal/mol of gas-phase MMH.

The rate-limiting step of the overall absorption reaction was assumed to be the rate of mass transfer of the solute gas to the solvent liquid; e.g., that MMH gas would react instantly with liquid  $\text{HNO}_3$  once they came into contact. The first-order reaction rate was then calculated from the mass transfer rate, treating the aerosol droplet as a sphere of diameter  $d$  and using a Sherwood number correlation for the mass-transfer coefficient [85–87]:

$$rate = k'_c \cdot \pi d^2 \cdot \frac{P}{RT} (y_{i,bulk} - y_{i,interface}) = \left( k'_c \cdot \pi d^2 \cdot \frac{P}{RT} \right) y_{i,bulk} \quad (3.1)$$

where  $k'_c = \frac{D_{i,mix}}{d} (2 + 0.552 Re^{0.53} Sc^{1/3})$

After absorption, the solvated complexes should be stable until they separate and vaporize around the ignition point. The primary contribution of the aerosol formation reaction to the overall mechanism is the addition of heat in the early reaction stages. For the work presented here, the subsequent vaporization and reversal of this aerosol formation during gas-phase combustion were not included explicitly.

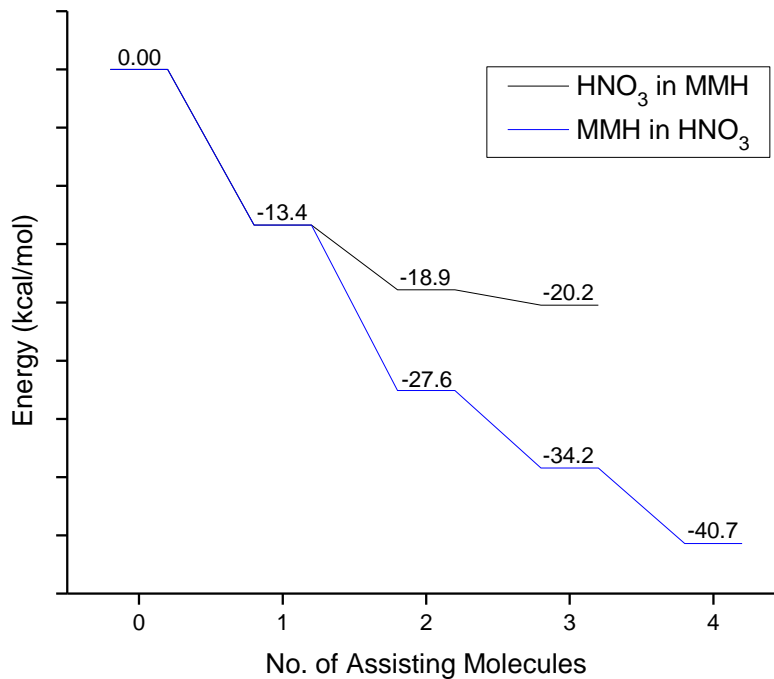


Figure 3.16: Potential energy diagram of system as assisting molecules are added.



### 3.6 *TMEDA/RFNA simulations*

TMEDA (tetramethylethylenediamine) has been investigated as a less harmful alternative to the current carcinogenic, hydrazine-based rocket fuels. To understand TMEDA's potential as a fuel, a chemical mechanism must be developed for its decomposition. So far, the study of the TMEDA/nitric acid hypergolic bipropellant pair (whether RFNA or WFNA) has been confined to experimental investigation of reaction products [88] and ab-initio simulation [89]. RMD simulations allow the intermediate steps of TMEDA/NA combustion to be studied at conditions more similar to those of the experiments. This work uses ReaxFF simulations in LAMMPS simulations to get a more complete picture of the mechanism of TMEDA/NA combustion. A TMEDA/NA ratio of 1:2 was chosen, based on experimental studies using an excess of NA [88] and favorable results from RMD simulations of other hypergolic bipropellants at that ratio [90]. Box sizes for the simulations were chosen so that the reactants were initially at experimental densities. Initial geometries were set up in Hyperchem Professional [91] and equilibrated using the software's built-in geometry optimization. The systems were then annealed by slowly scaling the temperature from 400K to the desired temperature and limiting the distance atoms were allowed to move per time step. After annealing, the simulations were run for varying times using a time step of 0.1 fs. All simulations reported here were NVE calculations run at an initial temperature of 2000 K to reduce time of computation. As a result, all data represents the behavior of the system at high temperature.

The first step in interpreting the simulation results was to determine the initiation route for combustion. The hypothesis was that H-abstraction was the main initiating channel, raising the question of whether the terminal hydrogens or the central hydrogens would be abstracted most. Figure 3.17 shows the proposed initial products of each H-abstraction channel and figure 3.18 shows simulated concentration profiles for three of these species.

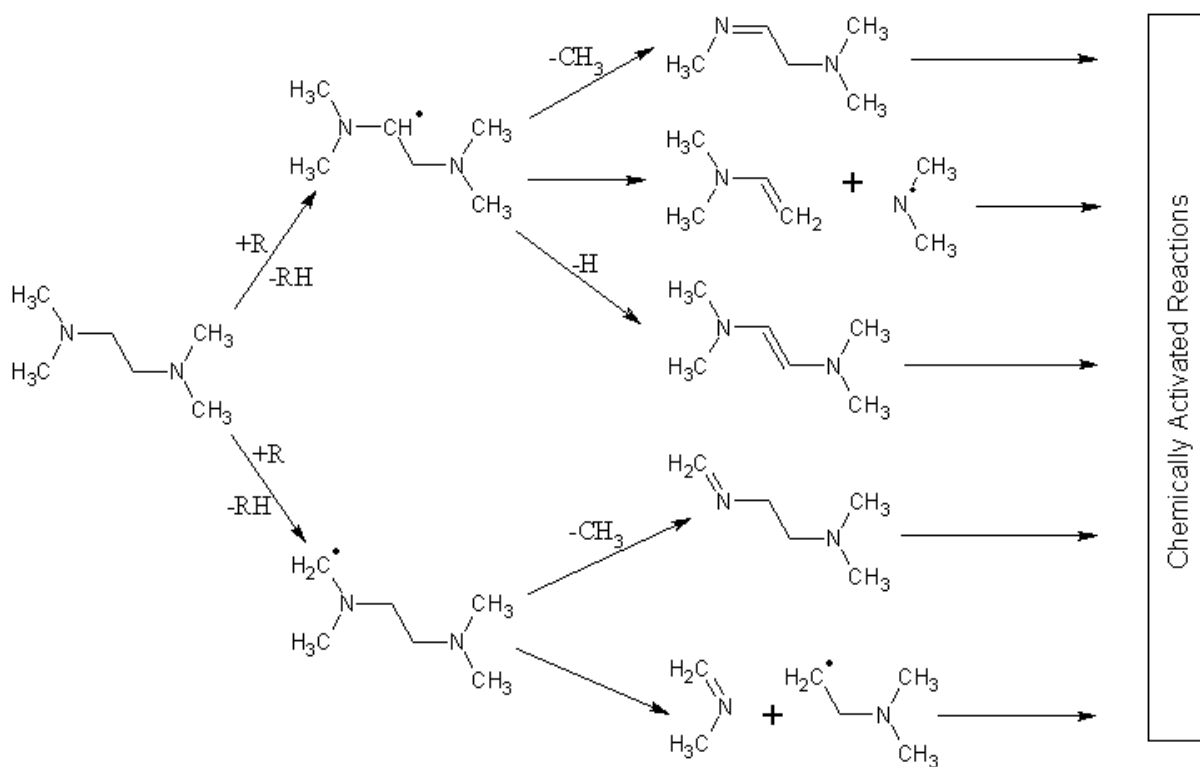


Figure 3.17: H-abstraction routes for TMEDA

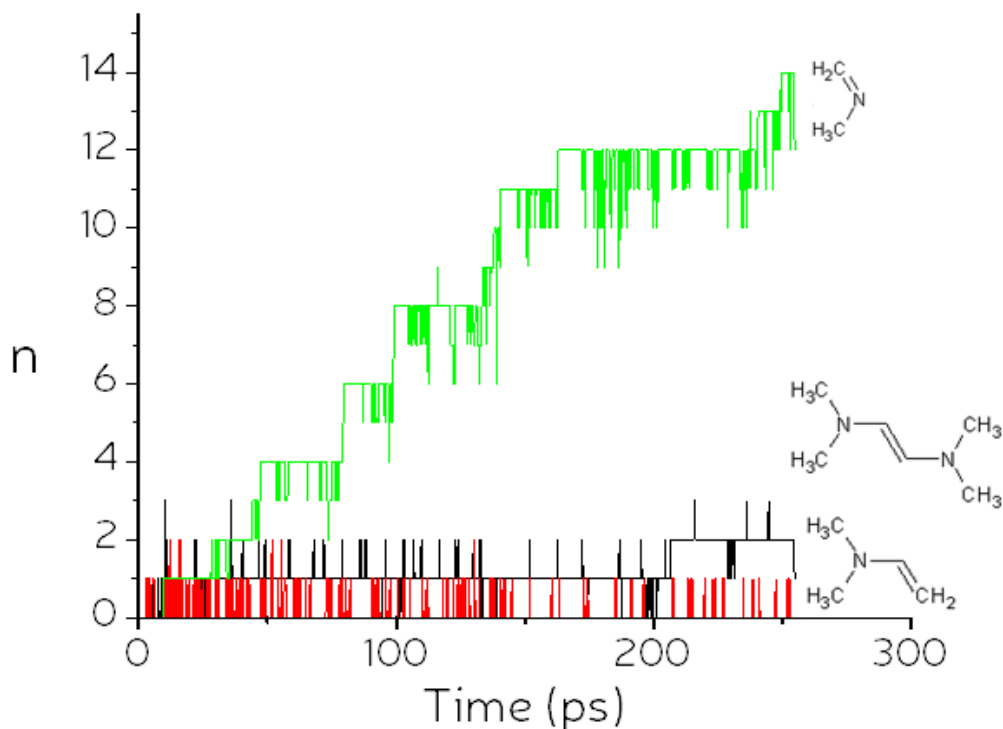


Figure 3.18: Concentration profiles for three species apposite for distinguishing the H-abstraction initiation channel of TMEDA/ $\text{HNO}_3$  combustion.

The high number of  $\text{CH}_2=\text{NCH}_3$  molecules compared to the other two species suggests that the terminal hydrogens are the dominant route, even though they are more tightly held than the central hydrogens. This effect is likely due to the fact that there are three times as many terminal hydrogens and they are more easily accessible. Figure 3.19 shows the other major species in the simulation.

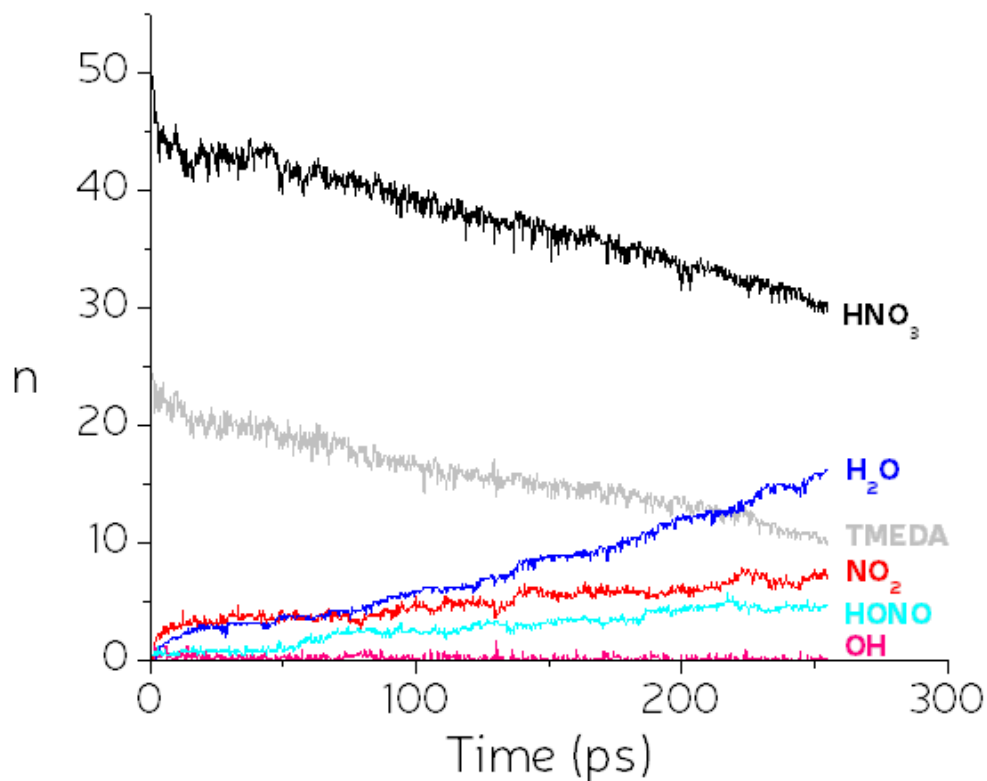


Figure 3.19: Major reactants, products, and abstractors in high temperature TMEDA/HNO<sub>3</sub> reaction.

The data suggests that HNO<sub>3</sub> primarily splits into NO<sub>2</sub> and OH, which go on to be the major abstractors in the system with NO<sub>2</sub> forming HONO upon abstracting a hydrogen and OH forming H<sub>2</sub>O. The data shows that there is negligible OH buildup in the system and that H<sub>2</sub>O fairly quickly becomes the major product. This suggests that OH is the main H-abstractor and that NO<sub>2</sub>, while a participant, is appreciably slower. The species OH and NO<sub>2</sub> being the main abstractors means that the rate of HNO<sub>3</sub> decomposition is the initial rate-limiting step in high-T combustion for TMEDA/HNO<sub>3</sub>. After abstraction, the amine radicals decompose by

beta scission into smaller molecules, mostly  $C_2H_4$  and more  $CH_2=NCH_3$ . The major decomposition pathway observed for TMEDA is shown in Figure 3.20.

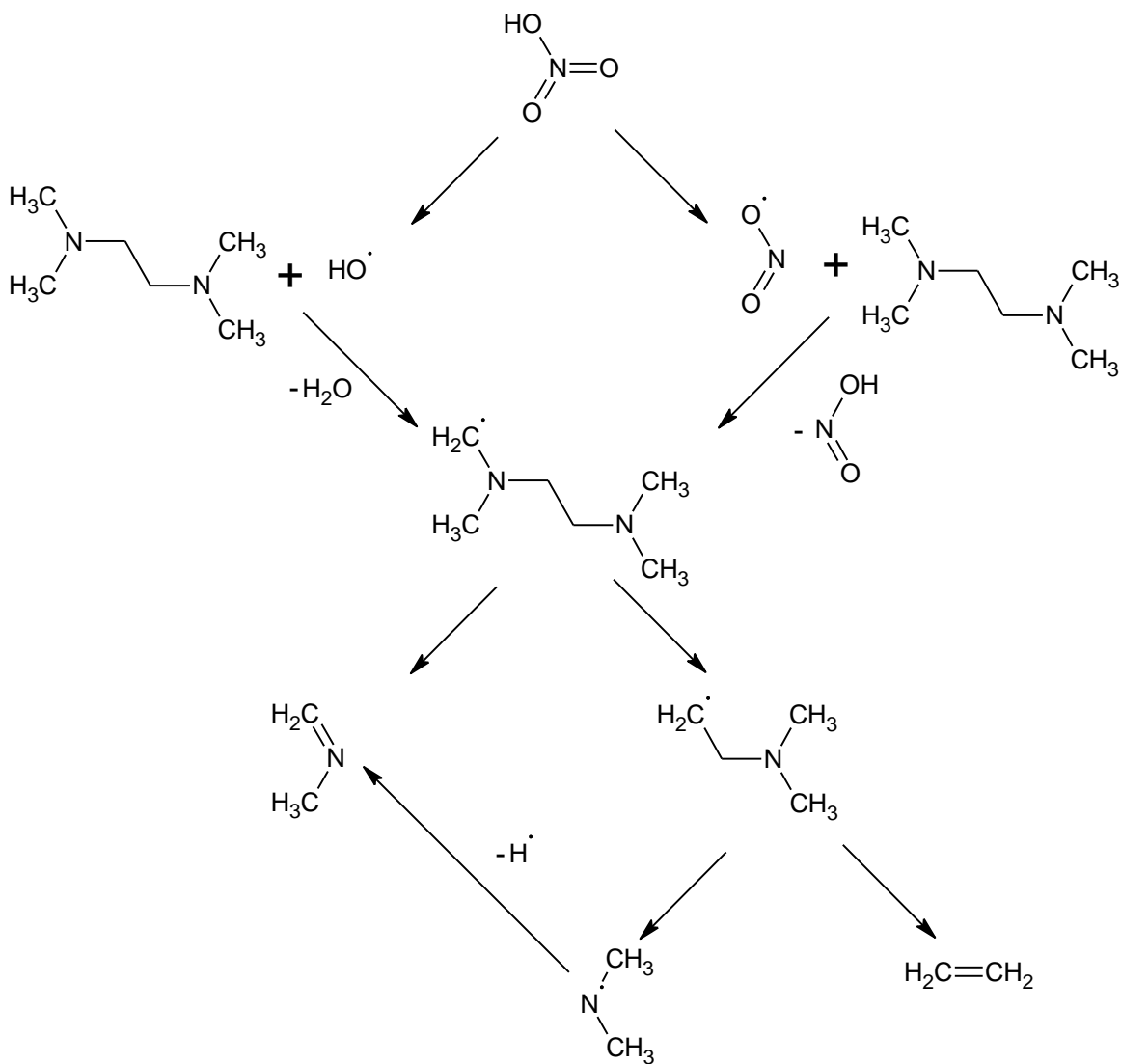


Figure 3.20: Major TMEDA decomposition pathway

Though papers on the subject of TMEDA combustion discuss the formation of nitrate salts, complexation was seen infrequently in the simulations. Any complexes formed were only present for a few time steps before disassociating back into TMEDA and NO<sub>3</sub>.

### 3.7 *Conclusion*

In this work, a mechanism for the combustion of MMH and RFNA was created by literature analysis. Both this mechanism and a previous mechanism for MMH/RFNA combustion from ARL were iteratively reduced for use with reactive CFD calculations. The resulting mechanisms were unable to achieve ignition in the CFD calculation. A hypothesis was discovered suggesting the formation of an aerosol cloud helped raise the system temperature from the boiling point of the liquids to the ignition point. QC simulations for the fuel solvating in excess oxidizer and vice versa were used to investigate the solvation energy gained by aerosolization. A reaction rate was arrived at by assuming the solvation was mass-transfer limited.

In addition, the combustion of TMEDA and HNO<sub>3</sub> was investigated at high temperatures using RMD. Results gave insight into the initiation steps for the system, suggesting that H-abstraction of the terminal hydrogens by OH formed from HNO<sub>3</sub> decomposition is responsible for the onset of combustion under these conditions.

## **CHAPTER 4. A COMBUSTION AND FLAMMABILITY REACTION MECHANISM FOR REFRIGERANT HFO-1234YF**

### *4.1 Introduction*

HFO-1234yf has been shown to be a desirable, low-environmental-impact alternative to the more common HFC-134a as an automotive refrigerant [92–96]. Accordingly, there is interest in the flammability characteristics of 1234yf as compared to 134a. A few experimental studies have been conducted [95–97], but more comprehensive analysis of the behavior of 1234yf in flames is desirable. Although some attempts have been made in the past to measure reaction rates of 1234yf with certain radicals [92,98], there has been no comprehensive chemical mechanism proposed.

A reaction mechanism is developed here to describe 1234yf combustion, serving as a useful aid for exploring the refrigerant's flammability behavior. By starting from the previously developed NIST mechanism describing the combustion of small, fluorinated hydrocarbons [12,99], the only reactions that need to be described are those that break 1234yf down into smaller molecules.

### *4.2 Methods for determining collisional-reaction rate coefficients*

For a number of the reactions discussed below it was necessary to derive their rate coefficients mathematically using collision rate theory [100,101]. The reason for treating certain rate constants this way was almost invariably due to the lack of a maximum in the electronic energy along the reaction coordinate, which is usually the case for radical

combination. Benson [100] derived a formula for calculating the rate of radical recombinations (i.e., two radicals colliding and forming one species) based on the collision-frequency rate constant,  $Z_r$ :

$$k_{rec} = g_e Z_r \beta_i \beta_j \quad (4.1)$$

where  $g_e$  is the ratio of the electronic partition function (i.e., electronic spin degeneracy) of the transition state and the two radicals:

$$g_e = \frac{g^\ddagger}{g_i g_j} \quad (4.2)$$

and  $\beta_i$  is the empirical fraction of the molecular surface area where a collision will produce a reaction, also called the “active” fraction of the surface area, for each radical. Though Benson’s derivation of an equation for  $Z_r$  has typographical errors, it can be corrected to [100,101]:

$$Z_r = \frac{2.25}{\sqrt{\mu/2}} V_0^{1/3} (RT)^{1/6} 1.019 \frac{\pi r_0^2 N_A}{\sigma} \quad (4.3)$$

where  $\mu$  is the reduced molecular weight of the two radicals,  $r_0$  is the equilibrium bond length of the bond being formed, and  $\sigma$  is a symmetry factor where  $\sigma = 2$  for combination of identical radicals and  $\sigma = 1$  for combination of different radicals.  $V_0$  is the energy of the new bond given by:

$$V_0 = D^\circ + \epsilon_Z^{AB} - \epsilon_Z^A - \epsilon_Z^B \quad (4.4)$$

where  $D^\circ$  is the bond-dissociation energy and  $\epsilon_Z$  is the zero-point energy, all of which were calculated using Gaussian.



To complete the calculation,  $\beta_i$ , must be estimated for each species involved in collision. Table 4.1 summarizes the active fractions used in this study and the methods used for estimation.

Table 4.1: Active fractions for species used in collisional rate derivations

Species	$\beta_i$
H	1.000 <sup>a</sup>
O	0.690 <sup>a</sup>
OH	0.640 <sup>a</sup>
CF <sub>3</sub>	0.380 <sup>b</sup>
CO	0.023 <sup>c</sup>
CH <sub>2</sub> CFCF <sub>3</sub>	0.400 <sup>d</sup>
CH <sub>2</sub> CF	0.420 <sup>e</sup>
<i>E</i> - or <i>Z</i> -CHCFCF <sub>3</sub>	0.400 <sup>f</sup>
CH <sub>3</sub> CFCF <sub>3</sub>	0.250 <sup>g</sup>
CHOCFCF <sub>3</sub>	0.350 <sup>f</sup>
CF <sub>3</sub> CFCO	0.023 <sup>h</sup>
CF <sub>2</sub> CF <sub>2</sub>	0.450 <sup>f</sup>

<sup>a</sup>[101]

<sup>b</sup>[100]

<sup>c</sup>analogy to O<sub>2</sub> in [101]

<sup>d</sup>analogy to allyl in [100]

<sup>e</sup>analogy to C<sub>2</sub>H<sub>3</sub> in [101]

<sup>f</sup>analogy to 1234yf

<sup>g</sup>analogy to *i*C<sub>3</sub>H<sub>7</sub> in [100]

<sup>h</sup>analogy to CO

### 4.3 Mechanism development

#### 4.3.1 Determining possible reaction pathways

The first step to creating a mechanism for 1234yf combustion was to analyze the molecule and enumerate the different routes by which it could decompose into species already

described by the NIST small-fluorocarbon combustion mechanism [12,99]. Figure 4.1 is a schematic showing the different decomposition routes that were determined.

There are three different classes of reactions by which the 1234yf molecule can be destroyed: unimolecular decomposition (denoted by  $u$  reactions), hydrogen abstraction (denoted by  $a$  reactions), and addition (of H, O, and OH denoted by  $b$ ,  $c$ , and  $d$  reactions, respectively). These reaction classes and the specific reactions included in each class are discussed below.

#### 4.3.2 *Unimolecular decomposition reactions*

Of the three unimolecular routes included, one is a homolytic bond scission ( $u_1$ ) and the other two are concerted, four-centered eliminations ( $u_2$  and  $u_3$ ).

Most of the bonds in the 1234yf molecule are very strong and are unlikely to undergo homolytic scission on their own. However, the C–C single bond between the CF<sub>3</sub> group and the double-bonded central carbon has a bond energy of only 109 kcal/mole meaning that it is possible for it to break given enough energy from collisions. This collision-mediated reaction is shown as reaction  $u_1$ . Given the nature of homolytic bond scission, this reaction is barrierless and therefore has no transition state, making it impossible to calculate the rate of reaction using classical transition-state theory. Instead, the reverse rate (i.e., the rate for radical recombination) was calculated using collisional rate theory.

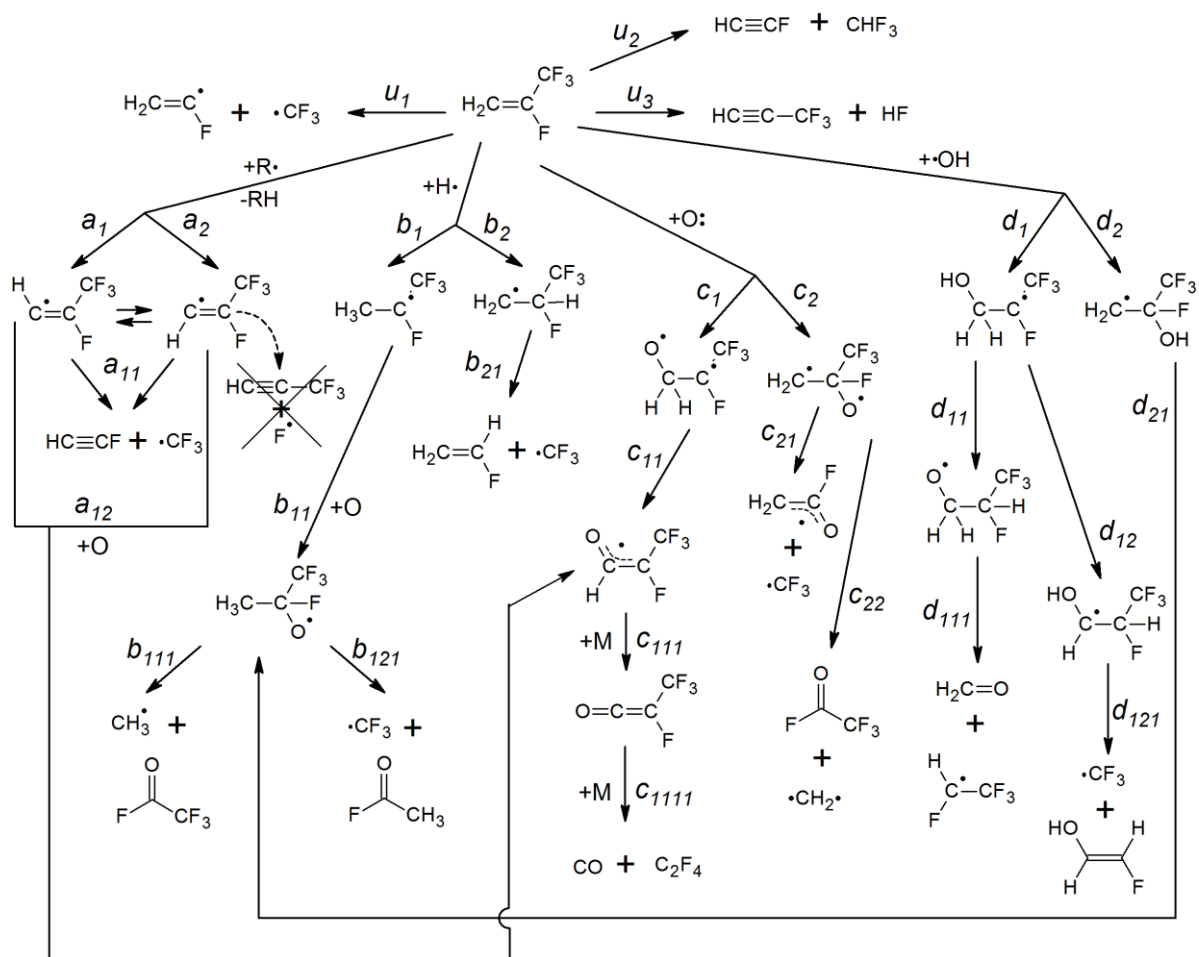


Figure 4.1: Sub-mechanism describing the decomposition of HFO-1234yf into small fluorocarbon species.

It is also possible for the 1234yf molecule to undergo a concerted elimination around the double bond, where either the  $\text{CF}_3$  group or the central fluorine proceeds through a four-centered transition state to combine with their respective hydrogen on the other side of the double bond and break away from the molecule. These two possibilities are represented by reactions  $u_2$  and  $u_3$ . Figure 4.2 shows an example of the electron movements involved in this type of pericyclic transition state, using  $u_3$  as a representative reaction.

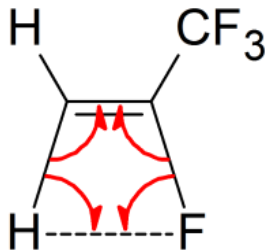


Figure 4.2: Schematic of the electron transfer occurring during reaction  $u_3$ .

The heats of formation of the species involved in reactions  $u_2$  and  $u_3$  are shown in Figure 4.3. For all energy diagrams, each plateau represents the standard heat of formation at 298 K of the reactants, the products, or the transition state of each reaction. The transition state is labeled according to which reaction it represents, and reactant or product species are shown near the plateau to which they correspond. The energy value of each plateau is also shown.

From the figure it is easy to see that  $u_3$  will be the most dominant of the three unimolecular reactions. Its energy barrier (i.e., the difference between the energy of the reactants and the energy of the transition state) is lower than any of the bond energies in the 1234yf molecule, lower than  $u_2$ , and it produces stable HF, giving low-energy products. Reactions  $u_1$  and  $u_2$  still have low enough energy barriers that they will occur as the combustion process heats up, so they are still necessary inclusions in the model.

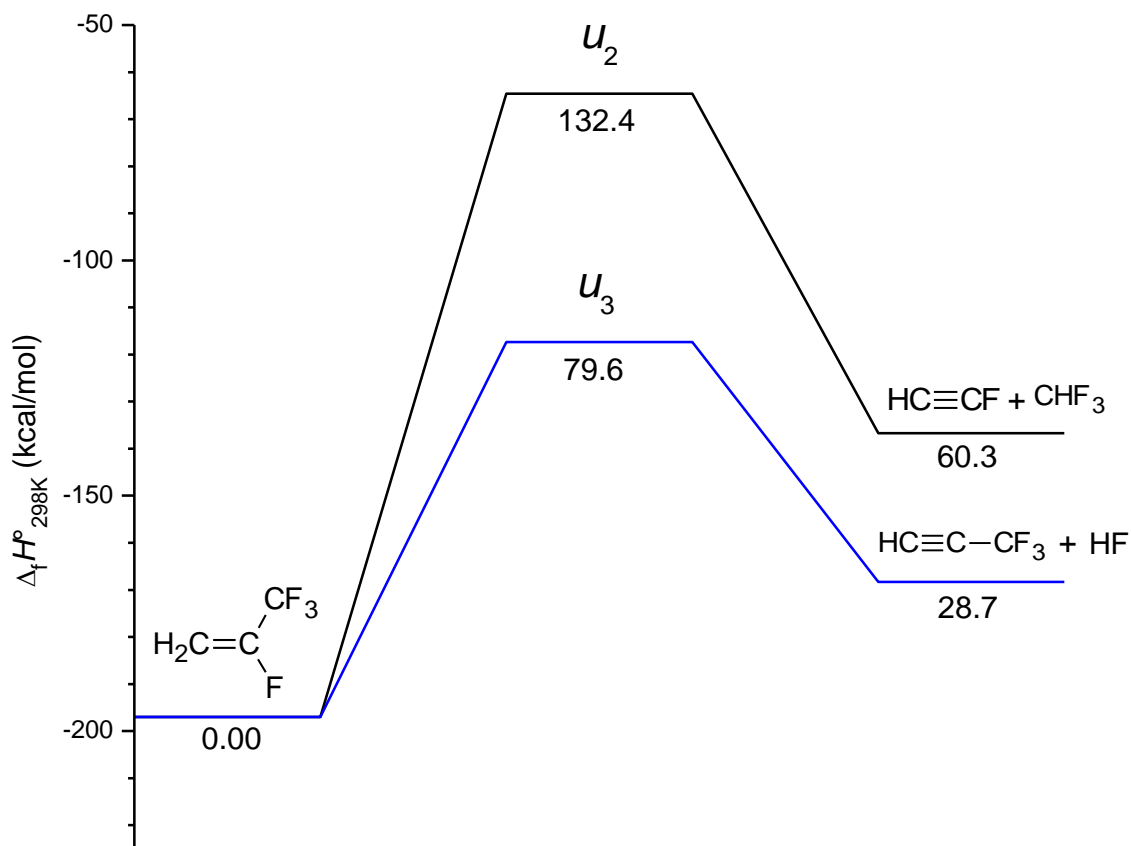


Figure 4.3: Energy diagram for unimolecular concerted reaction pathways  $u_2$  and  $u_3$ .

#### 4.3.3 Hydrogen abstraction reactions

The two hydrogens were the only two atoms considered for abstraction from the 1234yf molecule, given the strength of the carbon–fluorine bonds. The abstracting species considered were H, O, OH, CH<sub>3</sub>, and CF<sub>3</sub> radicals as well as O<sub>2</sub>. Abstraction through either reactions  $a_1$  or  $a_2$  produced 2,3,3,3-tetrafluoropropenyl radical with a single H, either cis to the CF<sub>3</sub> group (denoted as Z-CHCFCF<sub>3</sub> in the mechanism) or trans to it (denoted as E-CHCFCF<sub>3</sub>). Transition states calculations converged for all abstractors except O atom and

O<sub>2</sub>. Figure 4.4 shows the energy surfaces for the four abstractors with transition states. For abstraction by O and O<sub>2</sub> no maximum could be located on the reaction coordinate by transition-state calculations or potential energy scans, so kinetics parameters were estimated from similar structures. Parameters for abstraction by O were estimated from the rate given in Tsang et al. [102] for propene and parameters for abstraction by O<sub>2</sub> were estimated as half of the rate given in Hua et al. [103] for ethylene (2 Hs in 1234yf / 4 Hs in C<sub>2</sub>H<sub>4</sub>).

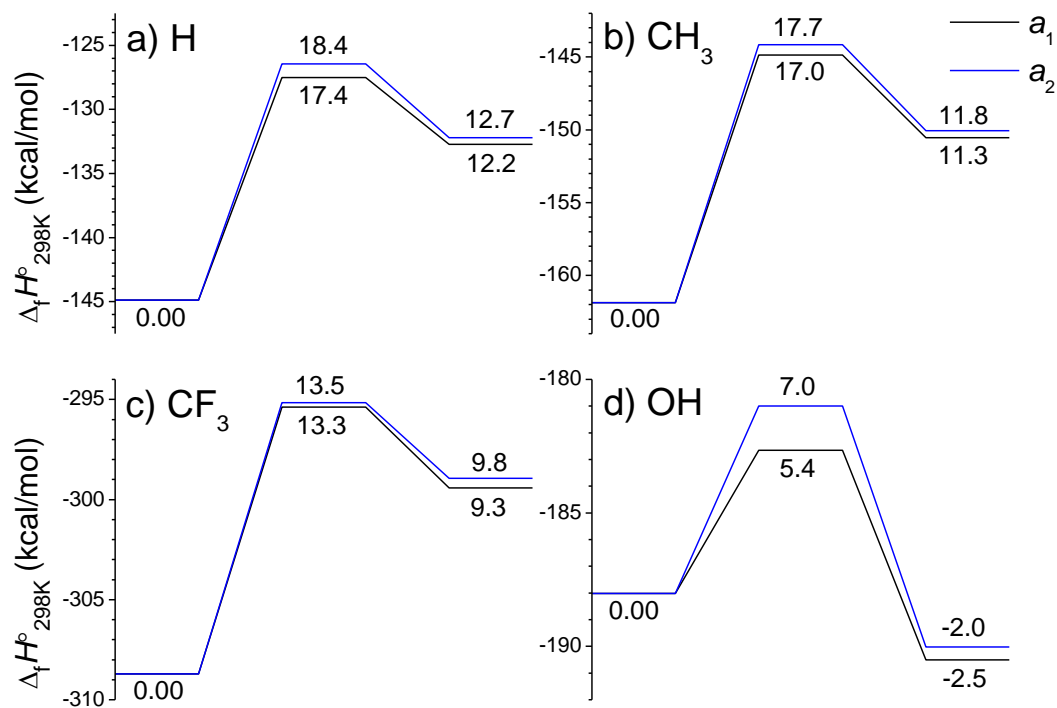


Figure 4.4: Energy surfaces for H-abstraction from 1234yf.

Of the four abstractors where transition states were found, OH has the smallest barrier and will likely be the dominant abstractor of H. The other three abstractors have very similar barriers in the 15-20 kcal/mol range and will play a smaller role in abstraction. Also important to note is that there is an approximately 0.5 kcal/mol energy difference between the two isomers of the radical, with the Z-tetrafluoropropenyl isomer being the lowest in energy. The E-tetrafluoropropenyl isomer will likely isomerize to the Z- form relatively quickly after its formation. The rate of isomerization was estimated using principles discussed in Benson's *Thermochemical Kinetics* [104]. He states that the A-factor for a cis-trans isomerization reaction can be estimated by the formula

$$A_{c-t} \sim 2 \left( \frac{ekT}{h} \right) \frac{q_{elec}}{q_{RC}} \quad (4.5)$$

where  $q_{elec}$  is the electronic partition function and  $q_{RC}$  is defined as the partition function corresponding to the reaction coordinate. When the vibrational frequency corresponding to the reaction coordinate is low,  $q_{RC}$  can be approximated by

$$q_{RC} = \frac{kT}{h\nu_{RC}} \quad (4.6)$$

reducing the A-factor equation to

$$A_{c-t} = 2q_{elec}\nu_{RC} \quad (4.7)$$

In this case, the radical makes  $q_{elec} = 2$  and  $\nu_{RC}$ , the vibrational frequency of the H-C=C scissoring motion, was calculated to be  $537 \text{ cm}^{-1}$ , giving  $A_{c-t}$  a value of  $6.4 \times 10^{13} \text{ s}^{-1}$ .

In addition to isomerizing, the Z- and E-tetrafluoropropenyl radicals can  $\beta$ -scission into fluoroacetylene and CF<sub>3</sub> radical ( $a_{11}$ ) or an O atom can add to the radical and produce a resonance stabilized structure ( $a_{12}$ ). Reaction  $a_{12}$  is a radical combination reaction that required the use of a collisional rate constant, discussed above. The decomposition of the product of reaction  $a_{12}$  is discussed in §4.3.4. There is an additional reaction possibility where the radicals can  $\beta$ -scission into 3,3,3-trifluoropropyne and an F radical, but the C–F bond is so strong in the molecule that the probability of this route occurring is small, so it is disregarded. This route is shown in figure 4.1 with a dashed arrow and an X though it to indicate its exclusion.

#### 4.3.4 Addition reactions

Addition reactions and the subsequent reactions of addition products constitute by far the largest portion of the 1234yf sub-mechanism. The three species considered for addition were H, O, and OH. Each can add to either side of the double bond.

Hydrogen addition can either produce a tetrafluoropropan-2-yl or tetrafluoropropan-1-yl radical ( $b_1$  and  $b_2$ , respectively). The product of reaction  $b_1$  is unlikely to undergo a unimolecular reaction into anything but 1234yf due to the tightly held fluorines in the CF<sub>3</sub> group. The n-propyl-like product of reaction  $b_2$  can easily  $\beta$ -scission into vinyl fluoride and CF<sub>3</sub> radical (reaction  $b_{12}$ ). Figure 4.5 shows the energy surface for reactions  $b_1$ ,  $b_2$ , and  $b_{21}$ . Of the two addition reactions,  $b_1$  has the lowest barrier and the most stable product. Although the  $b_2$  channel more easily decomposes, it is likely that  $b_1$  will be the most dominant H-addition channel.



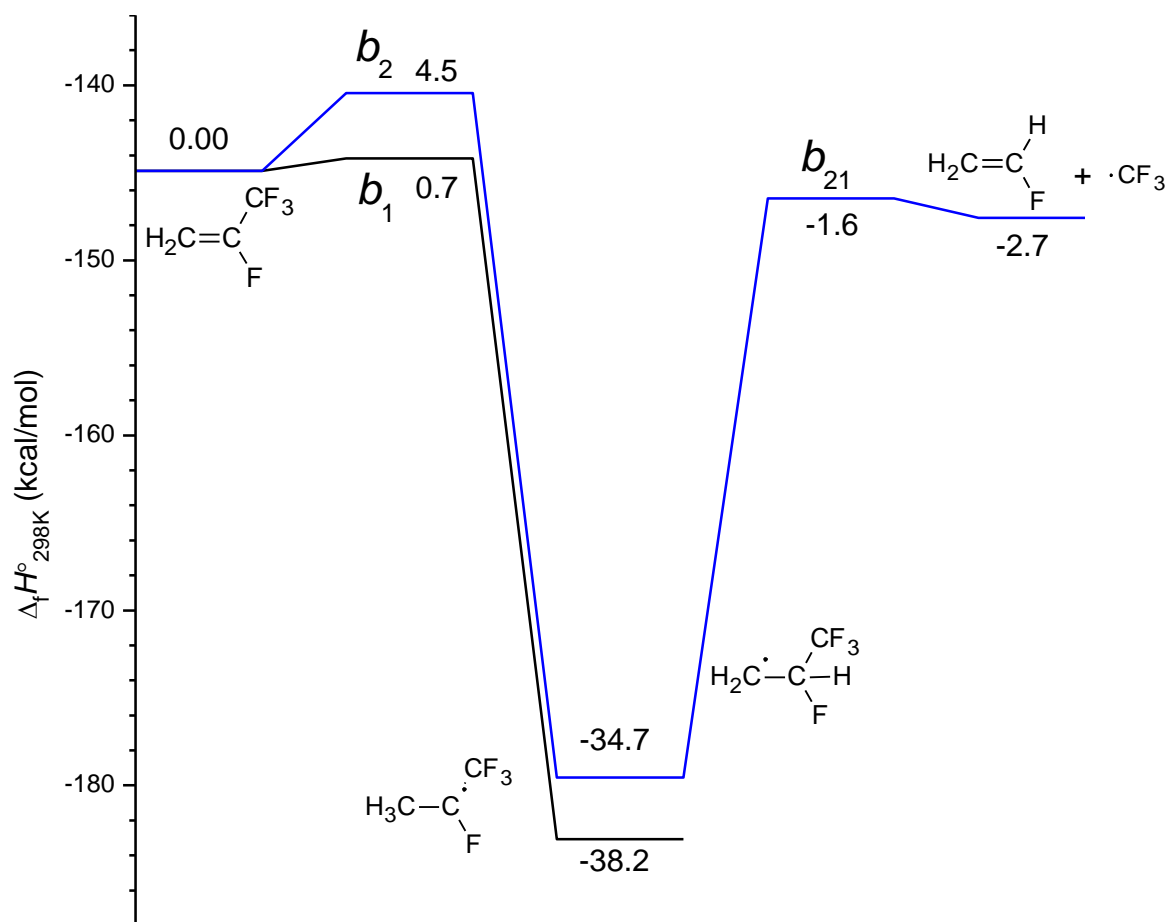


Figure 4.5: H addition to 1234yf and subsequent  $\beta$ -scission of tetrafluoropropan-1-yl

The relative stability of the tetrafluoropropan-2-yl radical means that it will possibly exist long enough to have an O atom add to it before it can scission back into 1234yf (reaction  $b_{11}$ ). This reaction is another O-atom addition requiring collisional treatment. The reaction will produce a tetrafluoropropoxyl radical that will  $\beta$ -scission into either trifluoroacetyl fluoride and  $\text{CH}_3$  ( $b_{111}$ ) or acetyl fluoride and  $\text{CF}_3$  ( $b_{112}$ ). Figure 4.6 shows the energy surface for reactions  $b_{111}$  and  $b_{112}$ . The figure shows that not only does  $b_{112}$  have products that are substantially more stable, but it also has a lower barrier by about 3 kcal/mol. The energy

disparity in the products is mostly due to the difference in stability between the  $\text{CH}_3$  and  $\text{CF}_3$  radicals, but combined with the difference in barrier height, it means that  $b_{112}$  will be the dominant channel.

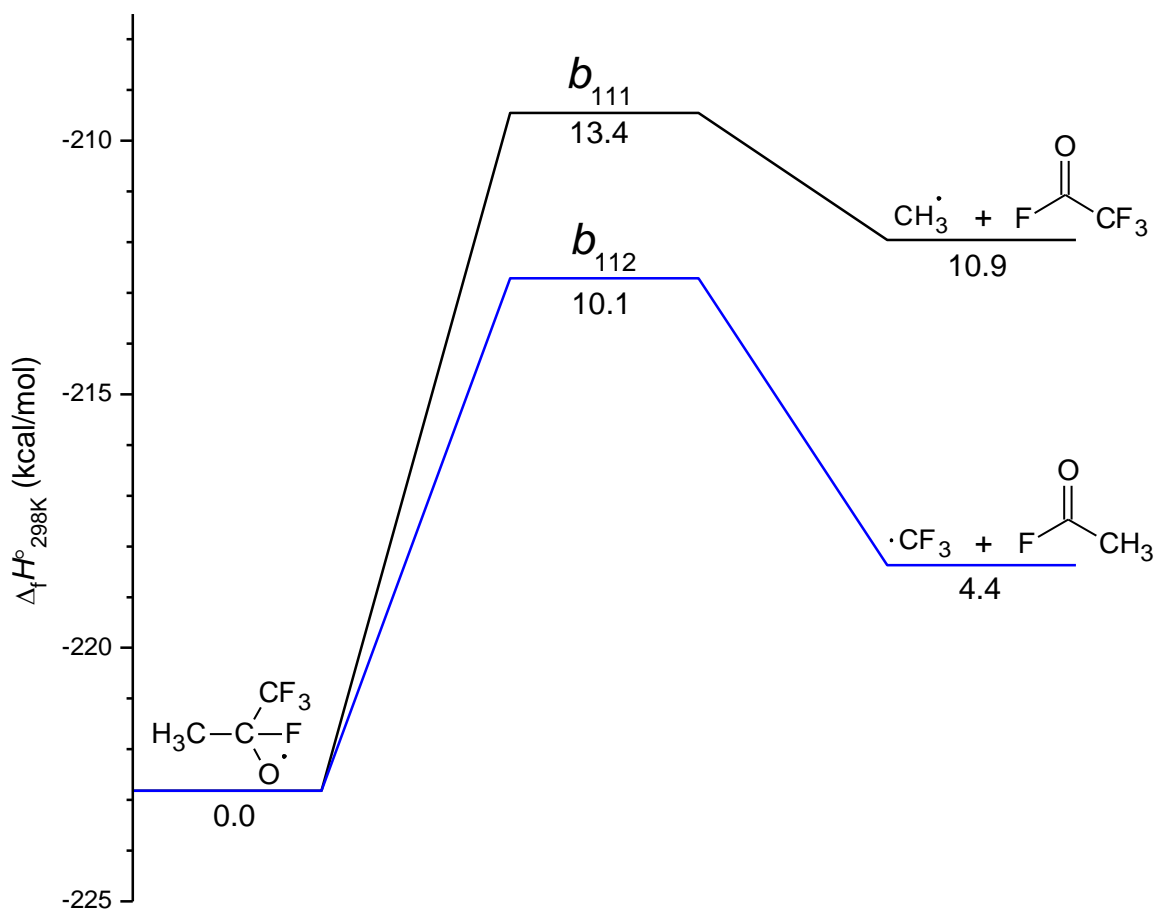


Figure 4.6: Decomposition channels of tetrafluoropropoxyl radical produced by reaction  $b_{12}$

Oxygen-addition reactions produce two oxygenated di-radical species with the oxygen atom attacking either the terminal carbon ( $c_1$ ) or the central carbon ( $c_2$ ). Potential energy scans revealed no maxima for either of these reactions, so they were both treated using collisional rate theory as discussed in §4.2. Of the two channels,  $c_2$  produces the most stable product by

almost 10 kcal/mol and should be the dominant channel for O-addition. As with the hydrogen addition products, these radicals can either  $\beta$ -scission back into 1234yf or proceed to different decomposition products. The product of reaction  $c_1$  can easily  $\beta$ -scission off a hydrogen atom and produce the resonance-stabilized structure (reaction  $c_{11}$ ) discussed earlier in reaction  $a_{12}$ . This species, once given enough energy through collisions, can lose the remaining hydrogen atom and form 2,3,3,3-tetrafluoroprop-1-en-1-one ( $c_{111}$ ). This species can then split into CO and C<sub>2</sub>F<sub>4</sub> in another collision mediated reaction ( $c_{1111}$ ). Each of the reactions in the  $c_1$  channel requires collisional treatment. The product of reaction  $c_2$  can  $\beta$ -scission into two different products depending on what C–C bond breaks. Breaking the C–CF<sub>3</sub> bond will produce a resonance-stabilized, oxygenated fluoroethyl radical and CF<sub>3</sub> radical ( $c_{21}$ ), while breaking the C–CH<sub>2</sub>· bond will produce a trifluoroacetyl fluoride and methylene radical ( $c_{22}$ ). Figure 4.7 shows the energy surfaces of these two competing decomposition routes. Based on its much lower barrier, as shown in the figure, the  $c_{21}$  route will be the dominant decomposition pathway.

Hydroxyl addition reactions can produce two tetrafluorohydroxypropyl radicals (reactions  $d_1$  and  $d_2$ ). Once again, potential energy scans revealed no maxima for these reactions, so the rates were calculated mathematically. Due to the weakness of the C–OH bond, these radicals are unlikely to  $\beta$ -scission into anything other than 1234yf. However, the hydroxyl hydrogen can easily transfer to the radical and produce a tetrafluoropropoxy radical. In the case where the hydroxyl adds to the terminal carbon ( $d_1$ ), hydrogen transfer can either produce the oxy radical ( $d_{11}$ ) or a hydrogen can transfer from the terminal carbon to the central

carbon and produce a different tetrafluorohydroxypropyl radical ( $d_{12}$ ). The oxidanyl radical produced from  $d_{11}$  will  $\beta$ -scission into formaldehyde and tetrafluoroethyl radical ( $d_{111}$ ). The hydroxypropyl radical produced from  $d_{12}$  will  $\beta$ -scission into  $\text{CF}_3$  radical and fluoroethenol ( $d_{121}$ ). In the case where the hydroxyl adds to the central carbon, the hydrogen transfer produces the same oxidanyl radical produced by reaction  $b_{11}$ .

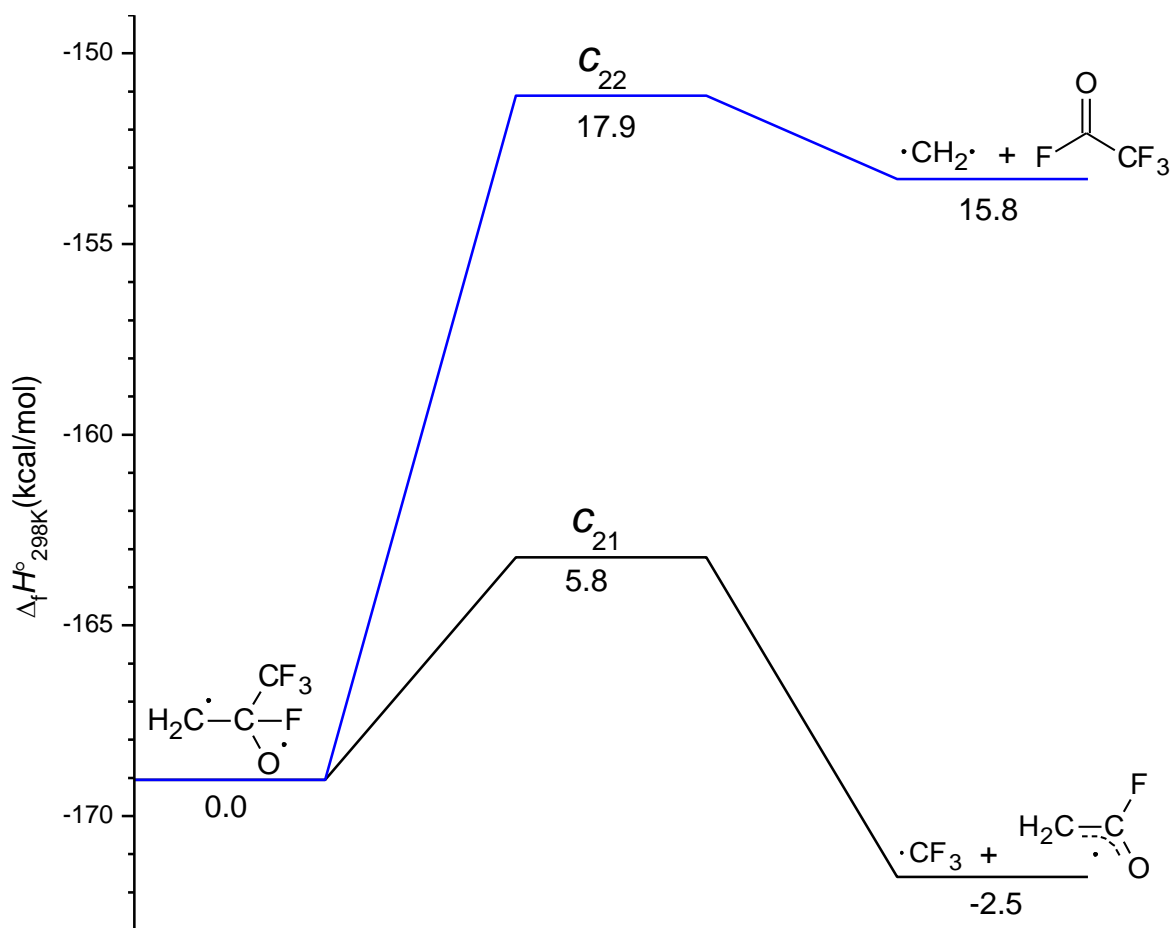


Figure 4.7: Decomposition of diradical product of reaction  $c_2$ .

Figure 4.8 shows the energy surface of the H-transfer isomerizations of the products of OH addition. All three of the isomerizations have relatively high barriers and will be slow;

however, the product of reaction  $d_2$  is the most stable and has the lowest barrier to H-transfer.

Thus it is probable that the  $d_2$  channel will be the most dominant OH-addition route.

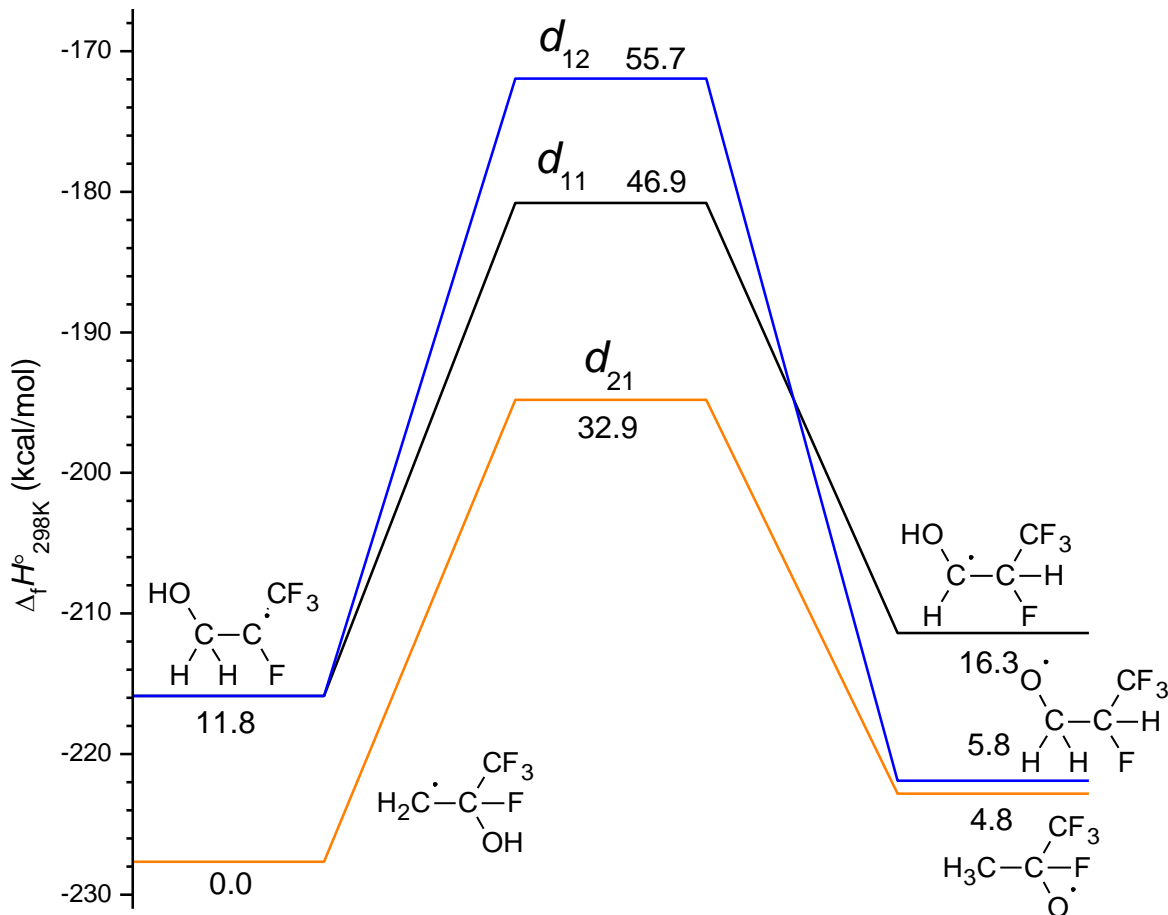


Figure 4.8: Isomerization pathways after OH addition.

#### 4.3.5 Mechanism summary

All reaction rates for the reactions described above can be found in Table 4.2. Note that this table shows only the sub-mechanism created for 1234yf combustion and not the small-

species reactions in the original NIST mechanism. Table 4.3 shows thermochemistry data for species not already included in the NIST mechanism.

Table 4.2: Sub-mechanism for the combustion of HFO-1234yf into small species

	Reaction		$A$	$n$	$E_a$	Ref.
1	$\text{CF}_3 + \text{CH}_2\text{CF} (+\text{M}) = \text{CH}_2\text{CFCF}_3 (+\text{M})$	$k_\infty$	6.81E14	0.00	0.00E00	
		$k_0$	2.53E18	-14.5	9.00E03	
2	$\text{CH}_2\text{CFCF}_3 (+\text{M}) = \text{CF}_3\text{CCH} + \text{HF} (+\text{M})$	$k_\infty$	9.68E10	0.98	7.99E04	
		$k_0$	3.85E50	-16.4	8.79E04	
3	$\text{CH}_2\text{CFCF}_3 = \text{HCCF} + \text{CHF}_3$		6.07E11	1.18	1.33E05	
4	$\text{CH}_2\text{CFCF}_3 + \text{H} = \text{Z-CHCFCF}_3 + \text{H}_2$		2.33E13	0.00	2.11E04	
5	$\text{CH}_2\text{CFCF}_3 + \text{H} = \text{E-CHCFCF}_3 + \text{H}_2$		2.04E14	0.00	2.22E04	
6	$\text{CH}_2\text{CFCF}_3 + \text{CH}_3 = \text{Z-CHCFCF}_3 + \text{CH}_4$		5.19E12	0.00	2.09E04	
7	$\text{CH}_2\text{CFCF}_3 + \text{CH}_3 = \text{E-CHCFCF}_3 + \text{CH}_4$		1.66E12	0.00	2.22E04	
8	$\text{CH}_2\text{CFCF}_3 + \text{CF}_3 = \text{Z-CHCFCF}_3 + \text{CHF}_3$		1.79E12	0.00	2.10E04	
9	$\text{CH}_2\text{CFCF}_3 + \text{CF}_3 = \text{E-CHCFCF}_3 + \text{CHF}_3$		8.79E11	0.00	2.12E04	
10	$\text{CH}_2\text{CFCF}_3 + \text{O} = \text{Z-CHCFCF}_3 + \text{OH}$		1.21E11	0.70	3.81E04	[102]
11	$\text{CH}_2\text{CFCF}_3 + \text{O} = \text{E-CHCFCF}_3 + \text{OH}$		1.21E11	0.70	3.81E04	[102]
12	$\text{CH}_2\text{CFCF}_3 + \text{OH} = \text{Z-CHCFCF}_3 + \text{H}_2\text{O}$		9.13E13	0.00	1.01E04	
13	$\text{CH}_2\text{CFCF}_3 + \text{OH} = \text{E-CHCFCF}_3 + \text{H}_2\text{O}$		1.52E13	0.00	1.16E04	
14	$\text{CH}_2\text{CFCF}_3 + \text{O}_2 = \text{Z-CHCFCF}_3 + \text{HO}_2$		3.58E13	0.00	6.00E04	[103] $\cdot\frac{1}{2}$
15	$\text{CH}_2\text{CFCF}_3 + \text{O}_2 = \text{E-CHCFCF}_3 + \text{HO}_2$		3.58E13	0.00	6.00E04	[103] $\cdot\frac{1}{2}$
16	$\text{E-CHCFCF}_3 = \text{Z-CHCFCF}_3$		6.44E13	0.00	0.00E00	[104]
17	$\text{Z-CHCFCF}_3 = \text{HCCF} + \text{CF}_3$		1.84E14	0.34	4.66E04	
18	$\text{Z-CHCFCF}_3 + \text{O} (+\text{M}) = \text{CHOCFCF}_3 (+\text{M})$	$k_\infty$	2.58E13	0.00	0.00E00	
		$k_0$	6.78E31	-17.1	9.61E03	
19	$\text{E-CHCFCF}_3 + \text{O} (+\text{M}) = \text{CHOCFCF}_3 (+\text{M})$	$k_\infty$	2.58E13	0.00	0.00E00	
		$k_0$	6.96E31	-17.1	9.41E03	
20	$\text{CH}_2\text{CFCF}_3 + \text{H} = \text{CH}_3\text{CFCF}_3$		1.14E14	0.00	4.09E03	
21	$\text{CH}_3\text{CFCF}_3 + \text{O} (+\text{M}) = \text{CH}_3\text{COFCF}_3 (+\text{M})$	$k_\infty$	1.70E13	0.00	0.00E00	
		$k_0$	1.39E39	-19.8	1.26E04	
22	$\text{CH}_3\text{COFCF}_3 = \text{CH}_3 + \text{CF}_3\text{COF}$		2.46E12	0.19	2.07E02	
23	$\text{CH}_3\text{COFCF}_3 = \text{CF}_3 + \text{CH}_3\text{COF}$		2.45E12	0.13	1.41E02	
24	$\text{CH}_2\text{CFCF}_3 + \text{H} = \text{CH}_2\text{CHFCF}_3$		2.26E14	0.00	7.75E03	
25	$\text{CH}_2\text{CHFCF}_3 = \text{CH}_2\text{CHF} + \text{CF}_3$		1.06E14	0.15	3.37E04	
26	$\text{CH}_2\text{CFCF}_3 + \text{O} (+\text{M}) = \text{CH}_2\text{OCFCF}_3 (+\text{M})$	$k_\infty$	3.42E13	0.00	0.00E00	
		$k_0$	2.92E01	-10.9	2.04E03	
27	$\text{CHOCFCF}_3 + \text{H} (+\text{M}) = \text{CH}_2\text{OCFCF}_3 (+\text{M})$	$k_\infty$	9.55E13	0.00	0.00E00	
		$k_0$	8.06E26	-17.3	8.98E03	
28	$\text{CF}_3\text{CFCO} + \text{H} (+\text{M}) = \text{CHOCFCF}_3 (+\text{M})$	$k_\infty$	8.36E12	0.00	0.00E00	
		$k_0$	2.60E15	-14.0	4.59E03	

Table 4.2 Continued

29	$\text{CO} + \text{CF}_2\text{CF}_2 = \text{CF}_3\text{CFCO}$		7.87E11	0.00	0.00E00
30	$\text{CH}_2\text{CFCF}_3 + \text{O} (+\text{M}) = \text{CH}_2\text{COFCF}_3 (+\text{M})$	$k_\infty$	3.00E13	0.00	0.00E00
		$k_0$	2.78E01	-11.0	2.06E03
31	$\text{CH}_2\text{COFCF}_3 = \text{CH}_2\text{COF} + \text{CF}_3$		9.86E11	0.88	4.02E03
32	$\text{CH}_2\text{COFCF}_3 = \text{CF}_3\text{COF} + \text{CH}_2$		8.62E11	1.13	1.85E04
33	$\text{CH}_2\text{CFCF}_3 + \text{OH} (+\text{M}) = \text{CH}_2\text{OHCFCF}_3 (+\text{M})$	$k_\infty$	1.64E13	0.00	0.00E00
		$k_0$	8.74E12	-14.2	5.05E03
34	$\text{CH}_2\text{OHCFCF}_3 = \text{CH}_2\text{OCHF}_3$		5.25E06	0.99	2.04E03
35	$\text{CH}_2\text{OHCFCF}_3 = \text{CHOHCHF}_3$		1.25E06	1.22	2.89E03
36	$\text{CH}_2\text{OCHF}_3 = \text{CH}_2\text{O} + \text{CF}_3\text{CHF}$		4.23E16	-0.99	6.85E03
37	$\text{CHOHCHF}_3 = \text{CF}_3 + \text{CHFCHOH}$		2.45E15	0.00	3.86E04
38	$\text{CH}_2\text{CFCF}_3 + \text{OH} (+\text{M}) = \text{CH}_2\text{COHFCF}_3 (+\text{M})$	$k_\infty$	1.68E13	0.00	0.00E00
		$k_0$	8.76E12	-14.1	5.36E03
39	$\text{CH}_2\text{COHFCF}_3 = \text{CH}_3\text{COFCF}_3$		7.25E09	0.39	5.31E03

Units are in  $\text{cm}^3 \text{ mol s cal K}$ ;  $k = AT^n \exp(-E_a/RT)$

Table 4.3: Thermochemistry data for new species

Species	$\Delta_f H^\circ$	$S^\circ$	$C_p^\circ(\text{T})$							
			298	298	300	400	500	600	800	1000
$\text{CH}_2\text{CFCF}_3$	-197.0	82.5	24.0	28.9	32.6	35.4	39.4	41.9	45.3	47.0
Z- $\text{CHCFCF}_3$	-132.7	82.7	24.0	28.3	31.4	33.7	36.7	38.6	40.8	42.0
E- $\text{CHCFCF}_3$	-132.2	82.9	24.1	28.3	31.4	33.7	36.7	38.6	40.9	42.0
$\text{CH}_3\text{CFCF}_3$	-183.1	87.1	26.1	31.0	35.0	38.2	42.8	45.9	50.1	52.3
$\text{CH}_2\text{CHF}_3$	-179.6	86.4	26.8	31.9	35.9	39.0	43.3	46.3	50.2	52.4
$\text{CH}_2\text{OCFCF}_3$	-160.7	88.9	27.1	32.2	36.3	39.5	44.1	47.2	50.9	52.9
$\text{CH}_2\text{COFCF}_3$	-169.1	85.6	26.3	31.9	36.3	39.7	44.3	47.3	50.9	52.9
$\text{CHOCFCF}_3$	-201.4	90.2	26.7	31.2	34.8	37.5	41.3	43.7	46.4	47.9
$\text{CH}_2\text{COF}$	-59.9	67.8	15.0	17.8	19.9	21.6	24.1	25.8	28.2	29.6
$\text{CF}_3\text{CFCO}$	-201.1	87.9	25.7	29.7	32.6	34.8	37.7	39.5	41.5	42.5
$\text{CH}_3\text{COFCF}_3$	-227.7	90.2	31.3	37.0	41.3	44.6	49.0	51.9	55.8	58.0
$\text{CH}_3\text{COF}$	-106.7	69.6	15.3	18.2	20.8	23.0	26.5	29.0	32.6	34.6
$\text{CH}_2\text{OHCFCF}_3$	-215.9	94.0	29.5	35.1	39.5	43.0	47.9	51.2	55.6	57.9
$\text{CH}_2\text{COHFCF}_3$	-227.7	90.2	31.3	37.0	41.3	44.6	49.0	51.9	55.8	58.0
$\text{CH}_2\text{OCHF}_3$	-211.4	90.5	28.8	34.6	39.2	42.9	48.0	51.5	55.9	58.2
$\text{CHOHCHF}_3$	-221.9	91.8	30.1	35.6	40.0	43.5	48.2	51.4	55.6	57.9
$\text{CHFCHOH}$	-74.2	68.5	15.4	18.7	21.4	23.6	26.8	29.1	32.5	34.4

Units for  $\Delta_f H^\circ$  are in kcal/mol; units for  $S^\circ$  and  $C_p$  are in  $\text{cal mol}^{-1} \text{ K}^{-1}$

#### 4.4 *Computational evaluation and reaction path analysis*

##### 4.4.1 *Mechanism evaluation by CHEMKIN-PRO*

To verify the mechanism's performance, it was necessary to compare simulation results from CHEMKIN-Pro to experimental data. Searching the literature turned up few data on 1234yf combustion and fewer data that could be simulated using CHEMKIN. Takizawa et al. [95] reported  $S_u$ , the burning velocity or adiabatic flame speed, of 1234yf in an O<sub>2</sub>-enriched environment (35% O<sub>2</sub> and 65% N<sub>2</sub>) in a series of experiments, giving sufficient experimental description for modeling. Simulations were performed to calculate the adiabatic flame speed of 1234yf at these conditions according to the mechanism, the results of which are shown in figure 4.9.

The results show that while the mechanism slightly under-predicts Takizawa's data, it also shows the same roughly linear trend with temperature. There are a few possible explanations for the difference. Takizawa provides no uncertainty estimate for the data and rather says "experimental uncertainty was rather large" [95] repeatedly over the course of the paper, though never in reference to this particular figure. If the uncertainty for this data is indeed somewhat large, the predictions likely fall into that uncertainty range given the two data sets are fairly close to one another.

Takizawa's data predict the burning velocity will start to decrease at about 450K, a trend to which he does not allude in the text. Calculations of stoichiometric 1234yf/air mixtures up to 1200K, shown in figure 4.10, do not show a similar trend but rather display a roughly exponential relationship between  $T$  and  $S_u$ .



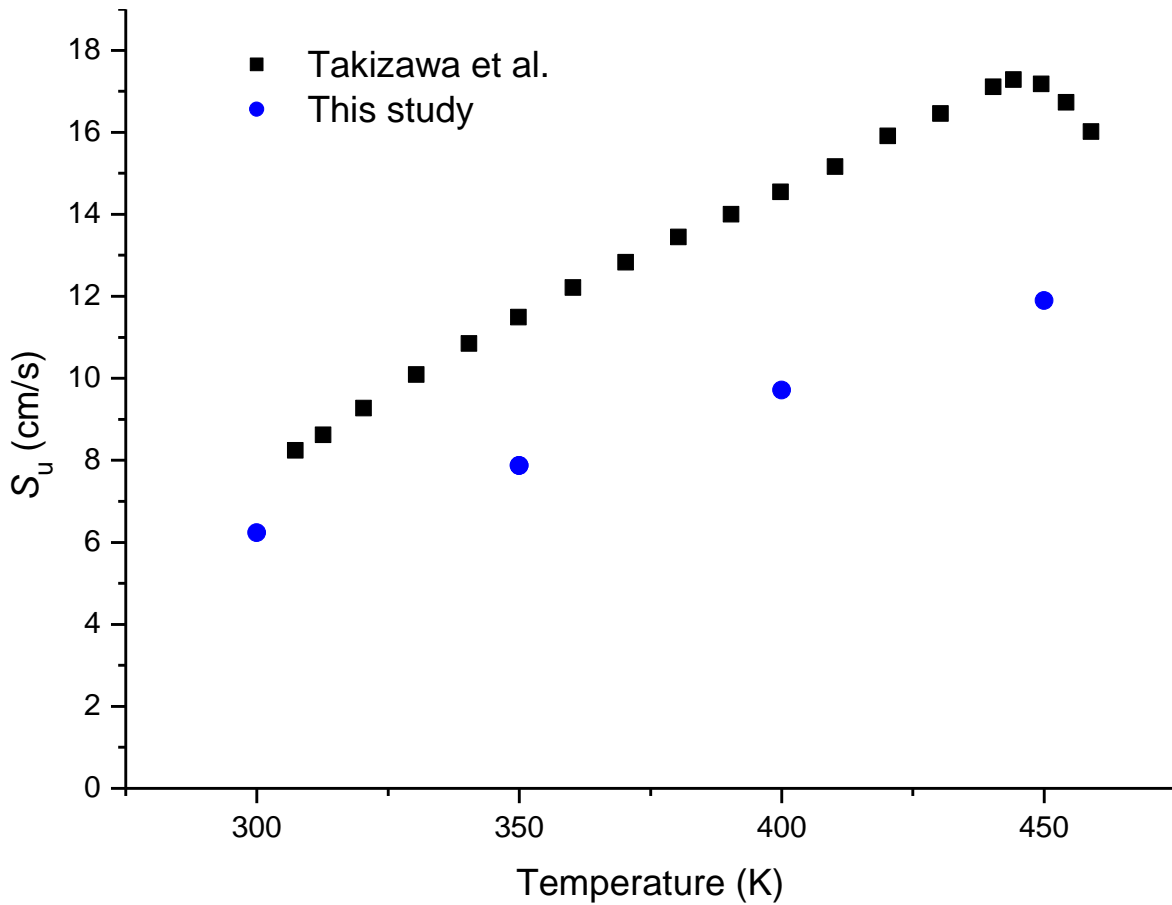


Figure 4.9: Burning velocity of stoichiometric 1234yf in 35% O<sub>2</sub>/65% N<sub>2</sub> mixture [95]. Note: experimental data (solid squares) shown are from Takizawa's 800 torr case. Calculations (solid circles) were performed at atmospheric conditions because the experimental data shows little variation with pressure.

Perhaps the drop off in Takizawa's data is due to some artifact of the experimental method and is not representative of the true relationship between  $S_u$  and  $T$ .

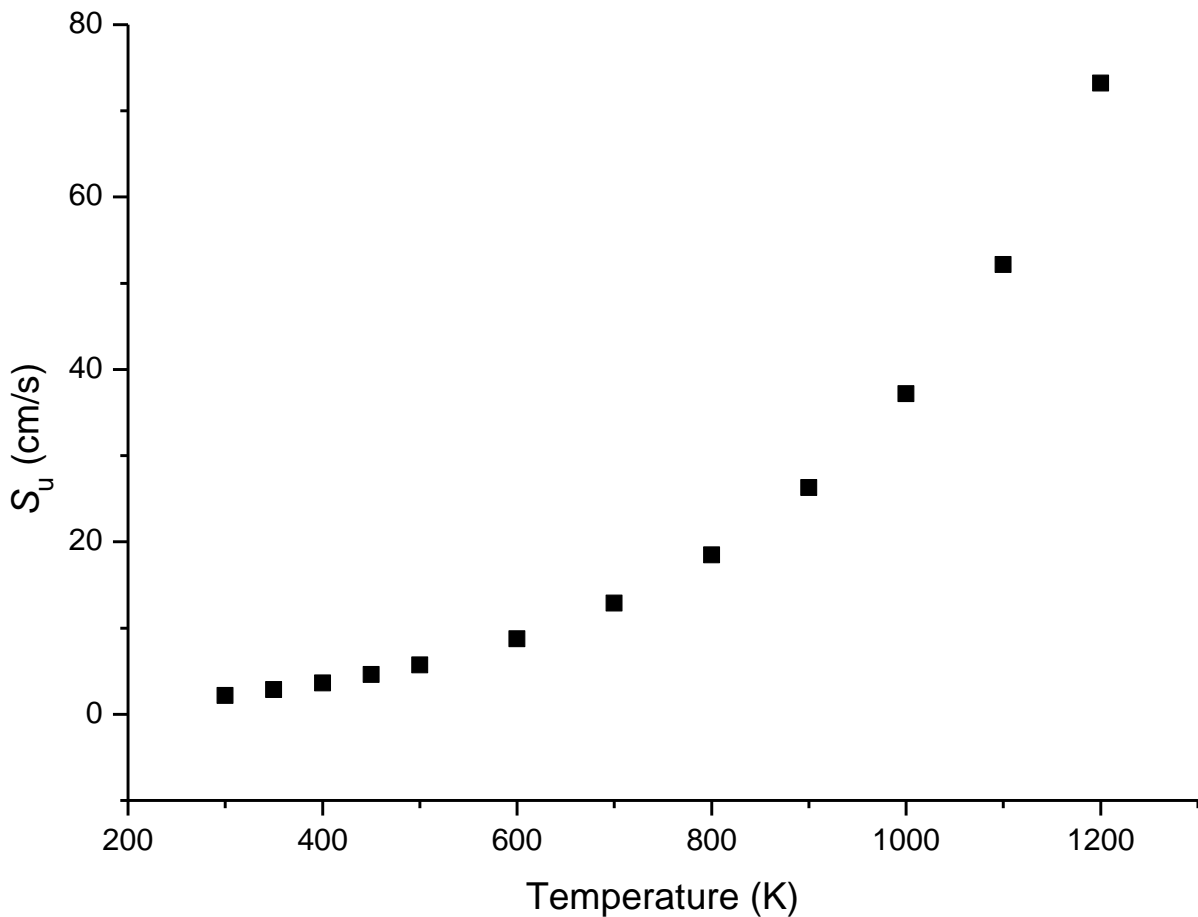


Figure 4.10: Burning velocity of stoichiometric 1234yf/air mixture.

#### 4.4.2 *Reaction-path analysis*

The major reaction routes of HFO-1234yf were determined using the reaction-path analysis tool included in the CHEMKIN-Pro software package, as well as the output from flame-speed simulations. Example simulation output in two figures below (4.11 and 4.12) shows the concentration profiles of various species in a 300K stoichiometric 1234yf/air flame.

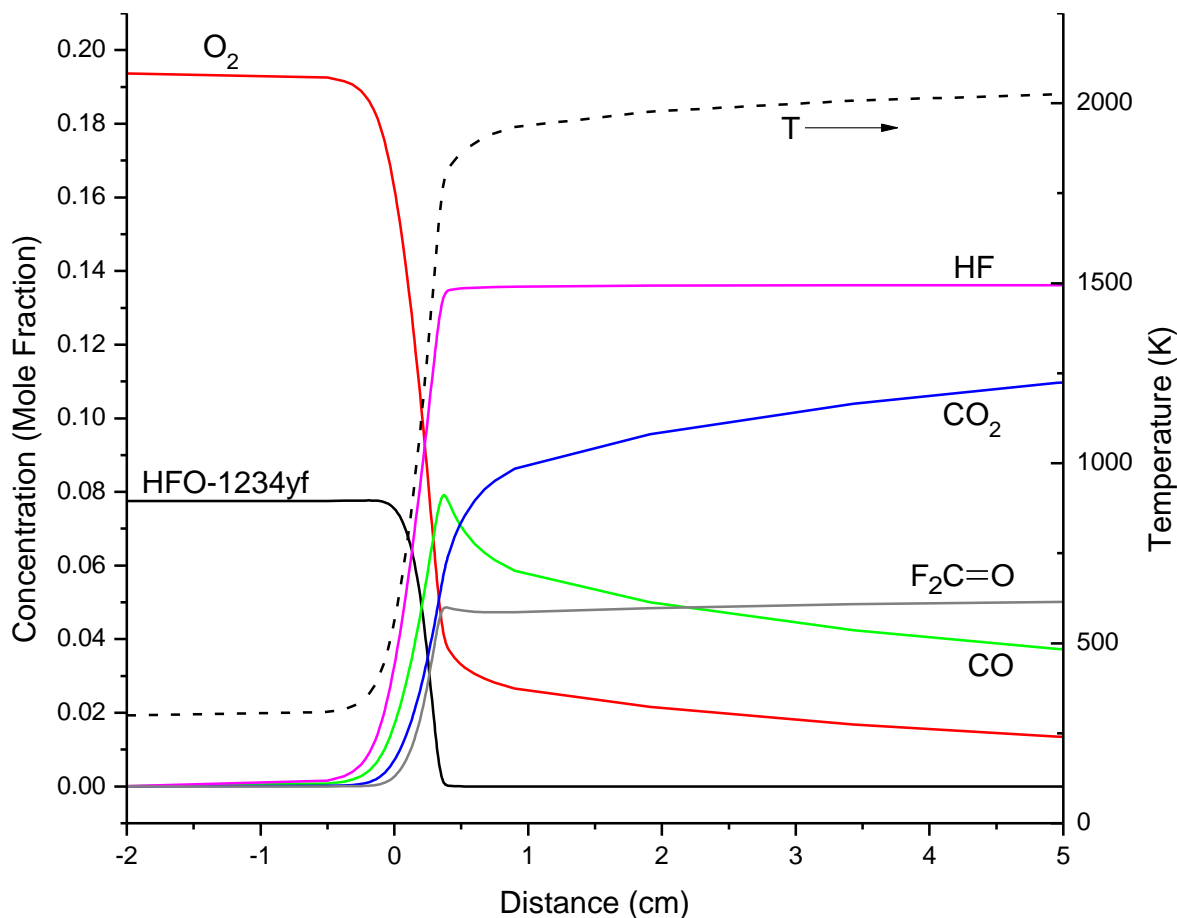


Figure 4.11: Concentration profiles for reactants and major products from combustion of stoichiometric 1234yf/air mixture at 300K.

At low initial temperatures, 1234yf does not undergo much decomposition until the system temperature reaches about 500K. The major decomposition route once destruction starts is H addition. Likely, the H radicals are produced by back diffusion of the species from hotter parts of the flame. As the temperature rises, H abstraction by OH contributing begins to dominate with the H-addition route beginning to produce acetyl fluoride. As the temperature nears its peak, the unimolecular routes,  $u_1$  and  $u_2$ , take over as the main decomposition reactions. Each of these decomposition routes quickly converts 1234yf into small, fluorinated

hydrocarbons that end up producing HF or F<sub>2</sub>CO, which can be seen as some of the major products in figure 4.11. The progression of intermediate-species peaks in figure 4.12 clearly shows the rise and fall of each dominant reaction. Overall, the unimolecular routes have the greatest effect on the system, and the abstraction and H-addition routes are each a few orders of magnitude behind.

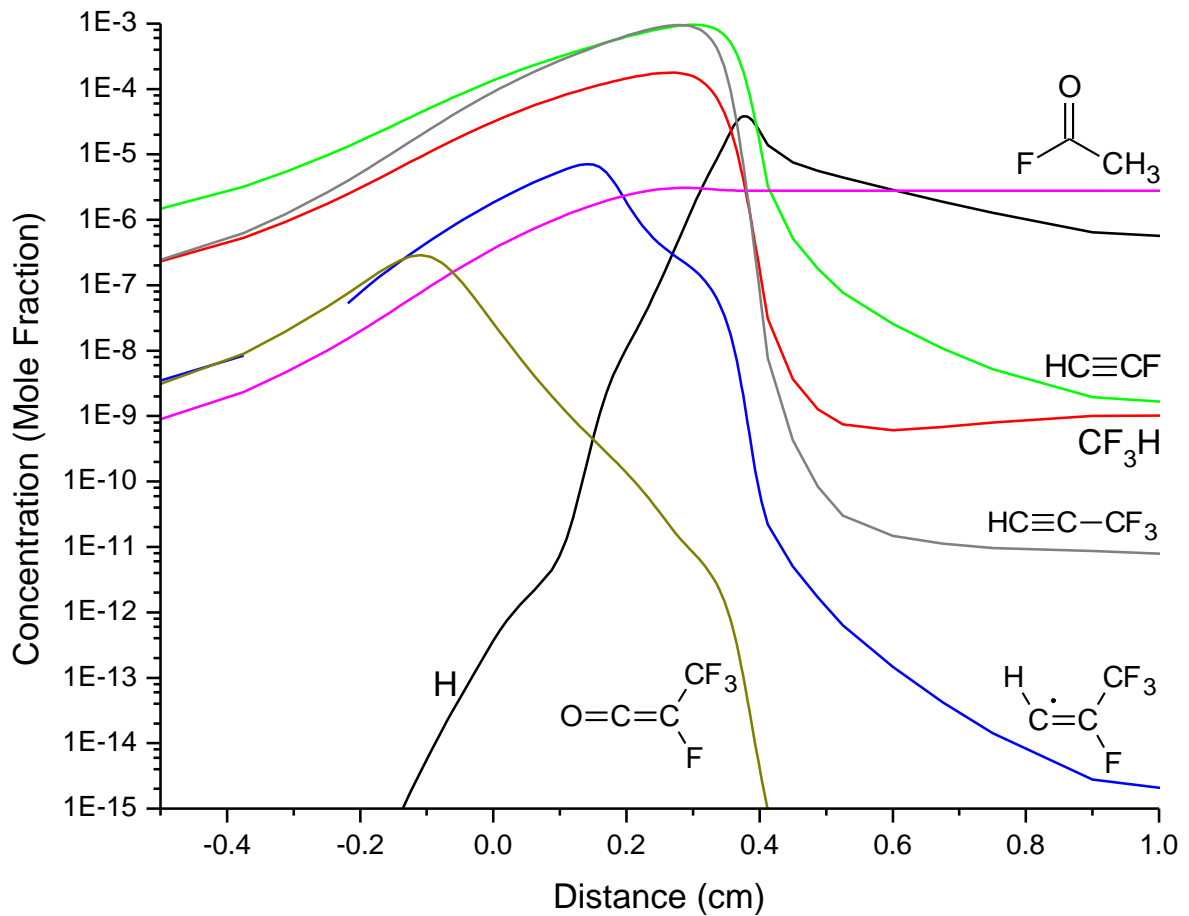


Figure 4.12: Concentration profiles for main intermediate from combustion of stoichiometric 1234yf/air mixture at 300K.

#### 4.5 *Conclusions*

In this work a series of reactions was proposed to describe the decomposition of the fluorocarbon refrigerant HFO-1234yf into smaller species. Rate and thermochemistry data for the proposed reactions were either calculated using quantum chemistry or estimated from published data for similar species. The new decomposition mechanism was combined with a mechanism from a previous study that describes the combustion of smaller fluorocarbon species. The combined mechanism was tested against published data for the flame speed of 1234yf. Results showed that while the mechanism under-predicted the experimental figures, it is likely that the predictions were within the uncertainty of the measurement. Further study may be needed to discern the true source of the discrepancy between prediction and measurement. A modeling study of the combustion of 1234yf at 300K was conducted to explore the major reaction routes of the refrigerant in a flame at ambient conditions. The results showed that unimolecular reactions dominated, followed by abstraction and H-addition reactions. While ambient conditions were investigated here, the mechanism is designed for use at temperatures ranging from 300 to 2300K and should be easy to incorporate into existing combustion models allow for extensive further study of HFO-1234yf and its behavior in applications.

## CHAPTER 5. DYNAMIC CHEMICAL MODEL FOR H<sub>2</sub>/O<sub>2</sub> COMBUSTION DEVELOPED THROUGH A COMMUNITY WORKFLOW

This work conducted in collaboration with of James Oreluk,<sup>1</sup> Sathya Baskaran,<sup>2</sup> S. Mani Sarathy,<sup>2</sup> Michael P. Burke,<sup>3</sup> Richard H. West,<sup>4</sup> Michael Frenklach<sup>1</sup>, and Phillip R. Westmoreland<sup>5\*</sup>

<sup>1</sup>Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA

<sup>2</sup>King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

<sup>3</sup>Department of Mechanical Engineering, Department of Chemical Engineering, and Data Science Institute, Columbia University, New York, NY 10027, USA

<sup>4</sup>Department of Chemical Engineering, Northeastern University, Boston, MA 02115, USA

<sup>5\*</sup>Corresponding author: Chemical and Biomolecular Engineering Dept., North Carolina State University, Raleigh, NC 27695

### *5.1 Contributions of this author to the work in this chapter*

The major roles of this author in the following work were entering or supervising the entry of flame data into the PrIME database, the selection of the three mechanisms used in optimization, and the transfer of those mechanisms from literature to PrIME format. The work presented below was highly collaborative, with roles for each step being presented in

figure 5.1. This work has been recently submitted for publication [105]. As such, all work presented in this chapter has been described in the words of this author.

## 5.2 *Introduction*

The system of H<sub>2</sub>/O<sub>2</sub> combustion has been a classic problem in the combustion community that receives considerable study even today [10,14,106–109]. With new information being published so frequently it is difficult for mechanisms to keep up. The need for a new approach where new information can be incorporated into a mechanism by anyone who has made a discovery is clear. This approach requires a framework that is universally accessible and easy to use. The present work presents the uncertainty quantification (UQ) tools in PrIme [19] as a solution to this problem and others encountered by the kinetics community. The H<sub>2</sub>/O<sub>2</sub> combustion system is used both as a proof of concept and as an example for the type of significantly well-studied system that can benefit most from the capabilities of PrIme.

## 5.3 *Theory*

### 5.3.1 *The architecture and use of PrIme*

PrIme is a cyberinfrastructure composed of a data warehouse and a workflow. The data warehouse is a large database of experiments, reactions, reaction rates, reaction mechanisms, references, and more all stored in XML format. The workflow is a set of applications that allow the user to perform many different computations upon data from the warehouse, such as reactor modeling and uncertainty quantification [109]. Both the data warehouse and the workflow application can be accessed on the PrIme website [19].

In the warehouse, data entries are assigned a PrIME ID that allows each entry to be easily linked to other related entries. For example, if rate coefficients derived by a publication are entered into the database, each rate receives its own PrIME ID and is linked to the ID of a separate file that contains information about the reaction (i.e., the species involved and their stoichiometric coefficients) and the ID of another separate file containing the reference information (i.e., the bibliographic record of the publication). The extensive interconnections of the database reduce redundancy (and, by extension, the size of the database) and simplify the process of accessing the data.

Within the workflow, various tools can be used to use or probe the data. The most basic of these tools simply allows the user to search the warehouse and submit new data to it. The tools that are used most heavily in this study are PrIME's reactor modeling and UQ tools, applied with the goal of using UQ to develop a new, optimized mechanism. Figure 5.1 lays out schematically the process required, showing which team took which role by the institution initials underneath.

The process begins by determining the base reaction set and the experimental data to which it will be compared. This determination involves ensuring that all reaction rates and datasets involved are entered into the PrIME warehouse and that uncertainty bounds are assigned to both rates and experiments wherever possible.

In this study, novel computational tools were used to check the model for consistency with literature data. The UQ tool in PrIME requires that Quantities of Interest (or QoIs) be defined for the experimental data. A QoI represents a specific point in the experimental data record



that is chosen as being characteristic of that set of data (e.g., peak OH concentration, ignition delay time, flame speed, etc.). Often, more than one QoI is chosen for a given dataset if that dataset is deemed especially trustworthy or important. These QoIs are entered in the warehouse as XML files of type “data attribute” (each with a unique PrIme ID), which contain descriptions of the experimental conditions and uncertainty bounds as well as the actual value of the QoI.

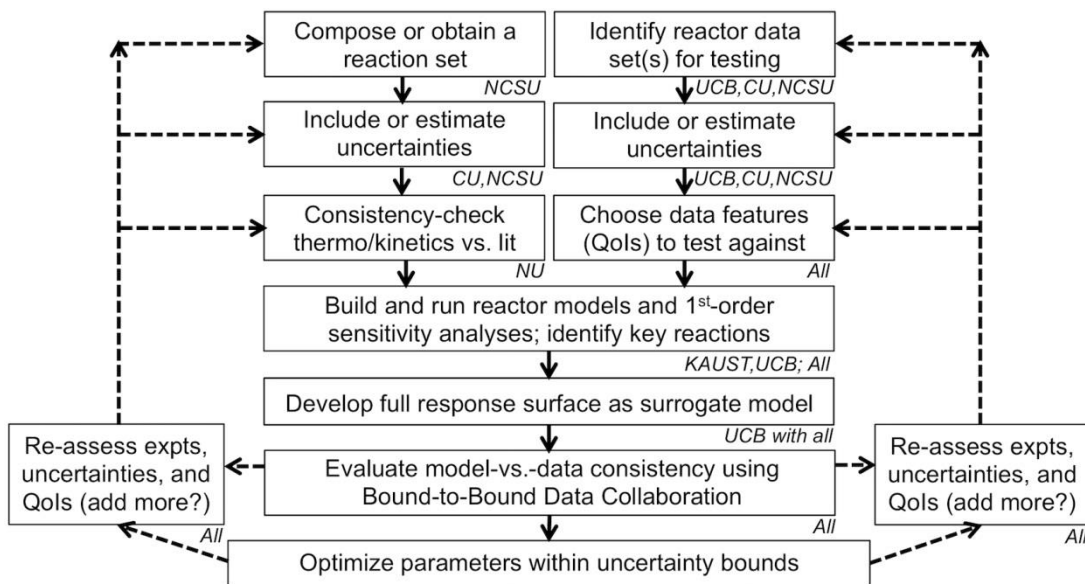


Figure 5.1: Step-by-step process for mechanism optimization using PrIme’s UQ capabilities. Lead investigators (grouped by institution) for each step are listed under the area description.

With reaction set and experimental QoIs defined, the next step is to use PrIme’s reactor modeling tools to simulate the experimental results with the reaction set. Shock-tube simulations used PrIme’s PFR reactor tool, described by You et al. [106]. Flame simulations used a cloud-based tool called CloudFlame [111–113], which interfaces with PrIme’s workflow.

The simulated and experimental datasets with uncertainties are compared to each other using Bound-to-Bound Data Collaboration (B2B-DC) [106,110,114–118] as part of PrIME’s UQ tool. The goal of this analysis is to determine whether the reaction set simulates the experimental data within the uncertainty bounds. If so, the dataset is said to be consistent and the reaction set and QoIs can be reevaluated to determine if more data is needed. If not, both the reaction set and QoIs need to be reevaluated to determine the source of the inconsistency. If the dataset is consistent and the data included are deemed sufficient, PrIME is able to optimize the reaction set to predict the experimental data more precisely. The user selects a set of active variables (in this work, the pre-exponential factors of the rate coefficients in the reaction set) which are adjusted within their uncertainty bounds to produce a new, optimized reaction set.

### 5.3.2 *Towards a more careful preservation of rate constants*

When a reaction rate is used in a mechanism, it is not uncommon that its parameters be changed from the units of its original publication to the units of the new author’s preference. Though this practice is necessary — it would be confusing if all reaction rate parameters in a published mechanism were reported in varying units — it is not always faithful in its duplication. West and co-workers have begun to look into the extent of the errors that are present in current mechanisms by comparing them with each other, with the results showing that “in many published and trusted models these parameters can differ by 100 kJ/mol and 30 orders of magnitude respectively” [119]. To ensure that these transposition errors were not included in the database, all reaction rates that were entered into the warehouse were taken

directly from the source in which they were first measured or reported, if possible. Along with this practice, an effort was made to catalogue the different sources that made use of each reaction. While no claims will be made towards complete coverage of the literature, the intention was to lead users to the correct source when they were searching for reaction rates from different mechanisms that come from the same original source. The ability to preserve and cross-reference reaction rate data in this way is PrIME's proffered solution to the problem of errors introduced by transfer of reaction rates from publication to publication.

The need to enter reaction rate data that matches the reaction direction listed in the database was discovered as an undesirable exception within PrIME's framework. Rate-coefficients written for the wrong direction needed to be reversed using thermochemistry data before being submitted to the warehouse. The reversal procedure involved using a program called RMG-Py [120] to regression-fit a modified-Arrhenius equation to 50 temperatures between 294 and 2000 K in an attempt to preserve any temperature dependencies in the original rate-coefficient expression. A future code modification should be to allow comparisons of forward and reverse data within the cyberinfrastructure.

#### *5.4 Data selection procedures*

##### *5.4.1 Reaction sets*

The reaction mechanism from Burke et al. [10] was selected for the base reaction set to be used in analysis. It was selected for the same reasons as it was used in Chapter 3, due to its consideration of many different types of experiments in its analysis, especially shock tubes and flames, and its good agreement when compared to the experimental data. A few updates

to the reactions in the Burke mechanism have already been published [121,122]. Though including these updates in the reaction set seemed natural, testing PrIME's reactor modeling by using it to reproduce data comparisons in the original publication [10] was a necessary consistency check. Are the rates entered into PrIME correctly? Are the PrIME reactor modeling tools working correctly? Therefore the original Burke mechanism was named Mechanism1 [123] and the mechanism with updates was named Mechanism2 [124]. A third mechanism, Mechanism3 [125], was created by adding kinetics for ozone,  $O(^1D)$ ,  $O(^1\Delta_g)$ , and  $OH^*$  ( $^2\Sigma$  state) from Konnov [14] to Mechanism2 intending that comparisons between the performance of the two mechanisms would yield insights about how excited species fit into the framework of  $H_2/O_2$  combustion.

#### 5.4.2 *Experimental data*

This work focused on testing models against a number of shock-tube and flame experiments. QoIs for shock tubes were chosen from experimental ignition time data of  $\log(\tau_{ign})$  vs.  $1/T$  at  $1/4$ ,  $1/2$ , and  $3/4$  maximum temperature. QoIs for flames were chosen as the measured laminar flame speed in each experiment. This resulted in 124 QoIs (114 from shock tubes and 10 from flames) from 12 shock-tube sources [126–137] and two flame studies [138,139].

#### 5.4.3 *Resolving data inconsistencies*

The B2B-DC approach was undertaken to determine the consistency of the dataset. Before analyzing the dataset as a whole, each QoI was checked for self-consistency. By definition, a QoI is self-consistent if the reaction set can simulate the QoI value within the uncertainty set

for that individual QoI. QoIs that don't meet this criterion are said to be self-inconsistent and need to be reevaluated. The analysis concluded that 29 shock-tube QoIs were self-inconsistent. Of these, 10 could be made self-consistent by reassessing the uncertainty bounds. The others were discarded.

The new dataset of self-consistent QoIs was then evaluated for consistency as a whole and found to be inconsistent. An inconsistent dataset means there exists no set of allowed values of the active variables that will be able to model all QoIs *simultaneously* (as opposed to individually, as with the self-consistency checks). Figure 5.2 shows the sensitivity of the dataset consistency to ten QoIs (denoted by their PrIME ID). As with the self-consistency check, experimental uncertainties were reassessed to attempt to resolve the issue. In this case, the two QoIs with the highest sensitivity required uncertainty-bound changes of more than 5% and were removed from the analysis. The discarded QoIs were not eliminated but werereserved in the PrIME warehouse for future study. After this process, the dataset was brought to consistency, and a new, optimized mechanism was produced. This mechanism was named DynamicMech151203 [140] with the intention of defining the set as a revisable mechanism that can be improved by the research community.

### 5.5 *Results and discussion*

Though the new mechanism represents a tangible result of this study, the analysis yielded a additional insights about the H<sub>2</sub>/O<sub>2</sub> system and the studies done upon it.

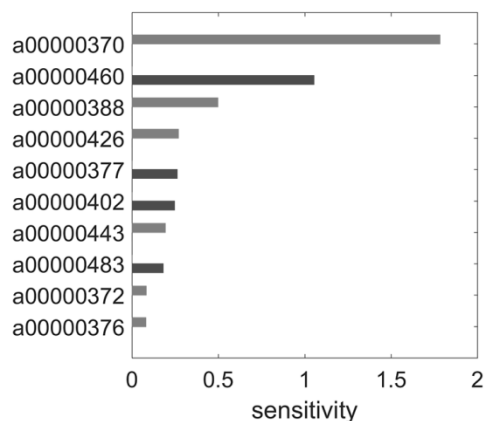


Figure 5.2: Normalized dataset consistency sensitivity to ten data attributes (QoIs) with highest sensitivity. All are shock-tube QoIs except a00000483, which is a flame speed. Black bars represent upper-bound sensitivity; gray, lower-bound sensitivity.

### 5.5.1 $O_2(^1\Delta_g)$

The comparison of Mechanism2 to Mechanism3 yielded interesting suggestions about the inclusion of excited species in  $H_2/O_2$  mechanisms. Of the greatest interest, it implied that  $O_2(^1\Delta_g)$  plays an unexpected role at higher pressures. Mechanism3 predicted the flame speed for QoI a00000484 (a high-P, fuel-rich flame) better, about 15% lower than Mechanism2. Figure 5.3 shows the reactions in Mechanism3 with the highest impact factor for this QoI. The reaction  $H_2+O_2(^1\Delta_g)=H+HO_2$  (more specifically its reverse) has been shown to inhibit high-pressure flames [139] and has one of the highest impact factors in the figure.

To test the hypothesis that this reaction aids its equivalent ground-state reaction  $H+HO_2=H_2+O_2(^3\Sigma_g^-)$  in quenching radicals, the reaction rate for the ground-state reaction in Mechanism2 was scaled by the flux through the excited-state reaction. Simulations using this modified Mechanism2 reproduced the flame speed predicted by Mechanism3 within 1%,

effectively confirming that the reduced flame speed was a result of including the excited-O<sub>2</sub> channel. Though this analysis accounted for the discrepancy with only one reaction, the results suggest that a more careful look at the role of excited species may be necessary and showed how the tools within PrIME are effective at investigating this type of issue.

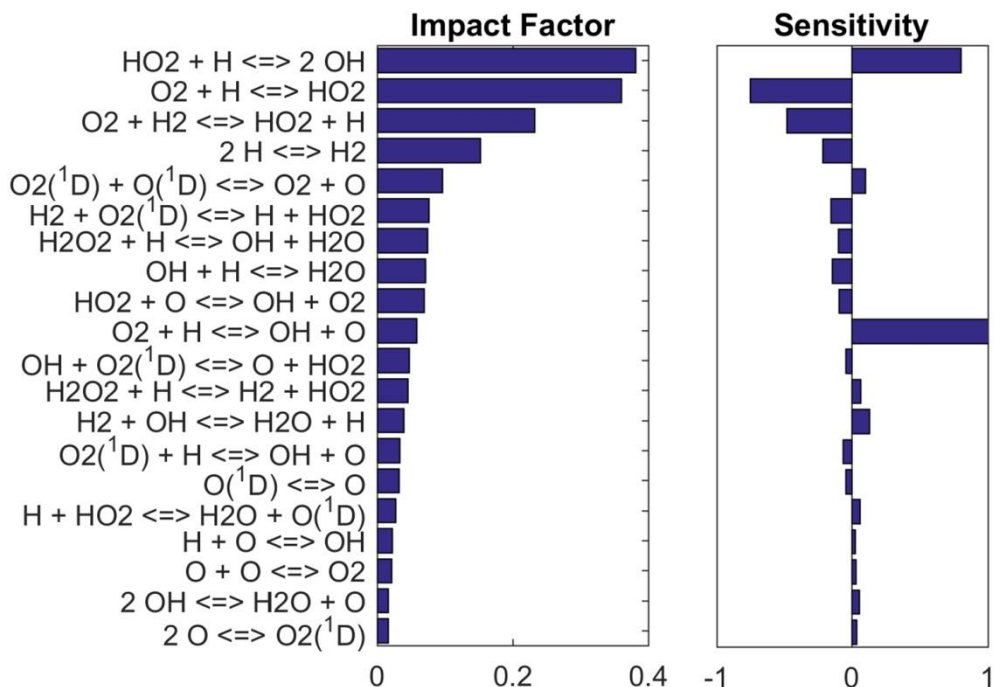


Figure 5.3: Impact factor and sensitivity of the prediction of flame speed QoI a00000484 to the top 20 reactions ranked by impact factor, where the impact factor is  $0.5\log(U_e/L_e)$  multiplied by the absolute sensitivity. Note: For font reasons,  $O_2(^1\Delta_g)$  is shown as  $O_2(^1D)$  in the PrIME database.

### 5.5.2 Insights from data inconsistency

The consistency analysis describe above discovered two QoIs that were self-inconsistent. In this case, the experimental time to OH maximum concentration in these experiments/QoIs was 40% or less of what was predicted by the model. Some studies [133,141] have shown

that these systems are not adequately predicted by the reactor model used here, instead needing more sophisticated codes that can incorporate heterogeneities in the reactor and pre-ignition energy release. The inconsistency of the data, therefore, points to the need for more complex simulation and not to some shortcoming of the experiments. In this way, inconsistent datasets, particularly with QoIs that are self-inconsistent, can be used to gather insights about how experimental results fit within the data already gathered by the community and whether new results indicate more complexity than expected.

## 5.6 Conclusion

Uncertainty-quantification procedures were carried out upon the H<sub>2</sub>/O<sub>2</sub> combustion system, resulting in an optimized model and a few discoveries about the system. O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>) was discovered to play a more important role than previously thought, and data inconsistencies pointed to the need for more rigorous codes for the simulation of some shock-tube experiments. All these discoveries were enabled by the PrIME framework, which has shown that it is a powerful tool for investigating reactive systems. The optimized mechanism [140] has been archived in the PrIME data warehouse and is now accessible and open to improvement by the community. This accessibility represents PrIME's most important strength, the capability of being easily usable by the entire scientific community to explore complex problems with data as it is measured.



**CHAPTER 6. TEMPERATURE-DEPENDENT REACTION BETWEEN  
TRIMETHYLALUMINUM AND POLY(METHYL METHACRYLATE) DURING  
SEQUENTIAL VAPOR INFILTRATION: EXPERIMENTAL AND *AB INITIO*  
ANALYSIS**

*6.1 Contributions of this author to the work in this chapter*

The major role of this author in the following publication was to perform quantum-chemical simulations of the species involved in the reaction between trimethylaluminum (TMA) and poly(methyl methacrylate) (PMMA) and to interpret the results of those simulations. Due to the previously unknown or, at best, poorly understood nature of the reaction being explored, potential reaction mechanisms first had to be proposed. These mechanisms were proposed by analyzing the molecules involved and using intuition gained from the study of physical chemistry and working with a multitude of elementary-reaction mechanisms while also drawing on the organic chemistry expertise of co-author Phillip S. Williams. The experimental spectra often offered clues that could eliminate a proposed product (and by extension the proposed mechanism) without the need for simulation. For example if a product lacked a C=O group, it would almost certainly not reproduce the vibration observed around 1600-1800  $\text{cm}^{-1}$ . In this way, mechanisms were proposed and eliminated until a few promising ones remained. The products of these select reaction schemes were simulated using computational quantum chemistry. The frequency data from these calculations was compared to the experimental spectra to discern which products, if any, would reproduce the experimental spectra. This comparison was done with the help of the other co-authors. If

none of the products was correct, the data were used to inform the proposal of new reaction schemes and new products to be simulated, essentially reiterating the process. More information on the experiments of co-author Erinn C. Dandley (Needham) and the results of the quantum chemical analysis described above can be found in the publication reproduced below.

The following work is reproduced with permission from Erinn C. Dandley, Craig D. Needham, Phillip S. Williams, Alexandra H. Brozena, Cristopher J. Oldham, and Gregory N. Parsons, “Temperature-dependent reaction between trimethylaluminum and poly(methyl methacrylate) during sequential vapor infiltration: experimental and *ab initio* analysis,” *Journal of Materials Chemistry C*, 44 (2014) 9416-9424 [142]. © 2014 Royal Society of Chemistry.

## 6.2 Introduction

Several active research groups currently explore polymer modification by vapor-phase, metal-organic reagents to understand reactions that alter material surface and bulk structure as well as functionality [143–150]. Improved understanding of vapor infusion and reaction mechanisms will help expand the use of current methods, and will lead to the discovery of novel approaches or process schemes to enable new and broader applications. For example, sequential vapor infiltration (SVI) proceeds by repeatedly exposing a polymer, or other material, to a vapor reactant, usually a metal-organic species, in a heated reactor environment. After the reagent vapor flows into the reactor the deposition chamber is closed for a set “hold” time, increasing the net reactant exposure. Sequential exposures are separated

by an inert gas purge to remove vapor byproducts and renew the reactant concentration. Co-reactants, such as water to produce metal oxide products, are also delivered either as an additional step within the reactant/inert gas sequence, or after completing the desired number of reactant infusion/purge cycles. This approach has grown from atomic layer deposition (ALD), which uses sequential, self-limiting reactant exposure steps to deposit conformal and uniform thin films on surfaces with monolayer precision [151–153]. Variations on the process take different names, including multiple pulse infiltration [143,144] and sequential infiltration synthesis [147,148]. Multiple pulse infiltration also uses a hold step after precursor exposure, whereas sequential infiltration synthesis typically uses co-reactant exposures after each precursor step, without hold steps [150].

Infiltration and reaction involving trimethylaluminum (TMA) vapor and the polymer poly(methyl methacrylate) (PMMA), the latter in a thin film [151,154] or block co-polymer (BCPs) such as polystyrene-*block*-poly(methyl methacrylate) (PS-*b*-PMMA) [147,148], is a commonly studied system. PMMA has reactive functional groups and a relatively large free volume. TMA is a common reagent for ALD of Al<sub>2</sub>O<sub>3</sub>; its small size and high reactivity make it a good candidate to study vapor infusion and reaction processes. Several recent studies show that TMA exposure to PS-*b*-PMMA BCPs lead to selective reaction within the PMMA which, upon subsequent plasma oxidation, produces a solid template of the original PMMA that can be used for pattern transfer and lithography [147,148].

Even with this interest in vapor infusion, the detailed chemical mechanisms associated with the reaction remain uncertain. A recent study from our group [154] using *in situ* infrared

transmission (IR) showed TMA infusion and reaction depends strongly on the nature of the starting polymer structure. Moreover, based on changes in IR, we hypothesized mechanisms for TMA/polymer reactions that included covalent bond formation between TMA and PMMA at moderate process temperature (80°C).

In this article we present more detailed results including temperature dependent IR, quartz crystal microbalance (QCM) mass uptake, and quantum chemical modeling analysis. We also show that at moderate temperatures TMA forms a non-covalent, metastable adduct coordinating to the PMMA carbonyl unit. TMA either desorbs from this coordinated complex under purge conditions or subsequently reacts, more readily at higher temperatures, to form a covalent Al-O bonding structure that remains present after water exposure. New insight from this analysis will be helpful to understand reaction products and mechanisms for this and other vapor-phase metal-organic interactions with polymers.

### *6.3 Experimental procedures*

#### *6.3.1 Chemicals and materials*

Poly(methyl methacrylate) (Fluka Analytical, MW 97,000) and trimethylaluminum (Strem Chemicals, min 98% pure) were used as received. TMA was co-reacted with deionized water after a specified number of TMA doses. The reactor was purged with high purity nitrogen gas (Machine & Welding Supply Co) that was further purified with an Entegris GateKeeper located directly upstream from the reactor input. PMMA was spun-cast onto silicon substrates (University Wafers, P-type, <100>) by first dissolving PMMA into toluene

(Fischer Scientific) from one to eight weight percent PMMA. Silicon wafers were cleaned with acetone (Fischer Scientific) and dried by spinning at 2000 rpm for one minute. The surface of the silicon was flooded with PMMA solution and then spun at 2000 rpm for one minute. The sample was then heated on a hot plate at 200°C for two minutes to remove toluene.

### 6.3.2 *Sequential vapor infiltration (SVI)*

SVI was used to infiltrate the PMMA thin film. Briefly, the sample was placed into a custom made, viscous-flow, hot-walled, vacuum reactor described previously [145,146,155]. The reactor was kept at roughly 800 mTorr, and operated at temperatures between 45 and 150 °C. TMA was introduced into the reactor and held by closing all ports into and out of the reactor for a set time period. The reactor was then purged with N<sub>2</sub> gas. This was repeated  $n$  times followed by a dose of water and a final purge. We anticipated that the final water step would help form a protective barrier on the outside of the polymer-TMA composite to block the rapid reaction of trapped TMA with atmospheric water. The typical dosing scheme for these experiments was a 1 second TMA dose, 60 second hold, and 30 second purge, all repeated as many times as desired. This is followed by a 1 second dose of water and a 45 second final purge. This scheme is denoted as  $[(1/60/30) \times n + (1/45)]$ . For the duration of this article a “TMA dose” will refer to one TMA dose, hold and purge step and will be reported as a number of repeats of the TMA dose ( $n$ ).

### 6.3.3 Characterization

PMMA layer thickness was determined by spectroscopic ellipsometry (J.A. Woollam Co., Inc) and by profilometry (Veeco Dektak 150). Mass gain was quantified using an *in situ* quartz crystal microbalance. For QCM analysis, 50 nm PMMA films were cast onto quartz crystals (gold plated, 6 MHz resonant frequency, Inficon). They were then affixed to a crystal drawer (Inficon) with conductive silver epoxy (MG Chemicals). The crystal drawer was then inserted into the sensor head and placed into the reactor. The set up was allowed to equilibrate at process temperature overnight. The oscillating frequency of the crystal was recorded every 150 milliseconds and converted into a mass gain using the Sauerbrey equation.

Changes in chemical bonding were measured using an *in situ* Fourier transform infrared spectrophotometer (Nicolet 6700 FTIR) incorporated into a custom built viscous flow vacuum reactor [145,146,154,156]. Samples were cast onto IR transparent silicon wafers. The sample was prebaked in the reactor to a temperature of 140°C for 30 minutes under vacuum and flowing N<sub>2</sub> gas to remove any volatile species from the PMMA. The system was then cooled to the infiltration temperature and allowed to equilibrate for 30 minutes. Spectra were taken after 10, 50, 100, and 150 TMA doses as well as after water dosing. After the prescribed number of TMA doses the chamber was purged for two minutes and then closed off. Gates to the IR windows were then opened and 200 spectra were obtained at a resolution of 4 cm<sup>-1</sup> in the frequency range of 4000 to 400 cm<sup>-1</sup>. An MCT-A detector was used through CsI IR windows.

#### 6.3.4 Quantum chemistry analysis

Optimized geometries and frequencies of PMMA, TMA, and the PMMA–TMA coordination complex were calculated using Gaussian09 [15]. The B3LYP Density Functional Theory method was implemented because of its ability to accurately predict frequency data through the use of a scaling factor. All calculations were performed using a 6-31G++(d,p) basis set. This basis set provides suitable accuracy and rapid system output. As is commonly done with the B3LYP functional [157,158] we used a multiplication factor of 0.961 to adjust the calculated frequencies to better replicate the experimental values. The as-calculated and adjusted values are reported. We also employed Gaussview [31] to construct the model structures and view the calculated vibrations to identify modes in the experimental spectra. All simulations used methyl trimethylacetate as a model molecule for PMMA due to its structural similarity to one PMMA repeat unit. It has been shown that methyl trimethylacetate has a similar carbonyl stretching frequency to PMMA [159].

### 6.4 Results

#### 6.4.1 *In situ* FTIR and QCM

Figure 6.1 shows *in situ* FTIR results following 150 TMA doses on PMMA films between 45 and 150°C. Each spectrum was collected from a separate experiment, starting each time with a fresh, spun-cast PMMA film. Spectra are shown in differential mode relative to the starting PMMA substrate. The starting PMMA spectrum shows peaks at 1732, 1260 and 1143  $\text{cm}^{-1}$  (noted with dashed lines in Figure 6.1). The spectra show notable changes upon TMA

exposure, especially in the region between 1100 and 1800  $\text{cm}^{-1}$ . The magnitude of mode intensity change upon TMA exposure could depend on temperature, TMA partial pressure, exposure time, purge time, and starting layer thickness. Therefore, to address the effect of temperature, we fixed the pressure, exposure, purge time and substrate thickness ( $< \pm 1\%$ ) for all spectra collected. With these considerations, the distinct mode changes in Figure 6.1 reasonably relate to different extents of reaction, or different reaction products produced at the temperatures studied.

Previously, we reported *in situ* IR analysis of reactions between TMA and various polymer thin films, including PMMA, at a fixed temperature (80°C) [154]; spectra were similar to those at 70 and 90°C shown here in Figure 6.1. We note here that PMMA modes can be seen for C=O stretching at 1732  $\text{cm}^{-1}$ , and for C-O stretching in the =C-O- and -O-CH<sub>3</sub> units near 1260 and 1143  $\text{cm}^{-1}$  (*vide infra*). Consider first the effect of TMA exposure at 70°C on the IR results in Figure 1. After 150 TMA exposure steps, the differential spectrum shows negative going modes at 1732, 1260 and 1143  $\text{cm}^{-1}$ , and positive going modes at 1670, 1305, and 1200  $\text{cm}^{-1}$ , indicating significant modification of the C=O and C-O bonds. We previously observed and quantified changes in IR signature upon TMA exposure, concluding that TMA readily diffuses and reacts in the polymer bulk. That work also reported changes in the C=O and C-O modes [154], where we assigned the mode near 1600  $\text{cm}^{-1}$  (at 1670  $\text{cm}^{-1}$  in Figure 6.1) to the reaction between TMA and the C=O forming O-C-O-Al units. Based on experimental and modeling results discussed in detail below, we revise this interpretation and assign the mode at 1670  $\text{cm}^{-1}$  to TMA complexed to the ester C=O in a Lewis acid-base



adduct [160]. Physisorbed TMA will also indirectly affect the non-carbonyl oxygen of the ester moiety *via* resonance, resulting in shifts in the C-O modes.

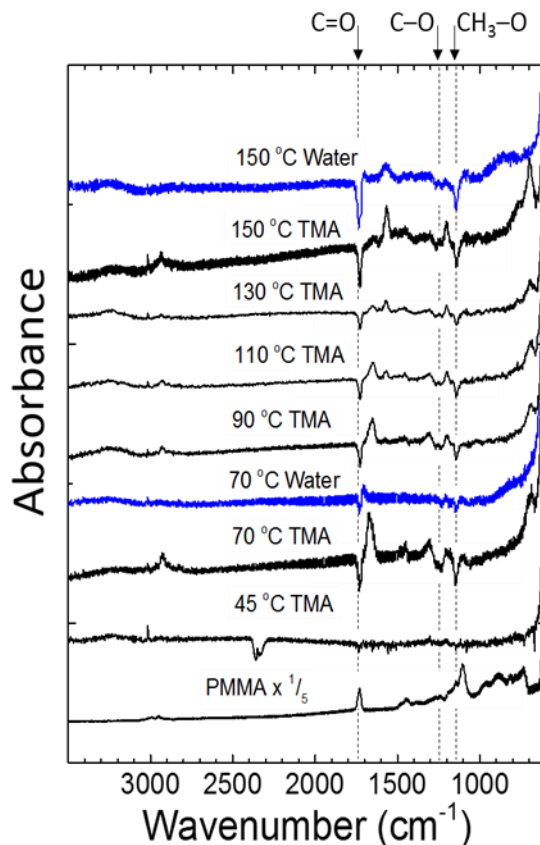


Figure 6.1: *In situ* FTIR spectra collected after 150 TMA doses on 170 nm thick PMMA films on silicon. The spectra are shown in differential mode, relative to the starting PMMA. Two spectra collected after TMA + water at 70 and 150 °C are also included, and similarly referenced to the starting PMMA.

Considering the data in Figure 6.1 collected at  $T = 45^\circ\text{C}$ , there is much less change in the IR modes than at  $70^\circ\text{C}$ . For  $T > 70^\circ\text{C}$  the  $1670\text{ cm}^{-1}$  mode also appears but it is less intense at increased temperature. Moreover, at  $T = 110^\circ\text{C}$  a small mode becomes visible at  $1568\text{ cm}^{-1}$

and it intensifies as the reaction temperature increases to 150°C. The identity of the 1568  $\text{cm}^{-1}$  mode is discussed in detail below.

In addition to spectra collected after TMA exposure, Figure 6.1 shows IR traces collected after water exposure (referenced to the starting PMMA) following TMA at 70 and 150°C. At 70°C, the TMA/water exposure sequence produced only small net changes in the PMMA features, indicating that the water step reverses or removes much of the change that occurred during the TMA step. TMA in the film will react with water to create Al-O clusters, consistent with the small broad feature near 820  $\text{cm}^{-1}$  due to Al-O stretching. The TMA/water sequence at 150 °C produces a very different outcome. The TMA step produces a negative-going peak at 1732  $\text{cm}^{-1}$  and a positive-going mode at 1568  $\text{cm}^{-1}$ , and it remains present after the water step (i.e. the spectra labeled “TMA” and “Water” at 150 °C look relatively similar). These results suggest the TMA forms a reversible product with the PMMA at low temperature (removed by water exposure), but at high temperature TMA reacts with the polymer to form a stable covalent product (not strongly modified by water). The =C-O- and -O-CH<sub>3</sub> modes at 1260 and 1143  $\text{cm}^{-1}$  in the starting PMMA show similar trends. At 70°C, the TMA exposure leads to changes that are largely reversed by the water dose, whereas at high temperature, the TMA leads to changes that are relatively stable upon water exposure (i.e. the spectra labeled “TMA” and “Water” are very different at low temperature, but are more similar at 150°C). In the Discussion section below, we consider possible PMMA–TMA reaction mechanisms and covalent bond products that can account for these IR results.

To further explore the reaction between TMA and PMMA, we performed quartz crystal microbalance (QCM) measurements during repeated TMA exposures to 50 nm spun-cast PMMA films at various reaction temperatures; results are shown in Figure 6.2. The QCM response over 60 TMA doses (Fig. 6.2a) show rapid net mass uptake during the first ~10 doses followed by slower uptake. For the three temperatures shown the net mass uptake is largest at 100 °C. Each TMA dose produced mass uptake followed by mass loss. The traces collected during TMA doses 41-43 (Fig. 6.2b) show that after the initial mass uptake the mass loss is nearly equal to the mass gain, with the largest gain and loss at 100 °C. The trace shape also varies with temperature. At 140 °C the mass gain jumps rapidly then continues more slowly. At 100 °C the mass increases continuously, whereas at 70 °C the mass uptake shows a peak followed by a small loss before continuing to grow. The QCM traces show TMA uptake and loss from the PMMA bulk during each hold/purge step. The trace shape at 70 °C is ascribed to relatively small amounts of TMA rapidly adsorbing and desorbing on the film surface, combined with slower TMA diffusion in and out of the PMMA bulk. Also, using QCM we find that after 50 dose steps at 70 °C a long (85 min) purge led to a loss of 60% of the mass gained, whereas the same experiment at 150 °C led to a mass loss of around 30 %. At 150 °C the mass loss plateaued after purging for approximately 15 minutes; at 70 °C the mass loss did not plateau during the extended purge. This mass uptake/loss during TMA exposure on polymers, including PMMA, has been observed [151] but has not previously been analyzed as a function of process temperature.

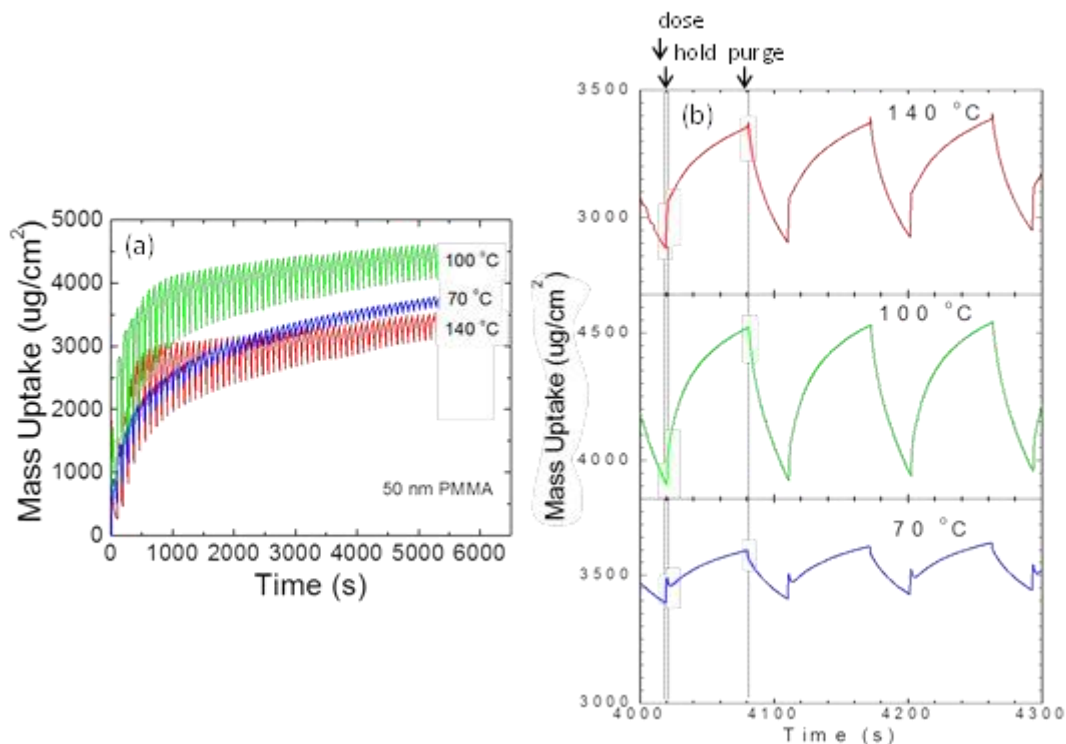


Figure 6.2: (a) Overall QCM mass response for 50 nm PMMA films exposed to 100 TMA doses at 70, 100 and 140 °C. (b) Magnified view of the mass response after 41-43 TMA doses.

To further understand the trend in mass uptake *versus* exposure and temperature, we measured *in situ* IR absorbance *versus* TMA exposure at 70 and 150 °C, as shown in Figure 6.3. The figure shows differential spectra relative to the previously plotted spectrum, where negative-going features correspond to modes removed and positive-going features to modes added. The spectrum labeled “10 doses TMA” corresponds to changes that occur between 0 and 10 doses, whereas “50 doses TMA” shows changes between 10 and 50 doses. Considering the data collected at 70 °C we see large changes during the first 10 doses including: loss of C=O stretching at 1732 cm<sup>-1</sup>; loss of C-O at 1260 and 1143 cm<sup>-1</sup>; and gains

at 1670, 1305, and 1200  $\text{cm}^{-1}$ . This change continues, but is less pronounced for the next 40 doses with only small changes appearing after 100 and 150 TMA doses. At 150 °C, these same changes are observed with the addition of a new mode appearing at 1568  $\text{cm}^{-1}$  after 10 doses (also seen in Figure 6.1) which was not observed at 70 °C. After 40 more TMA doses at 150 °C the spectrum shows a further decrease at 1732  $\text{cm}^{-1}$ . The mode at 1670  $\text{cm}^{-1}$  is now negative-going with an increase at 1568  $\text{cm}^{-1}$ . Note that the feature at 1670  $\text{cm}^{-1}$  that disappeared after 50 TMA doses at 150 °C is the same mode that appeared during the first 10 doses at both 150 and 70 °C. The degradation of the 1670  $\text{cm}^{-1}$  mode during TMA exposure was only observed at elevated temperature in our experiments. This trend—peak appearance followed by its disappearance—indicates the formation of a metastable intermediate (mode at 1670  $\text{cm}^{-1}$ ) that reacts at elevated temperature to create a more stable product state with a C=O mode at 1568  $\text{cm}^{-1}$ . Between 50 and 150 TMA doses we continue to observe the loss of the PMMA C=O mode at 1732  $\text{cm}^{-1}$  and corresponding gain in the 1568  $\text{cm}^{-1}$  feature consistent with stable product formation at the higher temperature.

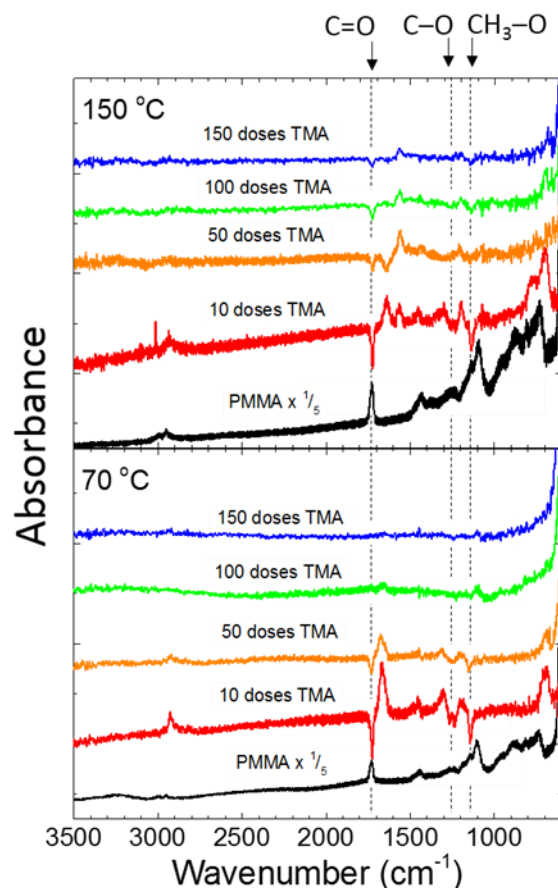


Figure 6.3: *In situ* FTIR data collected at 70 and 150 °C at several times during 150 TMA dose steps. Each differential spectrum is referenced to the preceding spectrum shown. The data shows different reaction trends at different temperatures, most noticeably in the region between 1500 and 1700  $\text{cm}^{-1}$ .

#### 6.4.2 Quantum chemical analysis

We performed quantum chemistry calculations as described above to minimize the potential energy for a PMMA analog, TMA and various possible reaction-product states. Figure 6.4 shows chemical structures for the species modeled, and the corresponding vibrational spectra. The calculated spectrum for the PMMA model (Fig. 6.4a) shows peaks at 1790, 1307, 1212 and 1182  $\text{cm}^{-1}$ . The peak at 1790  $\text{cm}^{-1}$  results from the C=O stretch, and the other

three peaks correspond to coupled =C-O- and -O-CH<sub>3</sub> stretching modes. Carbon-hydrogen stretching and deformation modes are also present at 3000-3200 and 1400-1550 cm<sup>-1</sup>, respectively. The starting PMMA spectrum in Figure 6.1 shows peaks at 1732 cm<sup>-1</sup> (C=O stretch), and at 1260 and 1143 cm<sup>-1</sup> (=C-O- and -O-CH<sub>3</sub> stretch) [161]. Table 6.1 lists the experimentally observed and calculated peak positions (as output and after frequency adjustment) for PMMA before and after TMA exposure. For the starting PMMA, the calculated peaks match well with the experimental values. An additional peak predicted near 1165 cm<sup>-1</sup> is not distinctly observed, but it could correspond to a shoulder that appears near 1189 cm<sup>-1</sup> on the 1143 cm<sup>-1</sup> peak.

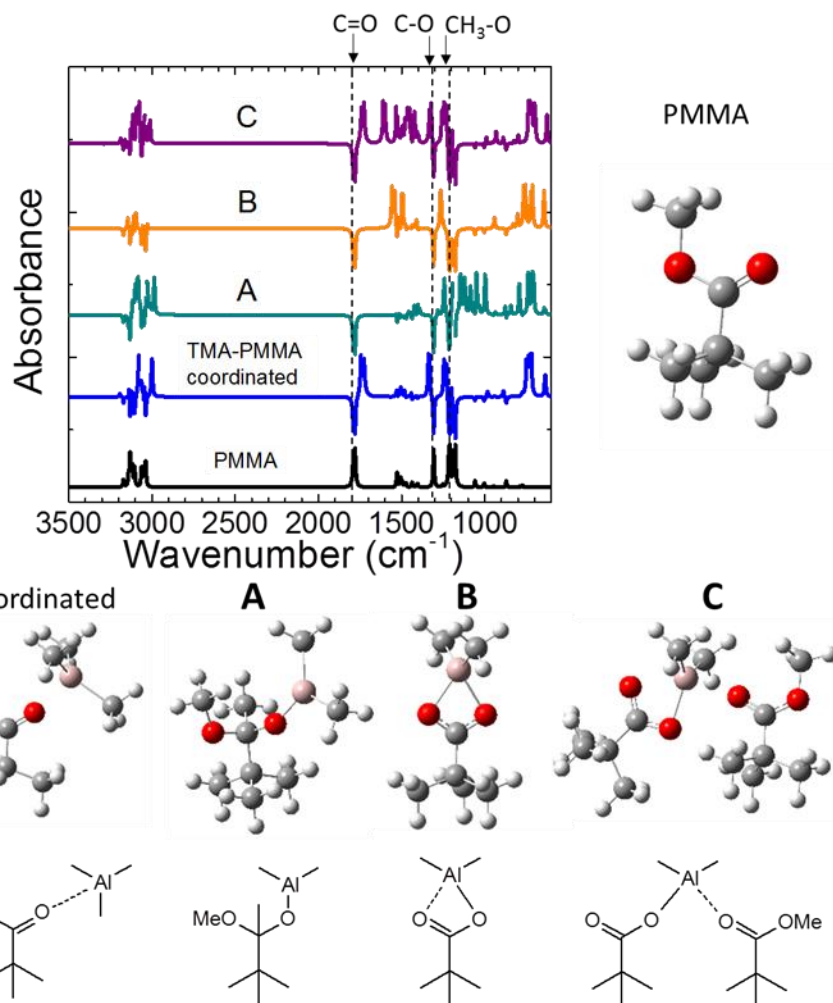


Figure 6.4: Relaxed chemical structures calculated using *ab initio* modeling, and their corresponding vibrational spectra referenced to spectra from structures calculated without TMA interaction. The bond models used for the calculations are also shown. The calculated spectrum for the PMMA model shows peaks at  $1790\text{ cm}^{-1}$  corresponding to C=O stretch, and features at  $1307$ ,  $1212$  and  $1182\text{ cm}^{-1}$  associated with =C-O- and -O-CH<sub>3</sub> coupled modes. For each structure, interaction with TMA leads to loss of the  $1790\text{ cm}^{-1}$  C=O mode and changes in the C-O vibrations. The peak at  $1725\text{ cm}^{-1}$  is TMA coordinated to the C=O in a physisorbed state, and is consistent with the IR and QCM results at lower temperature. Peaks between  $1750$  and  $1500\text{ cm}^{-1}$  in products **B** and **C** correspond to C=O coordinated with a neighboring covalently-bound Al-O, forming a resonant C=O $\cdots$ Al-O-C unit, consistent with the higher temperature product mode observed at  $1568\text{ cm}^{-1}$ .



Table 6.1: Experimental, calculated and adjusted IR peak positions for methyl trimethylacetate as a model for PMMA. Experimental and calculated peak positions are also shown for the starting material after exposure to trimethylaluminum.

Material	Experiment	Calculated	Adjusted <sup>a</sup>	Vibration
PMMA	1732 cm <sup>-1</sup>	1790 cm <sup>-1</sup>	1720 cm <sup>-1</sup>	C=O
	1260	1307	1256	=C-O- and -O-CH <sub>3</sub>
	--	1212	1165	
	1143	1182	1136	
PMMA + TMA	1670	1725	1658	C=O···Al-(CH <sub>3</sub> ) <sub>3</sub>
	1305	1323	1271	=C-O- and O-CH <sub>3</sub> with C=O···Al(CH <sub>3</sub> ) <sub>3</sub>
	1200	1237	1189	
	--	1197	1150	
	1568	1605 <sup>b</sup>	1542 <sup>b</sup>	C=O with =C-O-Al(CH <sub>3</sub> ) <sub>2</sub>

<sup>a</sup>The scaling factor used was 0.961. <sup>b</sup>Calculated and adjusted values are from structure **C** in Figure 6.4.

Previous quantum chemistry analysis of TMA interacting with surface hydroxyls during TMA/water ALD shows that TMA forms a short-lived metastable -O···Al(CH<sub>3</sub>)<sub>3</sub> adduct that subsequently reacts exothermically to yield stable -O-Al(CH<sub>3</sub>)<sub>2</sub> and methane [162]. Also, since TMA is a strong Lewis acid [163], we minimized the energy for TMA physisorbed to the C=O through a Lewis acid-base adduct state, producing the structure and corresponding vibrational spectrum shown in Figure 6.4. Like the experimental results, the calculated spectrum was plotted relative to the starting PMMA. The calculated spectrum for PMMA+TMA shows negative-going modes at 1790, 1307, 1212 and 1182 cm<sup>-1</sup> and new positive-going features at 1725, 1323, 1237 and 1197 cm<sup>-1</sup>. A peak near 730 cm<sup>-1</sup> corresponds to Al-methyl rocking modes in the Al-CH<sub>3</sub> groups. The Gaussview model confirms that the 1725 cm<sup>-1</sup> peak corresponds to stretching of the C=O unit coordinated with Al(CH<sub>3</sub>)<sub>3</sub>. Likewise the 1323, 1237 and 1197 cm<sup>-1</sup> peaks correspond to =C-O- and -O-CH<sub>3</sub> coupled vibrations neighboring the -C=O···Al(CH<sub>3</sub>)<sub>3</sub> coordinated structure. A shift in the

C=O frequency to smaller wavenumber is expected with an increase in the C=O bond length, which is consistent with TMA coordination. The coordination will also change the =C-O- and -O-CH<sub>3</sub> bond lengths, shifting the mode frequencies. These modes are expected to appear in the experimental spectra near 1658, 1271, 1189, and 1150 cm<sup>-1</sup>, respectively, as indicated in Table 6.1.

The experimental data collected at 70 °C shows three clear positive-going modes at 1670, 1305, and 1200 cm<sup>-1</sup> after TMA exposure. As in the PMMA spectrum before TMA exposure, the calculated peak near 1150 cm<sup>-1</sup> is not readily observed. The predicted peaks after TMA exposure are at generally smaller wavenumber than experimentally observed, *i.e.* the errors between the adjusted and measured peak positions are somewhat larger after TMA exposure than for neat PMMA. Since the calculations do not include thermal or matrix effects, and the base cluster size utilized was relatively small, we expect the calculation to exaggerate the interaction, shifting the peaks more than experimentally measured. With this consideration, the adjusted peaks agree well with the experimental values. The other frequencies included in Table 6.1 are discussed below.

#### 6.4.3 *Observed chromatic shift*

Bulk PMMA powder was exposed to TMA vapor at 90 and 150 °C in a fiber-encapsulated basket placed inside our reaction chamber, as previously described [164]. PMMA powder as received is white, as shown in Figure 6.5a. Upon 600 TMA doses at 90 °C, no color change was observed. When the reactor temperature was increased to 150 °C, the powder appeared black upon removal from the reactor. Faint popping sounds could be heard as the black

powder converted to orange, consistent with a rapid reaction between the TMA–PMMA composite and water in the air. After 24 hours the powder was reddish brown. The sample maintained a stable orange color for more than 9 months following exposure, as shown in Figure 6.5f. Color changes due to metal atoms bonded and coordinated to organic groups are often used as metal-complex dyes [165]. Complex-dyes have structures similar to that of alumina bound to multiple PMMA pendent groups as depicted in Figure 6.4c.

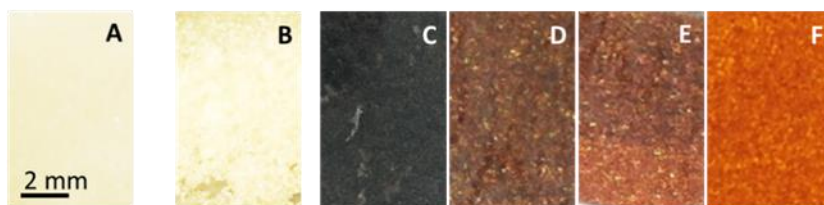


Figure 6.5: Bulk PMMA powder, as received, was treated with 600 TMA doses at varying temperatures. At increased temperatures a color change was observed that was not seen at lower temperatures. A) PMMA powder as received. B) PMMA powder with 600 SVI TMA doses at 90 °C. C) PMMA powder with 600 SVI TMA doses at 150 °C immediately after removal from the reactor, after D) 1.5 hrs E) 24 hrs and F) 9 months.

## 6.5 Discussion

Based on the IR and QCM data combined with the *ab initio* analysis results, we conclude that over a wide temperature range TMA diffuses into the polymer bulk and forms a metastable adduct, coordinating to the PMMA ester carbonyl. The physisorbed TMA shifts the C=O stretching frequency from 1732 to 1670  $\text{cm}^{-1}$ , which appears in the difference spectra in Figure 6.1 as a mode loss adjacent to a mode gain. By interaction with the carbonyl oxygen, the TMA Lewis acid increases the C=O bond length and decreases the stretching frequency.

The change in the C=O unit also draws some charge from the =C-O- and -O-CH<sub>3</sub> bonds, shifting the modes at 1260 and 1143 cm<sup>-1</sup>.

At low temperature, TMA can desorb from the C=O···Al(CH<sub>3</sub>)<sub>3</sub> complex, as shown in the QCM results, and subsequent water exposure leads to relatively small changes in the starting PMMA. At high temperature, the physisorbed structure converts to form a PMMA–TMA reaction product with a characteristic vibration at 1568 cm<sup>-1</sup>. This reaction proceeds relatively rapidly at higher temperature (within the first 10 TMA doses at 150 °C, Figure 6.3). Moreover, the PMMA–TMA reaction product is stable; the IR data in Figure 6.1 shows that it remains present after water exposure.

The QCM results (Fig. 6.2) also show TMA uptake in the PMMA bulk, followed by desorption. QCM analysis on a planar quartz crystal substrate typically shows a mass uptake of ~40 ng cm<sup>-2</sup> per cycle during steady-state TMA–water ALD [166,167]. We find that at 100 °C, one TMA dose onto PMMA produces a mass change > 500 ng cm<sup>-2</sup>. This large mass change is ascribed to TMA diffusing into the polymer bulk. This sub-surface diffusion of ALD precursors into several different polymers has been previously observed by IR, QCM, TEM and other methods [145–152]. We also note that the magnitude of overall mass uptake after 150 TMA doses (Fig 6.2a) increases with temperature between 70 and 100 °C, but it is not as large at 140 °C. At low temperature, where IR indicates that TMA does not react with PMMA, increasing the temperature will promote TMA diffusion. At high-temperature, the covalent reaction between TMA and PMMA will fix TMA and could slow sub-surface

diffusion. Therefore, the temperature-dependent QCM results further support the TMA adsorption–desorption and reaction mechanism described above.

We now consider possible PMMA–TMA reaction products that could account for the observed data, including the characteristic IR vibration at  $1568\text{ cm}^{-1}$ . One product we considered is structure **A** in Figure 6.4. This could be produced by breaking the carbonyl to form Al-O, transferring a methyl to the carbon. Even though this product was previously considered [154], this reaction scheme is not likely because methyl migration products from TMA adducts typically require stronger electron donating functional groups than ester carbonyls to adequately destabilize the aluminum complex [168]. Even so, we performed a geometry optimization for this structure and examined its vibrational modes using Gaussian, the resulting spectrum is plotted in Figure 6.4. The carbonyl stretch is lost and new C-O coupled modes appear between  $1000$  and  $1300\text{ cm}^{-1}$ . No new modes appear in the  $1500$ - $1700\text{ cm}^{-1}$  region where the stable product is experimentally observed. Since this product lacks the vibrational signature of the resulting product, and because the reaction scheme is not favorable, we looked for other possible stable products.

Another possibility is that the TMA in the coordination complex interacts with the neighboring methoxy group in a pericyclic reaction to yield a covalent bond between  $\text{Al}(\text{CH}_3)_2$  and the oxygen originally in the carbonyl. The methyl lost from the TMA reacts with the methoxy moiety forming ethane vapor and an ester carbonyl. The proximal Al center would then coordinate to the carbonyl oxygen in the same ester, as shown in product **B**, or in a neighboring ester as shown in product **C** and in Figure 6.6. The reaction scheme in

Figure 6.6 is energetically driven by formation of the strong Al-O and ethane bonds. The scheme is consistent with the relative stability of TMA reacting with esters, where TMA/ester complexes are known to catalyze Tischenko-like reduction of *beta*-ketoesters without degradation of the ester moiety [168,169]. These pericyclic reactions are common in organic/inorganic complex formation and in other synthetic routes where TMA is able to promote methyl translation to form C-C bonds [170]. Since products **B** and **C** are synthetically feasible, we considered them further for *ab initio* modeling. Figure 6.4 shows the minimized structures and characteristic vibrational spectra. Both products B and C show loss of the C=O and coupled C-O stretching in the starting PMMA. Most notably, new modes appear in the 1500 -1700  $\text{cm}^{-1}$  region that correspond to C=O stretching modes shifted to lower frequency due to Al coordination and near-neighbor bonding. In product **B**, the model constrains the Al coordination and bonding on the same ester unit and modes appear at 1520 and 1480  $\text{cm}^{-1}$ . For product **C**, Al binds to adjacent esters, producing a C=O stretch at 1605  $\text{cm}^{-1}$ . In highly TMA-saturated PMMA, further reactions between  $-\text{O}-\text{Al}(\text{CH}_3)_2$  and other esters would form additional bond/coordination pairs, leading to further mode shifting. Based on this result, we believe that the mode at 1568  $\text{cm}^{-1}$  arises from C=O stretching vibrations where the carbonyl carbon is also linked to  $-\text{O}-\text{Al}(\text{CH}_3)_2$  (or possibly  $-\text{O}-\text{Al}(\text{CH}_3)-\text{O}-$ ) with the Al further coordinated with oxygen on other chains, as depicted in Figure 6.6. To further support this scheme, we note that PMMA powder, which appears white as received, remains visibly unchanged after TMA exposure at low temperature, whereas TMA exposure at high temperature leads to a dramatic, visible color change to black that transitions to orange upon exposure to air. This coloration may therefore be due to products where the metal atom

bridges multiple organic groups, as commonly found in metal-complexed dyes [165]. The color shift could be attributed to atmospheric water slightly altering the metal-organic structure; the permanence of this color change attests to the stability of this final product.

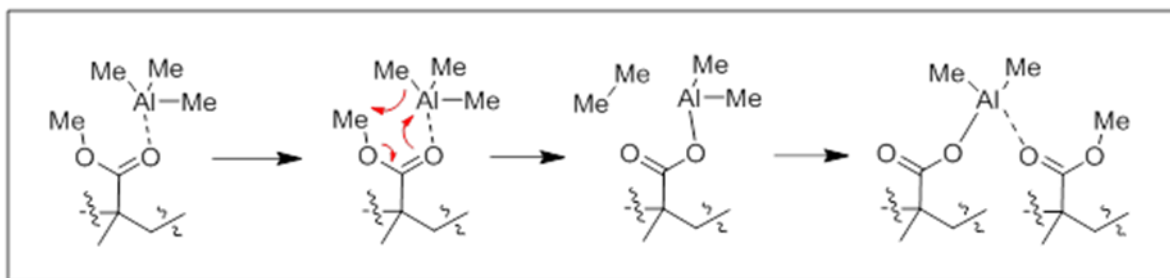


Figure 6.6: Proposed pericyclic activation of ester to form metal acetate.

## 6.6 Summary

Combining evidence from in situ infrared transmission and quartz crystal microbalance experiments with ab initio modeling analysis, we conclude that exposing TMA vapor to PMMA thin films leads to significant subsurface TMA infiltration where the TMA physisorbs onto C=O forming a metastable  $C=O \cdots Al(CH_3)_3$  structure. Upon TMA physisorption, the PMMA C=O stretching frequency at  $1732\text{ cm}^{-1}$  shifts to  $1670\text{ cm}^{-1}$  when the TMA Lewis base withdraws electrons from the C=O bond. At low temperatures (up to  $\sim 100\text{ }^\circ\text{C}$ ), the interaction does not produce C-O-Al covalent bonds [154] and the TMA readily desorbs. At higher temperatures an IR feature near  $1568\text{ cm}^{-1}$  arises, likely due to C=O stretching in resonant  $C=O \cdots Al-O-C$  units. These bonds could possibly form through a pericyclic reaction involving a PMMA methoxy group interacting with a neighboring TMA stabilized through coordination with the C=O ester. This improved understanding of the

mechanisms for TMA interaction with PMMA will also extend to other polymers and other Lewis-acidic metal-vapor reactants, helping to create knowledge and advance applications for sequential vapor infiltration processes.

### *6.7 Acknowledgements*

The authors acknowledge support from NSF project # 1344618. One co-author (C.D.N.) acknowledges support from the US Dept. of Education under the GAANN Fellowship program, project P200A09008.



## CHAPTER 7. CONCLUSIONS AND RECOMMENDATIONS

### 7.1 *Conclusions*

#### 7.1.1 *Hypergolic Bipropellants*

A mechanism for the simulation of MMH/RFNA hypergolic combustion was created by Dr. Nicole Labbe through literature analysis. During the construction of the mechanism it was tested against experimental data to ensure it was behaving realistically, This mechanism, along with one created by the Army Research Laboratory, was reduced by Dr. Labbe to the point where it could be used in reactive CFD codes, the computational costs of which prevent the use of reaction mechanisms with too many species. The two reduced mechanisms were tested with reactor modeling to ensure they produced results that were close to the original full mechanisms, although unpreventable loss in performance was both expected and observed.

Reactive CFD simulations using the reduced mechanisms, performed by collaborators, were unable to reach the ignition temperature, although some realistic behavior was observed. A survey of the literature revealed a hypothesis that energy from solvation of the fuel and oxidizer into aerosol droplets was responsible for raising the temperature from the boiling point of the liquids to the ignition temperature [83]. CQC was used to investigate the energy of solvation of the fuel in excess oxidizer and vice versa. The reaction was assumed to be mass-transfer limited, so a mass-transfer rate-coefficient was calculated and fitted to an Arrhenius form with the activation energy calculated from the CQC results. These new

reactions were added to the reactive CFD simulations and were able to push the simulation temperature above the ignition point.

Another bipropellant pair, TMEDA/RFNA, was of interest due to the relative safety of TMEDA as a chemical when compared to MMH. RMD in LAMMPS was employed to investigate the high temperature behavior of this system, though even at high temperatures only a few hundred picoseconds could be simulated. The simulations were able to reveal the major initiation pathway from TMEDA decomposition at high temperature. Specifically, the abstraction of terminal hydrogens from the four CH<sub>3</sub> groups dominates, and the dominant abstractor is OH produced by scission of HNO<sub>3</sub> into NO<sub>2</sub> and OH. NO<sub>2</sub> participates as an abstractor as well but in a much slower fashion.

### 7.1.2 *HFO-1234yf refrigerant combustion*

A sub-mechanism for the combustion of HFO-1234yf was created mainly using CQC methods. First, the possible decomposition routes were proposed based on physical/organic chemistry principles and based on previous experience with combustion mechanisms. For each proposed route, CQC was used to calculate the geometry and standard enthalpy of formation at 298K of the reactants, the products, and the transition state. The results of these calculations were then used to derive parameters for the rate coefficient of each reaction. For radical combination reactions (or their reverse: homolytic bond scission reactions), no maximum in the electronic energy was found along the reaction coordinate, meaning that transition-state calculations were unable to converge. Rate-coefficient parameters were derived mathematically for these reactions. Radical-combination/homolytic-bond-scission

reactions are known to be significantly pressure dependent, so low-pressure rate-coefficient parameters were also calculated for these reactions.

After rate-coefficient parameters were obtained for each proposed reaction, the sub-mechanism was added to a previously published mechanism for small fluorocarbon combustion [12,99]. The combined mechanism was used to simulate adiabatic flames speeds that were measured in experiments by Takizawa et al. [95]. Though the simulations under-predicted the experiments, the uncertainty in the data was rather large. The flame speed calculation results were also inspected to determine the major decomposition routes of HFO-1234yf. The analysis revealed that pericyclic, unimolecular decomposition routes dominated the reaction network, with abstraction and H-addition pathways also playing a large role.

### 7.1.3 *PrIMe investigation of H<sub>2</sub>/O<sub>2</sub> combustion*

The PrIMe data cyberinfrastructure was used to explore questions about the role of excited species and to create a new optimized mechanism from an amalgam of previously published mechanisms. First, selected mechanisms from the literature were entered into the PrIMe warehouse and combined to create a model which included reaction rates for O<sub>3</sub> and the excited species O(<sup>1</sup>D), O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>), and OH\*. In parallel, a large set of experimental datasets from many publications was entered into the database and QoIs were identified for each dataset. Reactor modeling tools from PrIMe were used to simulate each experimental dataset. The modeling results allowed use of the UQ tools in PrIMe to determine how accurately the model predicted each QoI and then to adjust the pre-exponential factors for each reaction to produce a new, optimized model. During the UQ analysis, it was revealed

that the reaction set was unable to predict certain QoIs within their uncertainty range. After discarding some QoIs and adjusting the uncertainties of others, the data inconsistency was reduced to the point where the reaction set could simulate each QoI individually, but the set of all QoIs were unable to be simulated simultaneously. Again, some QoIs were discarded and others had their uncertainties adjusted until the data inconsistency was resolved. The consistent dataset allowed the UQ tools to create the desired optimized model.

Analysis of the optimization results revealed that a reaction involving  $O_2(^1\Delta_g)$  was among the reactions to which the mechanism was highly sensitive. This reaction is known to inhibit high-pressure flames [139], which lowers the flame speed. The high sensitivity suggests that it is important to include this reaction in future  $H_2/O_2$  mechanisms. The data inconsistency that was encountered during the UQ process also suggests that PrIme's UQ tools may be useful in gauging whether a certain experimental result fits within the larger body of experiments and simulations in the literature. A self-inconsistent QoI may suggest some problems with that particular experiment, or it may point to some inadequacy of the model used for simulation, whether it be the reactor model or the reaction mechanism.

The optimization analysis performed on the  $H_2/O_2$  system shows that PrIme is a powerful tool for producing new mechanisms that are optimized for a specific application, for investigating the role of different chemistry, and for using experimental data to inform more intelligent simulations.

#### 7.1.4 *Interaction between TMA and PMMA*

A series of experiments was performed that yielded FTIR spectra of a PMMA substrate at different stages of TMA infiltration. The FTIR spectra showed peaks of unknown origin, hypothesized to be from the product of a reaction between TMA and PMMA that chemically binds the TMA to the PMMA molecules. Potential product molecules were proposed and simulated using CQC. The resulting calculated spectra were compared to the experimental spectra to identify if the proposed product was the species being formed in the experiments. The analysis determined that TMA first coordinates with the C=O in a PMMA side group. The coordination allows the TMA and PMMA to be in proximity for long enough that the TMA can bind to the PMMA through a six-centered pericyclic transition state that produces ethane as a side product. It is likely that the now-bound dimethylaluminum group will coordinate with another C=O group in the PMMA matrix and continue to react with the polymer substrate. The reaction mechanism discovered by this hybrid CQC/experimental analysis was previously unknown and will help to guide future study of TMA infiltration into PMMA.

#### 7.2 *Recommendations for future work*

As is the nature of research, there is always room for expansion and extension at the conclusion of a project. Each of the four studies described above has avenues which can still be pursued either simply to put the mechanisms that were developed to use, or to use the techniques involved to expand scientific knowledge.

Though the aerosol portion of the hypergols work was able to produce the desired results, it is based on many assumptions. The current model simulates the aerosol droplets as dummy species (e.g.,  $(\text{MMH}\cdot\text{H}^+)(\text{NO}_3^-)\cdot 2\text{MMH}$ ) rather than full, physical aerosol droplets. An extension of the CFD code to include droplet coagulation combined with elementary solvation reactions in the chemical mechanism could make reactive CFD results more accurate. Also, a deeper investigation of the effect of aerosol chemistry on other hypergolic bipropellant pairs could give insight onto how important aerosol chemistry is to hypergolic ignition in general, independent of the bipropellant pair used. This investigation could begin by using the same techniques used in this dissertation for determining the solvation energy and then taking advantages of extended reactive CFD codes to get more accurate results and more complete understanding.

TMEDA was only investigated briefly and only at high temperatures. To truly determine the usefulness of TMEDA as a safer MMH replacement, a full reaction mechanism needs to be created. A similar approach to the refrigerant combustion mechanism could be employed to create a combustion sub-mechanism for TMEDA. The sub-mechanism could be added to the MMH/RFNA mechanism with all MMH-specific reactions stripped out, leaving just the C/H/N/O base, which will adequately support the TMEDA sub-mechanism. With this new TMEDA/RFNA mechanism, a plethora of calculations could be performed comparing the performance of the two hypergolic fuels. The results would guide the application of TMEDA and show if it has potential to supplant MMH as the dominant hypergolic fuel. It would also be possible to reduce the new TMEDA mechanism with the same procedure used

for MMH and perform reactive CFD simulations. These studies would also fit well with the study of the effect of aerosols on general hypergolic combustion discussed in the preceding paragraph.

The refrigerant mechanism, as it is, only exists as a first attempt. Any and all further simulations will provide ideas for its expansion and improvement. Particularly, using it to simulate 1234yf-doped hydrocarbon flames could produce useful information about reactions that become important during more energetic combustion and could also give a good idea of the effect of the refrigerant on an already-burning system. In this way, these simulations would not only help improve the mechanism, but also drive experiments and lead to more intelligent applications of HFO-1234yf. Also, combustion simulations of the refrigerants that are currently in use, some of which are already represented in the NIST mechanism, could give insight about the combustion behavior of HFO-1234yf in comparison to the refrigerants that currently dominate the market. The unfortunate dearth of experimental data concerning HFO-1234yf also hinders improvements to the mechanism. Without data to compare to it is difficult to determine the weaknesses of the current mechanism. Performing laboratory measurements of 123yf-doped hydrocarbon flames (possibly using the Westmoreland group's molecular beam mass spectrometry system) would enable more directed study of improvements to the 1234yf mechanism.

The codes used in PrIME to investigate  $H_2/O_2$  combustion are constantly being improved and updated, leading to ever-increasing possibilities for future study. The current study only uses pre-exponential factors as optimization variables, a feature which is currently being expanded

to include all rate-coefficient parameters including temperature exponents and activation energies. Using the updated codes to run a full-parameter optimization would lead to a better-performing mechanism and more insights. Also, the inclusion of more data from more experimental sources (i.e., not just shock tubes and flames) in the optimization process would have a similar outcome. The ever-expanding nature of the set of tools in PrIME means that it is always possible to go back and improve upon previous results, which, by extension, means it is always possible to gather new insights and improve scientific understanding. Rigorous testing of the performance of the optimized models against published mechanisms would give a better idea of how well the optimization process works. The goal of PrIME is to produce the best mechanism through a community workflow but also to produce mechanisms that work well for a desired application; it is still advantageous to see how the performance of PrIME-created mechanisms compares to the current state of the literature.

The procedures used to discover the mechanism of reaction between TMA and PMMA would be easily applied to other precursor/substrate experiments. Given product spectra from ALD (or SVI) of any precursor on any substrate (even non-polymeric substrates), CQC techniques could be used to try to discover the mechanisms of those reactions. However, it is important to acknowledge that not all spectra may contain enough information or characteristic peaks to make this sort of analysis possible. More complete knowledge of precursor–substrate interactions enables researchers to more intelligently choose materials for their desired applications. Even the knowledge of what precursors and substrates don't react can be useful. As more precursor–substrate pairs are studied, a general method of



testing a precursor's interaction with a given substrate could be derived. CQC testing of precursors and substrates could precede experimental tests, saving researcher's time and avoiding expensive costs associated with experimental materials.

Though the reactive molecular dynamics method RxnMD is only briefly mentioned in this dissertation, it is an intriguing alternative to ReaxFF for RMD simulations. The goal of RxnMD is to be able to use the code with any equilibrium force field. Currently, the method lacks the code to handle coulombic interactions and the only species it can simulate are carbon and hydrogen. Coulombic interactions become very important in condensed-phase applications and when species have lone pairs. Code would need to be added not only to compute these forces, but also to speed up the pair interaction calculations so that the program would not be slowed to the point where it was unusable. Many calculation speedup methods already exist and could be incorporated into the RxnMD code in parallel with the coulombic-force calculations. To add in the capability for RxnMD to simulate more species, it is necessary to fit new switching functions. Going through the periodic table and fitting switching functions for every element is undesirable. It would be more apt to create generic switching functions for each reaction type that would work with all species, regardless of their constituent atoms. This development would require that the switching functions scale the activation energy of a reaction according to the heat of reaction of the species involved, based on the Evans–Polanyi relationship [171]. With these improvements, RxnMD would be closer to its goal of using any equilibrium force field for its calculations. This would allow RxnMD to be much more versatile than ReaxFF as an RMD simulation tool.

## REFERENCES

- [1] T.F.E. Rhead, R.V. Wheeler, *J. Chem. Soc. Trans.* 103 (1913) 461–489.
- [2] T.F.E. Rhead, R.V. Wheeler, *J. Chem. Soc. Trans.* 101 (1912) 846–856.
- [3] J. Warnatz, “Chapter 5: Rate Coefficients in the C/H/O System.” in W.C. Gardiner Jr (Ed.), *Combustion Chemistry*, Springer US, 1984, pp. 197–360.
- [4] J. Warnatz, *Combust. Sci. Technol.* 34 (1983) 177–200.
- [5] J. Warnatz, *Ber. Bunsenges. Phys. Chem.* 87 (1983) 1008–1022.
- [6] J. Warnatz, *Proc. Combust. Inst.* 18 (1981) 369–384.
- [7] M.T.H. Liu, K.J. Laidler, *Can. J. Chem.* 46 (1968) 479–490.
- [8] K.J. Laidler, M.T.H. Liu, *Proc. R. Soc. Lond. Math. Phys. Eng. Sci.* 297 (1967) 365–375.
- [9] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, T. Bowman, R.K. Hanson, S. Soonho, W.C. Gardiner, V.V. Lissianski, Z. Qin, *GRI-Mech 3.0* <[http://www.me.berkeley.edu/gri\\_mech](http://www.me.berkeley.edu/gri_mech)>
- [10] M.P. Burke, M. Chaos, Y. Ju, F.L. Dryer, S.J. Klippenstein, *Int. J. Chem. Kinet.* 44 (2012) 444–474.
- [11] W.R. Anderson, M.J. McQuaid, M.J. Nusca, A.J. Kotlar, *A Detailed, Finite-Rate, Chemical Kinetics Mechanism for Monomethylhydrazine-Red Fuming Nitric Acid Systems*, U.S. Army Research Laboratory, Report No. ARL-TR-5088 Aberdeen Proving Ground, MD, 2010.
- [12] D.R. Burgess Jr., M.R. Zachariah, W. Tsang, P.R. Westmoreland, *Prog. Energy Combust. Sci.* 21 (1995) 453–529.
- [13] G. Dixon-Lewis, D.J. Williams, “Chapter 1: The Oxidation of Hydrogen and Carbon Monoxide.” in C.H. Bamford and C.F.H. Tipper (Ed.), *Comprehensive Chemical Kinetics*, Elsevier, 1977, pp. 1–248.
- [14] A.A. Konnov, *Combust. Flame* 162 (2015) 3755–3772.
- [15] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery Jr., J.E. Peralta, F. Ogliaro, M. Bearpark,

- J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, Ö. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox, Gaussian-09 Revision B.01, Gaussian Inc., Wallingford, CT, 2010.
- [16] M.W. Schmidt, K.K. Baldrige, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A. Montgomery, *J. Comput. Chem.* 14 (1993) 1347–1363.
- [17] D. Van Der Spoel, E. Lindahl, B. Hess, G. Groenhof, A.E. Mark, H.J.C. Berendsen, *J. Comput. Chem.* 26 (2005) 1701–1718.
- [18] R. J. Kee, F. M. Rupley, J. A. Miller, M. E. Coltrin, J. F. Grcar, E. Meeks, H. K. Moffat, A. E. Lutz, G. Dixon-Lewis, M. D. Smooke, J. Warnatz, G. H. Evans, R. S. Larson, R. E. Mitchell, L. R. Petzold, W. C. Reynolds, M. Caracotsios, W. E. Stewart, P. Glarborg, C. Wang, Ola Adigun, CHEMKIN Collection, Release 3.6, Reaction Design, Inc., San Diego, CA, 2000.
- [19] "PrImE: Process Informatics Model," <<http://www.primekinetics.org>>, 2016.
- [20] D.G. Goodwin, H.K. Moffat, R.L. Speth, Cantera: An Object-Oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes, 2012, available at: <<http://www.cantera.org>>
- [21] CHEMKIN-PRO 15131, Reaction Design Inc., San Diego, 2013.
- [22] S. Glasstone, H. Eyring, K.J. Laidler, *The Theory of Rate Processes*, McGraw-Hill, 1941.
- [23] W.C. Gardiner Jr., J. Troe, "Chapter 4: Rate Coefficients of Thermal Dissociation, Isomerization, and Recombination Reactions" in W.C. Gardiner Jr. (Ed.), *Combustion Chemistry*, Springer US, 1984, pp. 173–196.
- [24] E. Schrödinger, *Phys. Rev.* 28 (1926) 1049–1070.
- [25] H. Eyring, J. Walter, G. Kimball, *Quantum Chemistry*, John Wiley & Sons Inc, New York, NY, 1944.
- [26] L. Pauling, E. Bright Wilson, *Introduction To Quantum Mechanics*, McGraw Hill Book Company Inc., New York, NY, 1935.
- [27] J.A. Montgomery Jr, M.J. Frisch, J.W. Ochterski, G.A. Petersson, *J. Chem. Phys.* 110 (1999) 2822–2827.

- [28] J.A. Montgomery Jr, M.J. Frisch, J.W. Ochterski, G.A. Petersson, *J. Chem. Phys.* 112 (2000) 6532–6542.
- [29] A.D. Becke, *Phys. Rev. A* 38 (1988) 3098–3100.
- [30] C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B* 37 (1988) 785–789.
- [31] R. Dennington, T. Keith, J. Millam, GaussView, Semichem Inc., Shawnee Mission KS, 2009.
- [32] C. Peng, P.Y. Ayala, H.B. Schlegel, M.J. Frisch, *J. Comput. Chem.* 17 (1996) 49–56.
- [33] C. Peng, H. Bernhard Schlegel, *Isr. J. Chem.* 33 (1993) 449–454.
- [34] H.P. Hratchian, H.B. Schlegel, *J. Chem. Theory Comput.* 1 (2005) 61–69.
- [35] H.P. Hratchian, H.B. Schlegel, *J. Chem. Phys.* 120 (2004) 9918–9924.
- [36] V. Mokrushin, V. Bedanov, W. Tsang, M. Zachariah, V. Knyazev, ChemRate, <<http://www.nist.gov/kinetics/chemrate/chemrate.html>>, Mokrushin Software, 2009.
- [37] B.J. McBride, S. Gordon, M.A. Reno, Coefficients for Calculating Thermodynamic and Transport Properties of Individual Species, National Aeronautics and Space Administration, Report No. NASA-TM-4513, 1993.
- [38] J.R. Barker, *Int. J. Chem. Kinet.* 41 (2009) 748–763.
- [39] B.J. Alder, T.E. Wainwright, *J. Chem. Phys.* 31 (1959) 459–466.
- [40] B.J. Alder, D.M. Gass, T.E. Wainwright, *J. Chem. Phys.* 53 (1970) 3813–3826.
- [41] M. Levitt, A. Warshel, *Nature* 253 (1975) 694–698.
- [42] S. Plimpton, *J. Comput. Phys.* 117 (1995) 1–19.
- [43] A.C.T. van Duin, S. Dasgupta, F. Lorant, W.A. Goddard III, *J. Phys. Chem. A* 105 (2001) 9396–9409.
- [44] A.C.T. van Duin, A. Strachan, S. Stewman, Q. Zhang, X. Xu, W.A. Goddard III, *J. Phys. Chem. A* 107 (2003) 3803–3811.
- [45] A. Strachan, A.C.T. van Duin, D. Chakraborty, S. Dasgupta, W.A. Goddard III, *Phys. Rev. Lett.* 91 (2003) 098301.
- [46] S. Cheung, W.-Q. Deng, A.C.T. van Duin, W.A. Goddard III, *J. Phys. Chem. A* 109 (2005) 851–859.

- [47] K.D. Nielson, A.C.T. van Duin, J. Oxgaard, W.-Q. Deng, W.A. Goddard III, *J. Phys. Chem. A* 109 (2005) 493–499.
- [48] K. Chenoweth, A.C.T. van Duin, W.A. Goddard III, *J. Phys. Chem. A* 112 (2008) 1040–1053.
- [49] J. Budzien, A.P. Thompson, S.V. Zybin, *J. Phys. Chem. B* 113 (2009) 13142–13151.
- [50] M.R. Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter, *J. Phys. Chem. A* 114 (2010) 5485–5492.
- [51] J.A. Keith, D. Fantauzzi, T. Jacob, A.C.T. van Duin, *Phys. Rev. B* 81 (2010) 235404.
- [52] A. Strachan, E.M. Kober, A.C.T. van Duin, J. Oxgaard, W.A. Goddard III, *J. Chem. Phys.* 122 (2005) 054502.
- [53] K. Smith, RxnMD, <<https://sourceforge.net/projects/rxnmd/?source=directory>>.
- [54] M.R. Nyden, D.W. Noid, *J. Phys. Chem.* 95 (1991) 940–945.
- [55] M.R. Nyden, G.P. Forney, J.E. Brown, *Macromolecules* 25 (1992) 1658–1666.
- [56] K.D. Smith, S.I. Stoliarov, M.R. Nyden, P.R. Westmoreland, *Mol. Simul.* 33 (2007) 361–368.
- [57] K.D. Smith, M. Bruns, S.I. Stoliarov, M.R. Nyden, O.A. Ezekoye, P.R. Westmoreland, *Polymer* 52 (2011) 3104–3111.
- [58] N. Labbe, Determining Detailed Reaction Kinetics for Nitrogen-and Oxygen-Containing Fuels, Ph.D. Dissertation, University of Massachusetts Amherst, 2013.
- [59] J. Bian, J. Vandooren, P.J. Van Tiggelen, *Proc. Combust. Inst.* 21 (1988) 953–963.
- [60] D.F. Davidson, K. Kohse-Höinghaus, A.Y. Chang, R.K. Hanson, *Int. J. Chem. Kinet.* 22 (1990) 513–535.
- [61] A.M. Dean, J.W. Bozzelli, “Combustion Chemistry of Nitrogen” in W.C. Gardiner Jr. (Ed.), *Gas-Phase Combustion Chemistry*, Springer New York, 2000, pp. 125–341.
- [62] C. Duynslaegher, H. Jeanmart, J. Vandooren, *Proc. Combust. Inst.* 32 (2009) 1277–1284.
- [63] A. Lucassen, K. Zhang, J. Warkentin, K. Moshhammer, P. Glarborg, P. Marshall, K. Kohse-Höinghaus, *Combust. Flame* 159 (2012) 2254–2279.
- [64] J.A. Miller, C.T. Bowman, *Prog. Energy Combust. Sci.* 15 (1989) 287–338.
- [65] Z. Tian, Y. Li, L. Zhang, P. Glarborg, F. Qi, *Combust. Flame* 156 (2009) 1413–1426.

- [66] W. Tsang, J.T. Herron, *J. Phys. Chem. Ref. Data* 20 (1991) 609–663.
- [67] J. Vandooren, J. Bian, P.J. Van Tiggelen, *Combust. Flame* 98 (1994) 402–410.
- [68] R.C. Sausa, G. Singh, G.W. Lemire, W.R. Anderson, *Proc. Combust. Inst.* 26 (1996) 1043–1052.
- [69] B. Lewis, G. von Elbe, “Chapter II: The Reaction between Hydrogen and Oxygen,” in B. Lewis, G. von Elbe (Eds.), *Combustion, Flames and Explosions of Gases*, Third Ed., Academic Press, San Diego, 1987, pp. 25–77.
- [70] M.A. Mueller, T.J. Kim, R.A. Yetter, F.L. Dryer, *Int. J. Chem. Kinet.* 31 (1999) 113–125.
- [71] J. Li, Z. Zhao, A. Kazakov, F.L. Dryer, *Int. J. Chem. Kinet.* 36 (2004) 566–575.
- [72] S.J. Klippenstein, L.B. Harding, P. Glarborg, J.A. Miller, *Combust. Flame* 158 (2011) 774–789.
- [73] L. Catoire, S.D. Chambreau, G.L. Vaghjiani, *Combust. Flame* 159 (2012) 1759–1768.
- [74] H. Sun, L. Catoire, C.K. Law, *Int. J. Chem. Kinet.* 41 (2009) 176–186.
- [75] J.A. Vanderhoff, W.R. Anderson, A.J. Kotlar, 29th JANNAF Combust. Subcomm. Meeting II (1992) 255.
- [76] D.A. Masten, R.K. Hanson, C.T. Bowman, *J. Phys. Chem.* 94 (1990) 7119–7128.
- [77] W. Li, *Initial Aromatics Growth in Different Hydrocarbon Flames*, Ph.D. Dissertation, North Carolina State University, 2011.
- [78] W. Li, M.E. Law, P.R. Westmoreland, T. Kasper, N. Hansen, K. Kohse-Höinghaus, *Combust. Flame* 158 (2011) 2077–2089.
- [79] T.A. Cool, J. Wang, N. Hansen, P.R. Westmoreland, F.L. Dryer, Z. Zhao, A. Kazakov, T. Kasper, K. Kohse-Höinghaus, *Proc. Combust. Inst.* 31 (2007) 285–293.
- [80] Personal communication to P.R. Westmoreland (2012).
- [81] O. Ubbink, *Numerical Prediction of Two Fluid Systems with Sharp Interfaces*, Ph.D. Dissertation, University of London UK, 1997.
- [82] S. Popinet, *J. Comput. Phys.* 190 (2003) 572–600.
- [83] S.Q. Wang, S.T. Thynell, *Combust. Flame* 159 (2012) 438–447.
- [84] F.-M. Tao, *J. Chem. Phys.* 108 (1998) 193–202.

- [85] R.E. Treybal, *Mass-Transfer Operations*, 3d ed., McGraw-Hill, New York, c1980.
- [86] R.B. Bird, W.E. Stewart, E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, New York, 2001.
- [87] W.E. Ranz, W.R. Marshall Jr, *Chem Eng Prog* 48 (1952) 173.
- [88] S. Wang, S.T. Thynell, A. Chowdhury, *Energy Fuels* 24 (2010) 5320–5330.
- [89] W.-G. Liu, S. Dasgupta, S.V. Zybin, W.A. Goddard III, *J. Phys. Chem. A* 115 (2011) 5221–5229.
- [90] Y. Liu, S.V. Zybin, J. Guo, A.C.T. van Duin, W.A. Goddard III, *J. Phys. Chem. B* 116 (2012) 14136–14145.
- [91] HyperChem(TM) Professional, Version 7.5.2, Hypercube, Inc., 1115 NW 4th St., Gainesville, FL 32601, USA, 2002.
- [92] O.J. Nielsen, M.S. Javadi, M.P.S. Andersen, M.D. Hurley, T.J. Wallington, R. Singh, *Chem. Phys. Lett.* 439 (2007) 18–22.
- [93] B. Minor, M. Spatz, *Int. Refrig. Air Cond. Conf.* (2008).
- [94] M. Koban, HFO-1234yf Low GWP Refrigerant LCCP Analysis, SAE Technical Paper 2009-01-0179, 2009.
- [95] K. Takizawa, K. Tokuhashi, S. Kondo, *J. Hazard. Mater.* 172 (2009) 1329–1338.
- [96] B.H. Minor, D. Herrmann, R. Gravell, *Process Saf. Prog.* 29 (2010) 150–154.
- [97] S. Kondo, K. Takizawa, K. Tokuhashi, *J. Fluor. Chem.* 144 (2012) 130–136.
- [98] V.L. Orkin, L.E. Martynova, A.N. Ilichev, *J. Phys. Chem. A* 114 (2010) 5967–5979.
- [99] M.R. Zachariah, P.R. Westmoreland, D.R. Burgess, W. Tsang, C.F. Melius, *J. Phys. Chem.* 100 (1996) 8737–8747.
- [100] S.W. Benson, *Can. J. Chem.* 61 (1983) 881–887.
- [101] P.R. Westmoreland, *Experimental and Theoretical Analysis of Oxidation and Growth Chemistry in a Fuel-Rich Acetylene Flame*, Ph.D. Dissertation, Massachusetts Institute of Technology, 1986.
- [102] W. Tsang, *J. Phys. Chem. Ref. Data* 20 (1991) 221–273.
- [103] H. Hua, B. Ruscic, B. Wang, *Chem. Phys.* 311 (2005) 335–341.
- [104] S.W. Benson, *Thermochemical Kinetics*, 2nd ed., Wiley, New York, 1976.

- [105] J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland, *Proc. Comb. Inst.* 2016, (submitted)
- [106] X. You, A. Packard, M. Frenklach, *Int. J. Chem. Kinet.* 44 (2012) 101–116.
- [107] Z. Hong, D.F. Davidson, R.K. Hanson, *Combust. Flame* 158 (2011) 633–644.
- [108] A. Kéromnès, W.K. Metcalfe, K.A. Heufer, N. Donohoe, A.K. Das, C.-J. Sung, J. Herzler, C. Naumann, P. Griebel, O. Mathieu, M.C. Krejci, E.L. Petersen, W.J. Pitz, H.J. Curran, *Combust. Flame* 160 (2013) 995–1011.
- [109] T. Varga, T. Nagy, C. Olm, I.G. Zsély, R. Pálvölgyi, É. Valkó, G. Vincze, M. Cserhádi, H.J. Curran, T. Turányi, *Proc. Combust. Inst.* 35 (2015) 589–596.
- [110] M. Frenklach, *Proc. Combust. Inst.* 31 (2007) 125–140.
- [111] G.L. Goteng, N. Nettyam, S.M. Sarathy, “CloudFlame: Cyberinfrastructure for Combustion Research”, in 2013 *Int. Conf. Info. Sci. Cloud Comput. Companion*, 2013, pp. 294–299.
- [112] G.L. Goteng, M. Speight, N. Nettyam, A. Farooq, M. Frenklach, S.M. Sarathy, “A Hybrid Cloud System for Combustion Kinetics Simulation”, 23rd *International Symposium on Gas Kinetics and Related Phenomena*, Hungary, 2014.
- [113] Z. Reyno-Chiasson, N. Nettyam, G.L. Goteng, M. Speight, B.J. Lee, S. Baskaran, J. Oreluk, A. Farooq, H.G. Im, M. Frenklach, S.M. Sarathy, “CloudFlame and PrIME: accelerating combustion research in the cloud,” 9th *Int. Conf. on Chemical Kinetics*, Ghent, Belgium, 2015.
- [114] M. Frenklach, A. Packard, P. Seiler, R. Feeley, *Int. J. Chem. Kinet.* 36 (2004) 57–66.
- [115] R. Feeley, P. Seiler, A. Packard, M. Frenklach, *J. Phys. Chem. A* 108 (2004) 9573–9583.
- [116] T. Russi, A. Packard, M. Frenklach, *Chem. Phys. Lett.* 499 (2010) 1–8.
- [117] T. Russi, A. Packard, R. Feeley, M. Frenklach, *J. Phys. Chem. A* 112 (2008) 2579–2588.
- [118] P. Seiler, M. Frenklach, A. Packard, R. Feeley, *Optim. Eng.* 7 (2006) 459–478.
- [119] V.R. Lambert, R.H. West, “Identification, Correction, and Comparison of Detailed Kinetic Models,” 9th *US Natl. Combust. Meeting*, Cincinnati, OH, May 18–20, 2015, Paper 3G03.
- [120] C. Gao, J.W. Allen, W.H. Green, R.H. West, *Comput. Phys. Comm.*, (submitted), available at: <<http://reactionmechanismgenerator.github.io/RMG-Py/>>



- [121] M.P. Burke, S.J. Klippenstein, L.B. Harding, *Proc. Combust. Inst.* 34 (2013) 547–555.
- [122] S.R. Sellevåg, Y. Georgievskii, J.A. Miller, *J. Phys. Chem. A* 113 (2009) 4457–4467.
- [123] J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland, Mechanism1, available at:  
<<http://warehouse.primekinetics.org/depositary/models/catalog/m00000007.xml>>.
- [124] J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland, Mechanism2, available at:  
<<http://warehouse.primekinetics.org/depositary/models/catalog/m00000008.xml>>.
- [125] J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland, Mechanism3, available at:  
<<http://warehouse.primekinetics.org/depositary/models/catalog/m00000009.xml>>.
- [126] T. Asaba, W.C. Gardiner, R.F. Stubbeman, *Symp. Int. Combust.* 10 (1965) 295–302.
- [127] N. Chaumeix, S. Pichon, F. Lafosse, C.-E. Paillard, *Int. J. Hydrog. Energy* 32 (2007) 2216–2226.
- [128] R.K. Cheng, A.K. Oppenheim, *Combust. Flame* 58 (1984) 125–139.
- [129] A. Cohen, J. Larsen, “Explosive mechanism of the H<sub>2</sub>-O<sub>2</sub> reaction near the second ignition limit,” BRL Report No. 1386, Ballistic Research Labs, Aberdeen Proving Ground, MD, 1967.
- [130] S. Fujimoto, M. Suzuki, *Mem. Def. Acad. Jpn.* 8 (1967) 1037–1046.
- [131] J. Herzler, C. Naumann, *Proc. Combust. Inst.* 32 (2009) 213–220.
- [132] C. Naumann, C. Herzler, P. Griebel, H. Curran, A. Keromnes, I. Mantzaras, “Results of ignition delay times for hydrogen rich and syngas fuel mixtures measure, Deliverable 1.1.3,” <<http://www.h2-igcc.eu/Pdf/SP1%20-Results%20of%20ignition%20delay%20times%20for%20hydrogen-rich%20and%20syngas%20fuel%20mixtures%20measured-%20D1.1.3%20-%20final.pdf>>, Project: Low Emission Gas Turbine Technology for Hydrogen Rich Syngas H<sub>2</sub>IGCC, Seventh Framework Programme Grant 239349, 2011.
- [133] G.A. Pang, D.F. Davidson, R.K. Hanson, *Proc. Combust. Inst.* 32 (2009) 181–188.
- [134] E.L. Petersen, D.M. Kalitan, M.J.A. Rickard, “Chemical Kinetics of OH\* Chemiluminescence in High-Temperature Reacting Flows,” Proceedings of the Third Joint Meeting of the U.S. Sections of the Combustion Institute, March 16-19, 2003, Chicago, IL.

- [135] E.L. Petersen, D.F. Davidson, M. Rohrig, R.K. Hanson, "Shock-Induced Ignition of High-Pressure H<sub>2</sub>-O<sub>2</sub>-Ar and CH<sub>4</sub>-O<sub>2</sub>-Ar Mixtures", 31st AIAA/ASME/SAE/ASEE Joint Propulsion Conference Exhibit, 1995.
- [136] G.L. Schott, J.L. Kinsey, *J. Chem. Phys.* 29 (1958) 1177–1182.
- [137] G.B. Skinner, G.H. Ringrose, *J. Chem. Phys.* 42 (1965) 2190–2192.
- [138] S.D. Tse, D.L. Zhu, C.K. Law, *Proc. Combust. Inst.* 28 (2000) 1793–1800.
- [139] M.P. Burke, M. Chaos, F.L. Dryer, Y. Ju, *Combust. Flame* 157 (2010) 618–631.
- [140] J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland, *DynamicMech151203*, available at: <http://warehouse.primekinetics.org/depositary/models/catalog/m00000010.xml>.
- [141] M. Ihme, Y. Sun, R. Deiterding, in R. Bonazza, D. Ranjan (Eds.), 29th Int. Symp. Shock Waves 1, Springer International Publishing, 2015, pp. 209–214.
- [142] E.C. Dandley, C.D. Needham, P.S. Williams, A.H. Brozena, C.J. Oldham, G.N. Parsons, *J. Mater. Chem. C* 2 (2014) 9416–9424.
- [143] S.-M. Lee, E. Pippel, U. Gösele, C. Dresbach, Y. Qin, C.V. Chandran, T. Bräuniger, G. Hause, M. Knez, *Science* 324 (2009) 488–492.
- [144] S.-M. Lee, E. Pippel, O. Moutanabbir, I. Gunkel, T. Thurn-Albrecht, M. Knez, *ACS Appl. Mater. Interfaces* 2 (2010) 2436–2441.
- [145] J.C. Spagnola, B. Gong, S.A. Arvidson, J.S. Jur, S.A. Khan, G.N. Parsons, *J. Mater. Chem.* 20 (2010) 4213–4222.
- [146] B. Gong, Q. Peng, J.S. Jur, C.K. Devine, K. Lee, G.N. Parsons, *Chem. Mater.* 23 (2011) 3476–3485.
- [147] Q. Peng, Y.-C. Tseng, S.B. Darling, J.W. Elam, *Adv. Mater.* 22 (2010) 5129–5133.
- [148] Q. Peng, Y.-C. Tseng, S.B. Darling, J.W. Elam, *ACS Nano* 5 (2011) 4600–4606.
- [149] Y.-C. Tseng, Q. Peng, L.E. Ocola, J.W. Elam, S.B. Darling, *J. Phys. Chem. C* 115 (2011) 17725–17729.
- [150] H.I. Akyildiz, R.P. Padbury, G.N. Parsons, J.S. Jur, *Langmuir ACS J. Surf. Colloids* 28 (2012) 15697–15704.
- [151] C.A. Wilson, R.K. Grubbs, S.M. George, *Chem. Mater.* 17 (2005) 5625–5634.
- [152] E. Farm, M. Kemell, M. Ritala, M. Leskela, *J. Phys. Chem. C* 112 (2008) 15791–15795.

- [153] G.N. Parsons, S.M. George, M. Knez, *MRS Bull.* 36 (2011) 865–871.
- [154] B. Gong, G.N. Parsons, *J. Mater. Chem.* 22 (2012) 15672–15682.
- [155] J.S. Jur, J.C. Spagnola, K. Lee, B. Gong, Q. Peng, G.N. Parsons, *Langmuir* 26 (2010) 8239–8244.
- [156] B. Gong, D.H. Kim, G.N. Parsons, *Langmuir* 28 (2012) 11915–11922.
- [157] M.W. Wong, *Chem. Phys. Lett.* 256 (1996) 391–399.
- [158] A.P. Scott, L. Radom, *J. Phys. Chem.* 100 (1996) 16502–16513.
- [159] K. Naito, G.E. Johnson, D.L. Allara, T.K. Kwei, *Macromolecules* 11 (1978) 1260–1265.
- [160] When this article was originally submitted, similar findings regarding the PMMA C=O/TMA Lewis acid/base adduct and related IR spectra were independently reported: M. Biswas, J. A. Libera, S. B. Darling and J. W. Elam, Nanopatterning of Inorganic Materials by Sequential Infiltration Synthesis: In Situ FTIR Investigation of the Precursor–Polymer Interaction, 2014 AVS Topical Conference on Atomic Layer Deposition (ALD 2014), Kyoto, Japan, 2014, AVS, Chico, CA, 2014.
- [161] I. Noda, A.E. Dowrey, J.L. Haynes, C. Marcott, in J.E. Mark (Ed.), *Phys. Prop. Polym. Handb.*, Springer New York, 2007, pp. 395–406.
- [162] Y. Xu, C.B. Musgrave, *Chem. Mater.* 16 (2004) 646–653.
- [163] M. Witt, H.W. Roesky, *Curr. Sci.* 78 (2000) 410.
- [164] C.K. Devine, C.J. Oldham, J.S. Jur, B. Gong, G.N. Parsons, *Langmuir* 27 (2011) 14497–14507.
- [165] K. Grychtol, W. Mennicke, in *Ullmanns Encycl. Ind. Chem.*, Wiley-VCH Verlag GmbH & Co. KGaA, 2000.
- [166] J.W. Elam, M.D. Groner, S.M. George, *Rev. Sci. Instrum.* 73 (2002) 2981–2987.
- [167] M.N. Rocklein, S.M. George, *Anal. Chem.* 75 (2003) 4975–4982.
- [168] D. Craig, F.W. Goldberg, R.W. Pett, N.T.H. Tholen, A.J.P. White, *Chem. Commun.* 49 (2013) 9275–9277.
- [169] S. Sano, H. Shimizu, Y. Nagao, *Tetrahedron Lett.* 46 (2005) 2887–2891.
- [170] K. Takai, I. Mori, K. Oshima, H. Nozaki, *Bull. Chem. Soc. Jpn.* 57 (1984) 446–451.
- [171] M.G. Evans, M. Polanyi, *Trans. Faraday Soc.* 34 (1938) 11–24.

## APPENDICES

## APPENDIX A. CHEMKIN MECHANISMS

All units in mole-cm-sec-K-cal unless otherwise noted.

### A.1 Labbe MMH/RFNA Sets

Thermochemistry parameters in CHEMKIN format

```

THERMO
  300.000  1000.000  5000.000
H          L 7/88H  1          G  200.000  3500.000  1000.000  1
  2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22  2
  2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15  3
  2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01  4
H2         TPIS78H  2          G  200.000  3500.000  1000.000  1
  3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14  2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05  3
  2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01  4
HE REF ELEMENT  g 5/97HE 1.  0.  0.  0.G  200.000  6000.000  1000.  1
  2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00  2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00  3
  0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01 0.00000000E+00  4
C          L11/88C  1          G  200.000  3500.000  1000.000  1
  2.49266888E+00 4.79889284E-05-7.24335020E-08 3.74291029E-11-4.87277893E-15  2
  8.54512953E+04 4.80150373E+00 2.55423955E+00-3.21537724E-04 7.33792245E-07  3
-7.32234889E-10 2.66521446E-13 8.54438832E+04 4.53130848E+00  4
CH         JUN03 C  1H  1          G  200.000  6000.000  1000.000  1
  0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-14  2
  0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-05  3
  0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01 0.71658188E+05  4
N          120186N  1          G  300.00  5000.00  1000.00  1
  0.02450268E+02 0.01066146E-02-0.07465337E-06 0.01879652E-09-0.01025984E-13  2
  0.05611604E+06 0.04448758E+02 0.02503071E+02-0.02180018E-03 0.05420529E-06  3
-0.05647560E-09 0.02099904E-12 0.05609890E+06 0.04167566E+02  4
CH2        JUN03 C  1H  2          G  200.000  6000.000  1000.000  1
  0.31463189E+01 0.30367126E-02-0.99647444E-06 0.15048358E-09-0.85733552E-14  2
  0.46041260E+05 0.47234171E+01 0.37175785E+01 0.12739126E-02 0.21734725E-05  3
-0.34885850E-08 0.16520887E-11 0.45872387E+05 0.17529794E+01 0.47050492E+05  4
CH2SING    JUN03 C  1H  2          G  200.000  6000.000  1000.000  1
  0.31350169E+01 0.28959393E-02-0.81666809E-06 0.11357270E-09-0.63626284E-14  2
  0.50504050E+05 0.40603062E+01 0.41933133E+01-0.23310518E-02 0.81567645E-05  3
-0.66298598E-08 0.19323320E-11 0.50366225E+05-0.74673431E+00 0.51572728E+05  4
NH         N  1H  1  0  OG  200.00  6000.00  1000.0  1
  0.27836929E+01 0.13298429E-02-0.42478047E-06 0.78348504E-10-0.55044470E-14  2
  0.42134514E+05 0.57407798E+01 0.34929084E+01 0.31179197E-03-0.14890484E-05  3
  0.24816442E-08-0.10356967E-11 0.41894294E+05 0.18483277E+01 0.42940822E+05  4
CH3        JUN03 C  1H  3          G  200.000  6000.000  1000.000  1
  0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-13  2
  0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-05  3
-0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01 0.17643935E+05  4
O          L 1/90O  1          G  200.000  3500.000  1000.000  1
  2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15  2

```

2.92175791E+04	4.78433864E+00	3.16826710E+00	-3.27931884E-03	6.64306396E-06						3
-6.12806624E-09	2.11265971E-12	2.91222592E+04	2.05193346E+00							4
NH2	121686N	1H	2	G	300.00	5000.00	1000.00			1
0.02961311E+02	0.02932699E-01	-0.09063600E-05	0.01617257E-08	-0.01204200E-12						2
0.02191977E+06	0.05777878E+02	0.03432493E+02	0.03299540E-01	-0.06613600E-04						3
0.08590947E-07	-0.03572047E-10	0.02177228E+06	0.03090111E+02							4
CH4	L 8/88C	1H	4	G	200.000	3500.000	1000.000			1
7.48514950E-02	1.33909467E-02	-5.73285809E-06	1.22292535E-09	-1.01815230E-13						2
-9.46834459E+03	1.84373180E+01	5.14987613E+00	-1.36709788E-02	4.91800599E-05						3
-4.84743026E-08	1.66693956E-11	-1.02466476E+04	-4.64130376E+00							4
OH	JUN03 O	1H	1	G	200.000	6000.000	1000.000			1
0.28385303E+01	0.11074129E-02	-0.29400021E-06	0.42069873E-10	-0.24228989E-14						2
0.36978081E+04	0.58449465E+01	0.39919842E+01	-0.24010666E-02	0.46166403E-05						3
-0.38791631E-08	0.13631950E-11	0.33688984E+04	-0.10399848E+00	0.44861538E+04						4
NH3	121386N	1H	3	G	300.00	5000.00	1000.00			1
0.02461904E+02	0.06059166E-01	-0.02004977E-04	0.03136003E-08	-0.01938317E-12						2
-0.06493270E+05	0.07472097E+02	0.02204352E+02	0.01011476E+00	-0.01465265E-03						3
0.01447235E-06	-0.05328509E-10	-0.06525488E+05	0.08127138E+02							4
H2O	L 8/89H	2O	1	G	200.000	3500.000	1000.000			1
3.03399249E+00	2.17691804E-03	-1.64072518E-07	-9.70419870E-11	1.68200992E-14						2
-3.00042971E+04	4.96677010E+00	4.19864056E+00	-2.03643410E-03	6.52040211E-06						3
-5.48797062E-09	1.77197817E-12	-3.02937267E+04	-8.49032208E-01							4
C2H	L 1/91C	2H	1	G	200.000	3500.000	1000.000			1
3.16780652E+00	4.75221902E-03	-1.83787077E-06	3.04190252E-10	-1.77232770E-14						2
6.71210650E+04	6.63589475E+00	2.88965733E+00	1.34099611E-02	-2.84769501E-05						3
2.94791045E-08	-1.09331511E-11	6.68393932E+04	6.22296438E+00							4
CN	C	1N	1	OG	200.00	6000.00	1000.0			1
3.39912871E+00	7.46548271E-04	-1.41493637E-07	1.86747261E-11	-1.26032174E-15						2
5.14665281E+04	4.67150296E+00	3.61256066E+00	-9.53015376E-04	2.13757148E-06						3
-3.05000108E-10	-4.70518899E-13	5.15179601E+04	3.98240466E+00	5.25707468E+04						4
C2H2	L 1/91C	2H	2	G	200.000	3500.000	1000.000			1
4.14756964E+00	5.96166664E-03	-2.37294852E-06	4.67412171E-10	-3.61235213E-14						2
2.59359992E+04	-1.23028121E+00	8.08681094E-01	2.33615629E-02	-3.55171815E-05						3
2.80152437E-08	-8.50072974E-12	2.64289807E+04	1.39397051E+01							4
H2CC	L12/89H	2C	2	OG	200.000	6000.000	1000.000			1
0.42780340E+01	0.47562804E-02	-0.16301009E-05	0.25462806E-09	-0.14886379E-13						2
0.48316688E+05	0.64023701E+00	0.32815483E+01	0.69764791E-02	-0.23855244E-05						3
-0.12104432E-08	0.98189545E-12	0.48621794E+05	0.59203910E+01	0.49887266E+05						4
HCN	110193H	1C	1N	1	G	0300.00	4000.00	1000.00		1
0.03426457E+02	0.03924190E-01	-0.01601138E-04	0.03161966E-08	-0.02432850E-12						2
0.01485552E+06	0.03607795E+02	0.02417787E+02	0.09031856E-01	-0.01107727E-03						3
0.07980141E-07	-0.02311141E-10	0.01501044E+06	0.08222891E+02							4
HNC	46.8	H	1C	1N	1	G	0300.00	5000.00	1500.00	1
0.05283464E+02	0.01092476E-01	-0.01170865E-05	-0.02308672E-09	0.03950673E-13						2
2.16142302E+04	-0.06388218E+02	0.03592377E+02	0.05561340E-01	-0.05936823E-04						3
0.03782329E-07	-0.09365092E-11	2.22826802E+04	0.02732160E+02							4
C2H3	OC	2H	3	OG	200.000	5000.000	1100.00		0	1
0.44767928E+01	0.72667722E-02	-0.25458602E-05	0.40524242E-09	-0.24034979E-13						2
0.33868175E+05	-0.70126031E-01	0.23280072E+01	0.99989781E-02	0.65780491E-06						3
-0.57360094E-08	0.23261669E-11	0.34648342E+05	0.11898753E+02							4
CO	TPIS79C	1O	1	G	200.000	3500.000	1000.000			1
2.71518561E+00	2.06252743E-03	-9.98825771E-07	2.30053008E-10	-2.03647716E-14						2
-1.41518724E+04	7.81868772E+00	3.57953347E+00	-6.10353680E-04	1.01681433E-06						3
9.07005884E-10	-9.04424499E-13	-1.43440860E+04	3.50840928E+00							4
N2	BUR0302	G 8/02N	2	0	OG	200.00	6000.00	1000.		1
2.95257637E+00	1.39690040E-03	-4.92631603E-07	7.86010195E-11	-4.60755204E-15						2
-9.23948688E+02	5.87188762E+00	3.53100528E+00	-1.23660988E-04	-5.02999433E-07						3
2.43530612E-09	-1.40881235E-12	-1.04697628E+03	2.96747038E+00	0.00000000E+00						4
CHNH	41687C	1H	2N	1	G	0300.00	4000.00	1000.00		1

```

0.04923293E+02 0.03332897E-01-0.03370897E-05-0.01901619E-08 0.03531825E-12 2
0.03132669E+06-0.01632509E+02 0.02759456E+02 0.06103387E-01 0.07713149E-05 3
-0.02063094E-07 0.01931920E-11 0.03217247E+06 0.01057489E+03 4
NCH2      41687H   2C   1N   1   G   0300.00  4000.00  1000.00  1
0.05209703E+02 0.02969291E-01-0.02855589E-05-0.01635550E-08 0.03043259E-12 2
0.02767711E+06-0.04444478E+02 0.02851661E+02 0.05695233E-01 0.01071140E-04 3
-0.01622612E-07-0.02351108E-11 0.02863782E+06 0.08992751E+02 4
C2H4      L 1/91C   2H   4   G   200.000  3500.000  1000.000  1
2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-1.25706061E-13 2
4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03 5.70990292E-05 3
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00 4
HCO       L12/89H   1C   10  1   G   200.000  3500.000  1000.000  1
2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-5.33508711E-14 2
4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05 3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 4
NNH      T 1/06N   2H   1   0   OG  200.000  6000.000  1000.  1 !
burcat 2010 *pw* change Hf=59.7 kcal/mole
3.42744423E+00 3.23295234E-03-1.17296299E-06 1.90508356E-10-1.14491506E-14 2
2.88067740E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-05 3
-1.33263744E-08 4.41023397E-12 2.88323793E+04 3.28551762E+00 3.02815661E+04 4
CH2NH     MELIUS 88   H   3C   1N   1   OG  300.000  5000.000  1577.000  01 !
DB00
4.54737795E+00 7.17720948E-03-2.47935299E-06 3.87692351E-10-2.26113075E-14 2
8.64056516E+03-1.16687427E+00 2.81849510E+00 5.11983235E-03 6.38887146E-06 3
-6.61374671E-09 1.65531940E-12 9.88442597E+03 1.03390629E+01 4
C2H5      L12/92C   2H   5   G   200.000  3500.000  1000.000  1
1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-1.49641576E-13 2
1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03 4.97142807E-05 3
-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00 4
NO        RUS 89N   1O   1   0   OG  200.00  6000.00  1000.  1 !
3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15 2
!H298 =91.097+/-0.085 kJ/mol [ATcT(RUS/PIN06)]
9.89456954E+03 6.36900469E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05 3
!S298 =50.36 cal/mol/K [BURCAT]
-9.34055507E-09 2.80554874E-12 9.81823786E+03 2.28060952E+00 4
!Cp [BURCAT]
CH2O      L 8/88H   2C   1O   1   G   200.000  3500.000  1000.000  1
1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14 2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05 3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01 4
N2H2      121286N   2H   2   G   300.00  5000.00  1000.00  1
0.03371185E+02 0.06039968E-01-0.02303854E-04 0.04062789E-08-0.02713144E-12 2
0.02418172E+06 0.04980585E+02 0.01617999E+02 0.01306312E+00-0.01715712E-03 3
0.01605608E-06-0.06093639E-10 0.02467526E+06 0.01379467E+03 4
H2NN     DBOZ00M93/JBPM3 96N  2H  2  0  OG  300.000  5000.000  1695.000  1
3.13531032E+00 5.68632569E-03-1.93983467E-06 3.01290501E-10-1.74978144E-14 2
3.33678346E+04 7.04815840E+00 2.88544262E+00 4.69495999E-03 7.01983230E-07 3
-1.53359038E-09 3.79345858E-13 3.36030690E+04 8.95096779E+00 4
CH3NH     THERM92   H   4C   1N   1   OG  300.000  5000.000  1404.000  11 !
DB00
4.90528413E+00 8.50385569E-03-2.82356461E-06 4.29267836E-10-2.45297886E-14 2
1.94541503E+04-1.35290137E+00 1.53882571E+00 1.62436539E-02-9.89573425E-06 3
3.49954504E-09-5.53823621E-13 2.06715086E+04 1.68295527E+01 4
CH2NH2    THERM92   H   4C   1N   1   OG  300.000  5000.000  1397.000  11 !
DB00
6.11432288E+00 7.69126269E-03-2.59025729E-06 3.97713575E-10-2.28883272E-14 2
1.55835138E+04-8.93053780E+00 2.56157769E+00 1.60730713E-02-1.05960335E-05 3
4.07638829E-09-6.95570548E-13 1.68563722E+04 1.01987687E+01 4
C2H6      L 8/88C   2H   6   G   200.000  3500.000  1000.000  1

```

```

1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-1.90002890E-13 2
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03 5.99438288E-05 3
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00 4
HNO ATcT/A H 1N 1O 1 OG 200.00 6000.00 1000. 1
!BURCAT
3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15 2
!H298 =106.842+/-0.125 kJ/mol [ATcT (BURCAT)]
1.17654289E+04 7.64513642E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05 3
!S298 =52.80 cal/mol/K
-1.71881225E-08 5.55818157E-12 1.16110981E+04 1.74318356E+00 4 !
HON HF MELIUS93H 1N 1O 1 OG 300.00 5000.00 1671.000 01
3.78577430E+00 2.86062728E-03-1.02423922E-06 1.64463139E-10-9.77943616E-15 2
2.93319701E+04 3.12193293E+00 3.33656431E+00 2.67682939E-03 5.61801303E-07 3
-1.11362279E-09 2.84076438E-13 2.95979751E+04 5.96343188E+00 4
CH2OH JUN03 C 1H 3O 1 G 200.000 6000.000 1000.000 1
0.50931437E+01 0.59476126E-02-0.20649746E-05 0.32300817E-09-0.18812590E-13 2
-0.40340964E+04-0.18469149E+01 0.44783436E+01-0.13507031E-02 0.27848498E-04 3
-0.36486906E-07 0.14790745E-10-0.35007289E+04 0.33091350E+01-0.20446277E+04 4
CH3O JUN03 C 1H 3O 1 G 200.000 6000.000 1000.000 1
0.47577924E+01 0.74414247E-02-0.26970518E-05 0.43809050E-09-0.26353710E-13 2
0.37811194E+03-0.19668003E+01 0.37118050E+01-0.28046331E-02 0.37655097E-04 3
-0.47307209E-07 0.18658842E-10 0.12956976E+04 0.65724086E+01 0.25257166E+04 4
N2H3 120186N 2H 3 G 300.00 5000.00 1000.00 1
0.04441846E+02 0.07214271E-01-0.02495684E-04 0.03920565E-08-0.02298950E-12 2
0.01664221E+06-0.04275205E+01 0.03174204E+02 0.04715907E-01 0.01334867E-03 3
-0.01919685E-06 0.07487564E-10 0.01727270E+06 0.07557224E+02 4
CH3NH2 SWS H 5C 1N 1 OG 300.000 5000.000 1387.000 11 !
DB00
5.23365618E+00 1.08525479E-02-3.65205276E-06 5.60552543E-10-3.22553444E-14 2
-5.52829576E+03-5.21507359E+00 1.69170293E+00 1.60389160E-02-4.99028441E-06 3
-3.83481304E-10 3.57345746E-13-3.94057426E+03 1.49835076E+01 4
O2 TPIS89O 2 G 200.000 3500.000 1000.000 1
3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14 2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06 3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00 4
NH2O 102290H 2N 1O 1 G 300.00 4000.00 1500.00 1
0.05673346E+02 0.02298837E-01-0.01774446E-05-0.01103482E-08 0.01859762E-12 2
0.05569325E+05-0.06153540E+02 0.02530590E+02 0.08596035E-01-0.05471030E-04 3
0.02276249E-07-0.04648073E-11 0.06868030E+05 0.01126651E+03 4
HNOH trans & Equ T11/11H 2N 1O 1 OG 200.000 6000.000 1000. 1
3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-14 2
1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-05 3
-3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00 1.21354115E+04 4
CH3OH L 8/88C 1H 4O 1 G 200.000 3500.000 1000.000 1
1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-1.17060220E-13 2
-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02 6.52441155E-05 3
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00 4
N2H4 121286N 2H 4 G 300.00 5000.00 1000.00 1
0.04977317E+02 0.09595519E-01-0.03547639E-04 0.06124299E-08-0.04029795E-12 2
0.09341219E+05-0.02962990E+02 0.06442606E+00 0.02749730E+00-0.02899451E-03 3
0.01745240E-06-0.04422282E-10 0.01045192E+06 0.02127789E+03 4
NH2OH JWB/SAND88 N 1H 3O 1 OG 300.000 5000.000 1412.000 1
5.12276969E+00 5.73428233E-03-1.86277359E-06 2.78938290E-10-1.57685159E-14 2
-7.42648110E+03-3.34064363E+00 1.59842441E+00 1.54722273E-02-1.24132635E-05 3
5.50996715E-09-1.00114333E-12-6.34935610E+03 1.50585859E+01 4
HO2 L 5/89H 1O 2 G 200.000 3500.000 1000.000 1
4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14 2
1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05 3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00 4

```



H2O2	L 7/88H	2O	2	G	200.000	3500.000	1000.000	1	
4.16500285E+00	4.90831694E-03	-1.90139225E-06	3.71185986E-10	-2.87908305E-14				2	
-1.78617877E+04	2.91615662E+00	4.27611269E+00	-5.42822417E-04	1.67335701E-05				3	
-2.15770813E-08	8.62454363E-12	-1.77025821E+04	3.43505074E+00					4	
C3H2	121686C	3H	2	G	0300.00	5000.00	1000.00	1	
0.06530853E+02	0.05870316E-01	-0.01720777E-04	0.02127498E-08	-0.08291910E-13				2	
0.05115214E+06	-0.01122728E+03	0.02691077E+02	0.01480366E+00	-0.03250551E-04				3	
-0.08644363E-07	0.05284878E-10	0.05219072E+06	0.08757391E+02					4	
C3H3	T 5/99C	3H	3	0	OG	200.000	6000.000	1	
7.14221880E+00	7.61902005E-03	-2.67459950E-06	4.24914801E-10	-2.51475415E-14				2	
3.89087427E+04	-1.25848436E+01	1.35110927E+00	3.27411223E-02	-4.73827135E-05				3	
3.76309808E-08	-1.18540923E-11	4.01057783E+04	1.52058924E+01	4.16139977E+04				4	
AR	120186AR	1	G	300.000	5000.000	1000.000		1	
0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2	
-0.07453750E+04	0.04366000E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00				3	
0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366000E+02					4	
NCN	103190C	1N	2	G	0300.00	4000.00	1500.00	1	
0.06652121E+02	0.06108034E-02	-0.01389727E-05	0.02695549E-10	0.01669944E-13				2	
0.05172403E+06	-0.01138517E+03	0.03101270E+02	0.09981674E-01	-0.09920701E-04				3	
0.04758919E-07	-0.08968626E-11	0.05285757E+06	0.07317579E+02					4	
AC3H4	L 8/89C	3H	4	0	OG	200.000	6000.000	1	
0.63168722E+01	0.11133728E-01	-0.39629378E-05	0.63564238E-09	-0.37875540E-13				2	
0.20117495E+05	-0.10995766E+02	0.26130445E+01	0.12122575E-01	0.18539880E-04				3	
-0.34525149E-07	0.15335079E-10	0.21541567E+05	0.10226139E+02	0.22962267E+05				4	
PC3H4	T 2/90H	4C	3	0	OG	200.000	6000.000	1	
0.60252400E+01	0.11336542E-01	-0.40223391E-05	0.64376063E-09	-0.38299635E-13				2	
0.19620942E+05	-0.86043785E+01	0.26803869E+01	0.15799651E-01	0.25070596E-05				3	
-0.13657623E-07	0.66154285E-11	0.20802374E+05	0.98769351E+01	0.22302059E+05				4	
HCCO	SRIC91H	1C	2O	1	G	300.00	4000.00	1000.000	1
0.56282058E+01	0.40853401E-02	-0.15934547E-05	0.28626052E-09	-0.19407832E-13				2	
0.19327215E+05	-0.39302595E+01	0.22517214E+01	0.17655021E-01	-0.23729101E-04				3	
0.17275759E-07	-0.50664811E-11	0.20059449E+05	0.12490417E+02					4	
HCNN	SRI/94C	1N	2H	1	G	300.000	5000.000	1000.000	1
0.58946362E+01	0.39895959E-02	-0.15982380E-05	0.29249395E-09	-0.20094686E-13				2	
0.53452941E+05	-0.51030502E+01	0.25243194E+01	0.15960619E-01	-0.18816354E-04				3	
0.12125540E-07	-0.32357378E-11	0.54261984E+05	0.11675870E+02					4	
CH2CNH	NL0512H	3C	2N	1	OG	200.00	5000.00	1000.00	1
5.66216832E+00	9.26107024E-03	-3.48651570E-06	6.07628542E-10	-4.01043359E-14				2	
1.97095267E+04	-5.55742628E+00	1.86949849E+00	1.78925908E-02	-5.52740583E-06				3	
-7.02394385E-09	4.78548967E-12	2.08046216E+04	1.43621039E+01					4	
AC3H5	PD5/98C	3H	5	0	OG	300.000	3000.000		1
0.65007877E+01	0.14324731E-01	-0.56781632E-05	0.11080801E-08	-0.90363887E-13				2	
0.17482449E+05	-0.11243050E+02	0.13631835E+01	0.19813821E-01	0.12497060E-04				3	
-0.33355555E-07	0.15846571E-10	0.19245629E+05	0.17173214E+02					4	
TC3H5	PD5/98C	3H	5	0	OG	300.000	3000.000		1
0.54255528E+01	0.15511072E-01	-0.56678350E-05	0.79224388E-09	-0.16878034E-13				2	
0.27843027E+05	-0.33527184E+01	0.17329209E+01	0.22394620E-01	-0.51490611E-05				3	
-0.67596466E-08	0.38253211E-11	0.29040498E+05	0.16568878E+02					4	
SC3H5	PD5/98C	3H	5	0	OG	300.000	3000.000		1
0.53725281E+01	0.15780509E-01	-0.59922850E-05	0.93089664E-09	-0.36550966E-13				2	
0.29614760E+05	-0.34186478E+01	0.91372931E+00	0.26432343E-01	-0.11758950E-04				3	
-0.23035678E-08	0.27715488E-11	0.30916867E+05	0.19989269E+02					4	
NCO	C	1H	ON	1O	1G	300.00	5000.00	1000.00	1
0.51511740E+01	0.25379660E-02	-0.10948080E-05	0.21129870E-09	-0.15056170E-13				2	
0.13463290E+05	-0.33718940E+01	0.45124190E+01	-0.32980770E-02	0.21963190E-04				3	
-0.26656140E-07	0.10269190E-10	0.13994080E+05	0.17322690E+01					4	
CH2CO	L 5/90C	2H	2O	1	G	200.000	3500.000	1000.000	1
4.51129732E+00	9.00359745E-03	-4.16939635E-06	9.23345882E-10	-7.94838201E-14				2	
-7.55105311E+03	6.32247205E-01	2.13583630E+00	1.81188721E-02	-1.73947474E-05				3	

9.34397568E-09-2.01457615E-12-7.04291804E+03	1.22156480E+01	4
CH2CHNH NL0512H 4C 2N 1 0g	200.00 5000.00 1000.00	1
5.50102729E+00 1.17702172E-02-4.46657421E-06	7.83031653E-10-5.19089322E-14	2
2.19556791E+04-3.60212879E+00 3.10187116E+00	6.36614579E-03 3.03829741E-05	3
-4.49078917E-08 1.85867428E-11 2.31285075E+04	1.15129893E+01	4
C3H6 120186C 3H 6 G	0300.00 5000.00 1000.00	1
0.06732257E+02 0.01490834E+00-0.04949899E-04	0.07212022E-08-0.03766204E-12	2
-0.09235703E+04-0.01331335E+03 0.01493307E+02	0.02092518E+00 0.04486794E-04	3
-0.01668912E-06 0.07158146E-10 0.01074826E+05	0.01614534E+03	4
HCNO C 1H 1N 1O 1G	300.00 5000.00 1000.00	1
0.60356200E+01 0.40593330E-02-0.15887770E-05	0.29204810E-09-0.20230570E-13	2
0.18339880E+05-0.91024050E+01 0.24825640E+01	0.14813560E-01-0.13687980E-04	3
0.60469050E-08-0.87705910E-12 0.19281540E+05	0.90325330E+01	4
HNCO C 1H 1N 1O 1G	300.00 5000.00 1000.00	1
0.53288440E+01 0.42143370E-02-0.16473930E-05	0.30184220E-09-0.20844800E-13	2
-0.15892150E+05-0.34500500E+01 0.34991880E+01	0.62636580E-02 0.31257680E-05	3
-0.86252000E-08 0.39133720E-11-0.15233280E+05	0.67449930E+01	4
HOCN C 1H 1N 1O 1G	300.00 5000.00 1000.00	1
0.48074750E+01 0.41918370E-02-0.16199240E-05	0.29436220E-09-0.20214190E-13	2
-0.33443110E+04 0.84660710E+00 0.47161980E+01	-0.12249760E-02 0.15769070E-04	3
-0.18447440E-07 0.68406900E-11-0.30276870E+04	0.27314860E+01	4
CH3CO JUN03 C 2H 3O 1 0G	200.000 6000.000 1000.0	1
0.53137165E+01 0.91737793E-02-0.33220386E-05	0.53947456E-09-0.32452368E-13	2
-0.36450414E+04-0.16757558E+01 0.40358705E+01	0.87729487E-03 0.30710010E-04	3
-0.39247565E-07 0.15296869E-10-0.26820738E+04	0.78617682E+01-0.12388039E+04	4
CH2CHO SAND86O 1H 3C 2 G	300.000 5000.000 1000.000	1
0.05975670E+02 0.08130591E-01-0.02743624E-04	0.04070304E-08-0.02176017E-12	2
0.04903218E+04-0.05045251E+02 0.03409062E+02	0.10738574E-01 0.01891492E-04	3
-0.07158583E-07 0.02867385E-10 0.15214766E+04	0.09558290E+02	4
CH3NN CH3-N=N T01/07C 1.H 3.N 2. 0.G	200.000 6000.000 1000.	1
5.03058624E+00 1.01655807E-02-3.80821408E-06	6.28676801E-10-3.81266093E-14	2
2.60782020E+04-1.37768696E+00 3.03556733E+00	7.89116568E-03 1.45352429E-05	3
-2.24777249E-08 8.99425199E-12 2.70660675E+04	1.09501412E+01 2.84101033E+04	4
nC3H7 P11/94C 3H 7 0 0G	300.000 3000.000	1
0.77097479E+01 0.16031485E-01-0.52720238E-05	0.75888352E-09-0.38862719E-13	2
0.79762236E+04-0.15515297E+02 0.10491173E+01	0.26008973E-01 0.23542516E-05	3
-0.19595132E-07 0.93720207E-11 0.10312346E+05	0.21136034E+02	4
iC3H7 P11/94C 3H 7 0 0G	300.000 3000.000	1
0.65192741E+01 0.17220104E-01-0.57364217E-05	0.84130732E-09-0.44565913E-13	2
0.73227193E+04-0.90830215E+01 0.14449199E+01	0.20999112E-01 0.77036222E-05	3
-0.18476253E-07 0.71282962E-11 0.94223724E+04	0.20116317E+02	4
CO2 L 7/88C 1O 2 G	200.000 3500.000 1000.000	1
3.85746029E+00 4.41437026E-03-2.21481404E-06	5.23490188E-10-4.72084164E-14	2
-4.87591660E+04 2.27163806E+00 2.35677352E+00	8.98459677E-03-7.12356269E-06	3
2.45919022E-09-1.43699548E-13-4.83719697E+04	9.90105222E+00	4
N2O 121286N 2O 1 G	300.00 5000.00 1000.00	1
0.04718977E+02 0.02873714E-01-0.01197496E-04	0.02250552E-08-0.01575337E-12	2
0.08165811E+05-0.01657250E+02 0.02543058E+02	0.09492193E-01-0.09792775E-04	3
0.06263845E-07-0.01901826E-10 0.08765100E+05	0.09511222E+02	4
C2H4O J 9/65C 2H 4O 1 0G	300.000 5000.000	1
0.59249249E 01 0.11120714E-01-0.37434083E-05	0.55413918E-09-0.29549886E-13	2
-0.93028008E 04-0.93792849E 01-0.24173594E 00	0.20761095E-01 0.21481201E-05	3
-0.16948157E-07 0.81075771E-11-0.71720117E 04	0.24432190E 02	4
CH3CHO L 8/88C 2H 4O 1 G	200.000 6000.000 1000.000	1
0.54041108E+01 0.11723059E-01-0.42263137E-05	0.68372451E-09-0.40984863E-13	2
-0.22593122E+05-0.34807917E+01 0.47294595E+01	-0.31932858E-02 0.47534921E-04	3
-0.57458611E-07 0.21931112E-10-0.21572878E+05	0.41030159E+01	4
CH3NNH OC 1H 4N 2O 0G	200.000 6000.000 1000.00	1
5.48334026D+00 1.17117818D-02-4.12106147D-06	6.54262200D-10-3.86199590D-14	2

```

1.86890527D+04-4.73384237D+00 3.51484036D+00 5.56200324D-03 2.14472257D-05 3
-2.41589770D-08 7.32461054D-12 1.99403457D+04 8.65997982D+00 4
C3H8 P11/94C 3H 8 0 OG 300.000 3000.000 1
0.75244152E+01 0.18898282E-01-0.62921041E-05 0.92161457E-09-0.48684478E-13 2
-0.16564394E+05-0.17838375E+02 0.92851093E+00 0.26460566E-01 0.60332446E-05 3
-0.21914953E-07 0.94961544E-11-0.14057907E+05 0.19225538E+02 4
HOCO 103190C 1H 10 2 G 0300.00 4000.00 1500.00 1
0.07517634E+02 0.01259029E-01-0.01910901E-05-0.03136391E-09 0.07547673E-13 2
-0.02634121E+06-0.01448392E+03 0.02285122E+02 0.01351435E+00-0.01160407E-03 3
0.05047011E-07-0.09032231E-11-0.02448416E+06 0.01367874E+03 4
HNNO MELIUS N 2H 10 1 OG 300.000 5000.000 1389.000 1
6.24922910E+00 3.26983002E-03-1.14794284E-06 1.81383141E-10-1.06538637E-14 2
2.53822106E+04-7.09495778E+00 2.40143922E+00 1.26718648E-02-1.00828306E-05 3
4.10522736E-09-6.79228705E-13 2.66782646E+04 1.34257436E+01 4
CH3NO 103190C 1H 3N 10 1G 0300.00 4000.00 1500.00 1
0.08820547E+02 0.03706233E-01-0.02894741E-05-0.01897910E-08 0.03237544E-12 2
0.05362862E+05-0.02213220E+03 0.02109955E+02 0.01517822E+00-0.07071789E-04 3
0.01510611E-07-0.01604204E-11 0.08293612E+05 0.01569702E+03 4
C2H5O JUN03 C 2O 1H 5 G 200.000 6000.000 1000.00 1
0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-13 2
-0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-04 3
-0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-0.16357022E+04 4
CH3NNH2 OC 1H 5N 2O OG 200.000 6000.000 1000.00 1
6.48248625D+00 1.31416200D-02-4.55408099D-06 7.15495219D-10-4.19235501D-14 2
2.18344199D+04-9.10020638D+00 2.89725447D+00 1.52571928D-02 5.46573210D-06 3
-1.13299263D-08 3.45334525D-12 2.33342324D+04 1.16815443D+01 4
HNNNH2 MOPAC/JWB N 3H 3 0 OG 300.000 5000.000 1387.000 1
6.69002957E+00 7.47314756E-03-2.57645360E-06 4.02077699E-10-2.34100069E-14 2
2.41665871E+04-1.12237235E+01 1.77934210E+00 1.84512489E-02-1.22068382E-05 3
4.40169354E-09-6.88479465E-13 2.59657722E+04 1.53992810E+01 4
NO2 L 7/88N 1O 2 0 OG 200.00 6000.00 1000. 1 !
4.88475400E+00 2.17239550E-03-8.28069090E-07 1.57475100E-10-1.05108950E-14 2
!H298 =34.025+/-0.085 kJ/mol [ATcT (RUS/PIN06)]
2.29397777E+03-1.17416951E-01 3.94403120E+00-1.58542900E-03 1.66578120E-05 3
!S298 =57.40 cal/mol/K [BURCAT]
-2.04754260E-08 7.83505640E-12 2.87409757E+03 6.31199190E+00 4
!Cp [BURCAT]
NH2NO H2NN=O T 1/12H 2N 2O 1 OG 200.000 6000.000 1000. 1
5.78592771E+00 6.03964151E-03-2.08624357E-06 3.28153040E-10-1.92960549E-14 2
7.61382696E+03-5.32127808E+00 3.68835855E+00 5.97978170E-03 1.22601857E-05 3
-2.07157226E-08 8.83557926E-12 8.44917678E+03 6.85576793E+00 9.88619462E+03 4
NHNHO M/B686 N 2H 2O 1 OG 300.000 5000.000 1382.000 1
6.87844514E+00 5.97768876E-03-2.32835297E-06 3.91753162E-10-2.40352995E-14 2
9.95321692E+03-1.33617968E+01 5.11596626E-01 1.95396787E-02-1.31481264E-05 3
4.26547517E-09-5.54657119E-13 1.23230195E+04 2.13441672E+01 4
CH3NHNH2 OC 1H 6N 2 OG 298.150 6000.000 1000.00 1
6.46195602D+00 1.54661452D-02-5.29188310D-06 8.22877488D-10-4.78182997D-14 2
8.08517920D+03-1.06506405D+01-1.55617356D-01 3.41164172D-02-3.21289044D-05 3
2.50164209D-08-9.43703969D-12 1.01527490D+04 2.41129608D+01 4
HONO RUS 89 H 1N 10 2 OG 200.00 6000.00 1000. 1
!BURCAT
0.57919018E+01 0.36515212E-02-0.12928936E-05 0.20688716E-09-0.12315254E-13 2
!H298 =-18.74 kcal/mol
-0.11565589E+05-0.40558233E+01 0.32141709E+01 0.81276869E-02 0.16602559E-05 3
!S298 =60.72 cal/mol/K
-0.95285182E-08 0.48715058E-11-0.10753237E+05 0.98219504E+01-0.94355439E+04 4 !
HNO2 103190 H 1N 10 2 G 300.00 4000.00 1500.00 1
!RAS/GLA08a

```

6.47963000E+00 1.99527400E-03-1.74038700E-07-9.69587200E-11 1.70148000E-14 2  
 !H298 = -9.80 kcal/mol [RAS/GLA08a]  
 -7.80950291E+03-1.06771518E+01 1.93483800E+00 1.01003600E-02-4.96461600E-06 3  
 !S298 =56.73 cal/mol/K [Sandia]  
 8.70112000E-10-2.32413500E-15-5.91571591E+03 1.47282082E+01 4 !  
 HNOO MELIUS88 N 1H 10 2 OG 300.000 5000.000 1685.000 1  
 6.22843297E+00 3.99232107E-03-1.71329587E-06 3.09055124E-10-1.99408751E-14 2  
 2.57303316E+04-7.82004870E+00 2.82368890E+00 9.26020228E-03-3.10307876E-06 3  
 -6.57987763E-10 3.64688961E-13 2.71092460E+04 1.13391387E+01 4  
 NH2NHO m93/jwb96pm3 N 2H 30 1 OG 300.000 5000.000 1405.000 1  
 6.76839963E+00 6.93278545E-03-2.28605862E-06 3.45978133E-10-1.97094457E-14 2  
 1.42869505E+04-9.16405703E+00 2.56091917E+00 1.79916569E-02-1.37740397E-05 3  
 5.87277161E-09-1.04140760E-12 1.56384602E+04 1.30177571E+01 4  
 HONHO M/JB86 N 1H 20 2 OG 300.000 5000.000 1416.000 1  
 9.01087354E+00 3.23941301E-03-1.18327845E-06 1.91943898E-10-1.14815574E-14 2  
 -1.48028338E+03-2.30114112E+01 1.05169569E-02 2.58437554E-02-2.25307323E-05 3  
 9.16861679E-09-1.42700071E-12 1.39517739E+03 2.46124525E+01 4  
 C4H P 1/93C 4H 1 0 OG 300.000 3000.000 1  
 0.77697593E+01 0.49829976E-02-0.17628546E-05 0.28144284E-09-0.16689869E-13 2  
 0.94345900E+05-0.14165274E+02 0.13186295E+01 0.38582956E-01-0.71385623E-04 3  
 0.65356359E-07-0.22617666E-10 0.95456106E+05 0.15567583E+02 4  
 C4H2 P 1/93C 4H 2 0 OG 300.000 3000.000 1  
 0.86637708E+01 0.67247189E-02-0.23593397E-05 0.37506380E-09-0.22230940E-13 2  
 0.53252275E+05-0.21093503E+02-0.39201030E+00 0.51937565E-01-0.91737340E-04 3  
 0.80471986E-07-0.26898218E-10 0.54845266E+05 0.20957794E+02 4  
 iC4H3 OC 4H 3 0 OG 200.000 5000.000 1200.00 0 1  
 0.87092233E+01 0.88631021E-02-0.31303011E-05 0.50137975E-09-0.29878650E-13 2  
 0.57500575E+05-0.18391950E+02 0.37694948E+01 0.23256639E-01-0.18531943E-04 3  
 0.76188028E-08-0.12128742E-11 0.58835310E+05 0.69616708E+01 4  
 nC4H3 82489C 4H 3 G 0300.00 4000.00 1000.00 1  
 0.10752738E+02 0.05381153E-01-0.05549637E-05-0.03052266E-08 0.05761740E-12 2  
 0.61979123E+05-0.02973025E+03 0.04153881E+02 0.01726287E+00-0.02389374E-05 3  
 -0.10187000E-07 0.04340504E-10 0.64145633E+05 0.06036506E+02 4  
 C4H4 H6W/94C 4H 4 0 OG 300.000 3000.000 1  
 0.66507092E+01 0.16129434E-01-0.71938875E-05 0.14981787E-08-0.11864110E-12 2  
 0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-04 3  
 0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02 4  
 C2N2 Dicyanogen ATcT/AC 2.N 2. 0. 0.G 200.000 6000.000 1000. 1  
 6.70549520E+00 3.64271185E-03-1.30939702E-06 2.16421413E-10-1.31193815E-14 2  
 3.48824335E+04-1.04803146E+01 2.32928126E+00 2.61540993E-02-4.90009889E-05 3  
 4.61923035E-08-1.64325831E-11 3.56900732E+04 9.86348075E+00 3.71976220E+04 4  
 n-C4H5 82489C 4H 5 G 0300.00 4000.00 1000.00 1  
 0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12 2  
 0.38695564E+05-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04 3  
 -0.11482454E-07 0.03197823E-10 0.42282224E+05 0.12894539E+02 4  
 i-C4H5 82489C 4H 5 G 0300.00 4000.00 1000.00 1  
 0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12 2  
 0.33423896E+05-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04 3  
 -0.09306953E-07 0.02386116E-10 0.36407556E+05 0.09842152E+02 4  
 CHCHNCH2 NL0512H 4C 3N 1 Og 200.00 5000.00 1000.00 1  
 7.02829199E+00 1.35098428E-02-5.23747631E-06 9.32145327E-10-6.24710034E-14 2  
 4.76681967E+04-9.71920936E+00 2.28897829E+00 1.73684484E-02 1.33889942E-05 3  
 -3.07663318E-08 1.38741396E-11 4.93973364E+04 1.69179788E+01 4  
 iiC4H6 A 8/83C 4H 6 0 OG 300. 3000. 1000.0 1  
 0.1781557E 02 -0.4257502E-02 0.1051185E-04 -0.4473844E-08 0.5848138E-12 2  
 0.1267342E 05 -0.6982662E 02 0.1023467E 01 0.3495919E-01 -0.2200905E-04 3  
 0.6942272E-08 -0.7879187E-12 0.1811799E 05 0.1975066E 02 0.1950807E+05 4  
 iic4H6 H6W/94C 4H 6 0 OG 300.000 3000.000 1  
 0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-12 2

0.91338516E+04-0.23328171E+02	0.11284465E+00	0.34369022E-01-0.11107392E-04	3							
-0.92106660E-08	0.62065179E-11	0.11802270E+05	0.23089996E+02	4						
C2H3CO C3H3O	T05/99C	3H	3O	1	OG	200.000	6000.000	1		
6.95842227E+00	1.07193211E-02-3.85218494E-06	6.22009064E-10-3.72401640E-14	2							
5.64826498E+03-1.14745786E+01	3.21169467E+00	1.18422105E-02	1.67462582E-05	3						
-3.06947176E-08	1.33048816E-11	7.12815750E+03	1.00881663E+01	8.70564832E+03	4					
CH2CHNCH2	NL0512H	5C	3N	1	Og	200.00	5000.00	1000.00	1	
6.46267020E+00	1.67980010E-02-6.50097404E-06	1.15557676E-09-7.73743161E-14	2							
1.64952732E+04-7.60355530E+00	2.70686712E+00	1.09849355E-02	3.70034076E-05	3						
-5.58051692E-08	2.29301182E-11	1.82832281E+04	1.56229034E+01	4						
C4H7	AM1/94C	4H	7	0	OG	300.000	3000.000	1000.000	1	
0.11963392E+02	0.11425305E-01	0.78948909E-06-0.19858872E-08	0.36873645E-12	2						
0.16962977E+05-0.37542908E+02	0.28698254E+00	0.36964495E-01-0.86277441E-05	3							
-0.15051821E-07	0.89891263E-11	0.20551301E+05	0.24484467E+02	4						
NCNO	92789C	1N	2O	1	OG	300.000	4000.000	1000.00	1	
0.73266358E+01	0.17882655E-02-0.20288753E-06-0.94724527E-10	0.18667134E-13	2							
0.36704793E+05-0.10886014E+02	0.49251637E+01	0.53706546E-02	0.27844874E-06	3						
-0.21986761E-08	0.46036536E-12	0.37592273E+05	0.24706030E+01	4						
NCHCHO	NL0512H	2C	2N	10	1g	200.00	5000.00	1000.00	1	
6.44159689E+00	8.76156545E-03-3.47897897E-06	6.29479906E-10-4.26839588E-14	2							
1.29189347E+04-5.19292137E+00	3.28273760E+00	1.07949442E-02	9.12178960E-06	3						
-1.91878297E-08	8.28309072E-12	1.41429825E+04	1.28099292E+01	4						
C2H3CHO	T 6/92C	3H	4O	1	OG	298.150	3000.0	1000.0	1	
0.48353180E+01	0.19772601E-01-0.10426628E-04	0.26525803E-08-0.26278207E-12	2							
-0.11557837E+05	0.18853144E+01	0.11529584E+01	0.28040214E-01-0.15072153E-04	3						
0.15905842E-08	0.84930371E-12-0.10417694E+05	0.21453279E+02-0.89572567E+04	4							
CH2NHCH2	NL0512H	6C	3N	1	Og	200.00	5000.00	1000.00	1	
7.50196587E+00	1.74773808E-02-6.58383837E-06	1.14807651E-09-7.58107388E-14	2							
2.33814706E+04-1.07082718E+01	2.57728607E+00	2.24497938E-02	1.01983386E-05	3						
-2.94479134E-08	1.36722613E-11	2.51162220E+04	1.66980623E+01	4						
CH2CH2NCH2	NL0512H	6C	3N	1	Og	200.00	5000.00	1000.00	1	
6.83108119E+00	1.87496609E-02-7.24470207E-06	1.28609137E-09-8.60231248E-14	2							
2.76999696E+04-7.71271290E+00	3.26656995E+00	1.24529614E-02	3.59690850E-05	3						
-5.44100284E-08	2.22352278E-11	2.94559526E+04	1.45710410E+01	4						
IC4H8	T 6/83C	4H	8	0	OG	300.000	5000.000	1		
0.20535841E+01	0.34350507E-01-0.15883197E-04	0.33089662E-08-0.25361045E-12	2							
-0.21397231E+04	0.15543201E+02	0.11811380E+01	0.30853380E-01	0.50865247E-05	3					
-0.24654888E-07	0.11110193E-10-0.17904004E+04	0.21062469E+02	4							
nC4H9	BURCAT	T 6/93C	4H	9	0	G	200.000	6000.000	1000.	1
8.97401527E+00	2.39704154E-02-8.48703645E-06	1.35644127E-09-8.06234913E-14	2							
5.19161526E+03-2.31075609E+01	4.73737837E+00	9.69051565E-03	6.63846383E-05	3						
-9.24799302E-08	3.74006099E-11	7.57382332E+03	4.91063455E+00	9.83838903E+03	4					
C2H3CH2O	96PRW1C	3H	5O	1	OG	300.00	3000.00	1000.00	1	
+2.75835879D+00+2.71781452D-02-1.44239030D-05+3.66635155D-09-3.64832209D-13	2									
+1.09685129D+04+1.15870981D+01+4.48935705D-01+3.24335892D-02-1.58843257D-05	3									
+4.03948822D-10+1.43106465D-12+1.15934429D+04+2.36532883D+01	4									
CH2CHOCH2	T 9/92C	3H	5O	1	OG	298.150	3000.000	1		
!rCH2OCHCH2 in old mech										
0.91206991E+01	0.12196117E-01-0.42929777E-05	0.12616892E-08-0.15705367E-12	2							
0.91765012E+04-0.22071447E+02	0.70599393E+00	0.25629797E-01	0.71080411E-05	3						
-0.29693495E-07	0.14360721E-10	0.11909268E+05	0.23610039E+02	0.13269823E+05	4					
NHCH2CHO	NL0512H	4C	2N	10	1g	200.00	5000.00	1000.00	1	
6.65451690E+00	1.34611580E-02-5.23712324E-06	9.34385840E-10-6.27315718E-14	2							
5.41174749E+03-5.10878592E+00	3.92385121E+00	7.15579388E-03	3.25906178E-05	3						
-4.68246266E-08	1.88885802E-11	6.82584683E+03	1.23163070E+01	4						
OCH2CHNH	NL0512H	4C	2N	10	1g	200.00	5000.00	1000.00	1	
6.88692946E+00	1.37500525E-02-5.36155188E-06	9.58262578E-10-6.44217673E-14	2							
1.09153616E+04-8.85641597E+00	3.10309188E+00	9.14738168E-03	3.45167980E-05	3						
-5.20699744E-08	2.14575673E-11	1.26500440E+04	1.42283131E+01	4						

CH3NNCH3	C&S-02	C	2N	2H	6	OG	300.000	4000.000	1000.00	1
0.49863152E+01	0.24070809E-01	-0.10732555E-04	0.22441162E-08	-0.17961655E-12						2
0.15409582E+05	-0.15606158E+01	0.19013815E+01	0.27280859E-01	-0.53752194E-05						3
-0.57609693E-08	0.23430172E-11	0.16600457E+05	0.15898338E+02	1.83222625E+04						4
C2H3OO	PRW84	C	2O	2H	3	G	0300.00	5000.00	1000.00	1
+1.07095497D+00	+2.93293018D-02	-2.26481331D-05	+8.68753392D-09	-1.30462650D-12						2
+1.27909845D+04	+2.07891307D+01	+3.93381061D+00	+1.98311250D-02	-1.14186387D-05						3
+3.09270357D-09	-3.22330856D-13	+1.21364287D+04	+6.51468027D+00							4
H2CNO2	103190C	1H	2N	1O	2G	0300.00	4000.00	1500.00		1
0.01127481E+03	0.02584711E-01	-0.03934331E-05	-0.05614969E-09	0.01392400E-12						2
0.01360470E+06	-0.03461951E+03	0.01165696E+02	0.02890490E+00	-0.02817663E-03						3
0.01387569E-06	-0.02727595E-10	0.01694546E+06	0.01888293E+03							4
CH3NO2	103190C	1H	3N	1O	2G	0300.00	4000.00	1500.00		1
0.01090158E+03	0.04326381E-01	-0.04203548E-05	-0.01893071E-08	0.03417444E-12						2
-0.01370862E+06	-0.03073183E+03	0.03224717E+01	0.02665147E+00	-0.01930574E-03						3
0.07762620E-07	-0.01398746E-10	-0.09597527E+05	0.02726156E+03							4
CH3ONO	103190C	1H	3N	1O	2G	0300.00	4000.00	1500.00		1
0.01136129E+03	0.04159349E-01	-0.04145670E-05	-0.01695140E-08	0.03028732E-12						2
-0.01281482E+06	-0.03545435E+03	0.01490345E+02	0.02645433E+00	-0.02112332E-03						3
0.09414399E-07	-0.01811205E-10	-0.09125782E+05	0.01813766E+03							4
C2H5OO	PW3/94C	2O	2H	5	G	0300.00	5000.00	1000.00		1
+2.10630563D+00	+2.77943799D-02	-1.44630852D-05	+3.25545688D-09	-2.46592854D-13						2
-2.64777663D+03	+1.80691037D+01	+2.10630563D+00	+2.77943799D-02	-1.44630852D-05						3
+3.25545688D-09	-2.46592854D-13	-2.64767408D+03	+1.80671959D+01							4
C5H2	OC	5H	2	0	OG	200.000	5000.000	900.00	0	1
0.10912226E+02	0.77090390E-02	-0.28335089E-05	0.46991021E-09	-0.28842258E-13						2
0.85484262E+05	-0.29829361E+02	0.25183751E+01	0.44292500E-01	-0.62601709E-04						3
0.43850625E-07	-0.11831256E-10	0.87024418E+05	0.99443064E+01							4
NO3	ATcT/AN	1O	3	0	OG	200.00	6000.00	1000.		1
!BURCAT										
7.48347702E+00	2.57772064E-03	-1.00945831E-06	1.72314063E-10	-1.07154008E-14						2
!H298 =17.83 kcal/mol										
6.12990474E+03	-1.41618136E+01	2.17359330E+00	1.04902685E-02	1.10472669E-05						3
!S298 =60.37 cal/mol/K										
-2.81561867E-08	1.36583960E-11	7.81290905E+03	1.46022090E+01	8.97563416E+03						4 !
NH2NO2 NITRAMIDE	tpis89N	2H	2O	2	G	200.000	6000.000	1000.00		1
7.38890844E+00	7.65188287E-03	-2.75087184E-06	4.44623197E-10	-2.66488354E-14						2
-6.21766970E+03	-1.32736914E+01	2.17310160E+00	1.43162238E-02	1.09031816E-05						3
-2.76714916E-08	1.29868784E-11	4.45906123E+03	1.53831146E+01	-3.12706341E+03						4
H2CCCCCH	OC	5H	3	0	OG	200.000	5000.000	1000.00	0	1
0.10024302E+02	0.10655411E-01	-0.38709251E-05	0.63462431E-09	-0.38550202E-13						2
0.65691196E+05	-0.25065161E+02	0.23963519E+01	0.36748178E-01	-0.36381526E-04						3
0.17889326E-07	-0.32474675E-11	0.67437737E+05	0.12840045E+02							4
HCCCHCCH	OC	5H	3	0	OG	200.000	5000.000	1000.00	0	1
0.10313636E+02	0.10278554E-01	-0.37086568E-05	0.60568664E-09	-0.36721455E-13						2
0.65859508E+05	-0.26380088E+02	0.10442368E+01	0.44574721E-01	-0.50980758E-04						3
0.29338989E-07	-0.65246891E-11	0.67852460E+05	0.19034765E+02							4
HNO3	T 8/03	H	1N	1O	3	OG	200.00	6000.00	1000.	1
!BURCAT										
8.03098942E+00	4.46958589E-03	-1.72459491E-06	2.91556153E-10	-1.80102702E-14						2
!H298 =-134.112+/-0.18 kJ/mol [ATcT(BURCAT)]										
-1.92821685E+04	-1.62616720E+01	1.69329154E+00	1.90167702E-02	-8.25176697E-06						3
!S298 =63.76 cal/mol/K										
-6.06113827E-09	4.65236978E-12	-1.73882411E+04	1.71839655E+01							4 !
C5H5	HR 6/01BLYP00C	5H	5	0	G	300.000	5000.000	1403.000		1
1.26805871E+01	1.27575785E-02	-4.34788920E-06	6.73442111E-10	-3.90092992E-14						2
2.55507801E+04	-4.67103980E+01	-3.35979212E+00	5.80041481E-02	-5.41839461E-05						3
2.56964859E-08	-4.80036435E-12	3.03384665E+04	3.66689604E+01							4
1-C5H5	BurcatC	5H	5	0	OG	300.000	5000.000	1402.000	01	

1.38816308E+01	1.14454546E-02	-3.83729159E-06	5.88208430E-10	-3.38379570E-14	2				
4.27127349E+04	-4.87035050E+01	-8.60045246E-01	5.18320271E-02	-4.67951024E-05	3				
2.14122502E-08	-3.87182913E-12	4.71932361E+04	2.82849534E+01		4				
H2C4O	120189H	2C	4O	1	G	300.000	4000.000	1000.000	1
1.02688800E+01	4.89616400E-03	-4.88508100E-07	-2.70856600E-10	5.10701300E-14	2				
2.34690300E+04	-2.81598500E+01	4.81097100E+00	1.31399900E-02	9.86507300E-07	3				
-6.12072000E-09	1.64000300E-12	2.54580300E+04	2.11342400E+00		4				
C5H6	HR11/99BLYP00C	5H	6	0	G	300.000	5000.000	1402.000	1
1.26575005E+01	1.53301203E-02	-5.23821364E-06	8.12867095E-10	-4.71504821E-14	2				
1.03083446E+04	-4.75386061E+01	-4.78259036E+00	6.09873033E-02	-5.17363931E-05	3				
2.25173536E-08	-3.92621113E-12	1.58382836E+04	4.43226201E+01		4				
CH2CHCH2CCH	C	5H	6		G	300.000	5000.000	1000.000	1
2.27091750E+01	-3.00201330E-03	3.55710540E-06	-9.23306040E-10	7.65447070E-14	2				
2.29371430E+04	-9.59871140E+01	3.25148510E+00	3.10524290E-02	-1.09708150E-05	3				
-1.24545210E-09	4.37795310E-13	3.02185390E+04	1.16484310E+01		4				
CH2CHCHCCH2	C	5H	6		G	300.000	5000.000	1000.000	1
1.16185120E+01	1.61550680E-02	-5.49912650E-06	8.78380530E-10	-5.41899260E-14	2				
2.53440310E+04	-3.52899400E+01	1.21979650E-01	4.73406170E-02	-3.22280940E-05	3				
7.08673830E-09	7.66264600E-13	2.84412680E+04	2.40296630E+01		4				
C6H2	P 1/93C	6H	2	0	OG	300.000	3000.000		1
0.13226281E+02	0.73904302E-02	-0.22715381E-05	0.25875217E-09	-0.55356741E-14	2				
0.80565258E+05	-0.41201176E+02	-0.15932624E+01	0.80530145E-01	-0.14800649E-03	3				
0.13300031E-06	-0.45332313E-10	0.83273227E+05	0.27980873E+02		4				
C6H3	H6W/94C	6H	3	0	OG	300.000	3000.000		1
0.58188343E+01	0.27933408E-01	-0.17825427E-04	0.53702536E-08	-0.61707627E-12	2				
0.85188250E+05	-0.92147827E+00	0.11790619E+01	0.55547360E-01	-0.73076168E-04	3				
0.52076736E-07	-0.15046964E-10	0.85647312E+05	0.19179199E+02		4				
l-C6H4	H6W/94C	6H	4	0	OG	300.000	3000.000		1
0.12715182E+02	0.13839662E-01	-0.43765440E-05	0.31541636E-09	0.46619026E-13	2				
0.57031148E+05	-0.39464600E+02	0.29590225E+00	0.58053318E-01	-0.67766756E-04	3				
0.43376762E-07	-0.11418864E-10	0.60001371E+05	0.22318970E+02		4				
c-C6H4	H6W/94C	6H	4	0	OG	300.000	3000.000		1
0.13849209E+02	0.78807920E-02	0.18243836E-05	-0.21169166E-08	0.37459977E-12	2				
0.47446340E+05	-0.50404953E+02	-0.30991268E+01	0.54030564E-01	-0.40839004E-04	3				
0.10738837E-07	0.98078490E-12	0.52205711E+05	0.37415207E+02		4				
n-C6H5	H6W/94C	6H	5	0	OG	300.000	3000.000		1
0.16070068E+02	0.81899539E-02	0.17325165E-05	-0.20624185E-08	0.36292345E-12	2				
0.64616867E+05	-0.56163742E+02	-0.61135769E+00	0.65082610E-01	-0.78262397E-04	3				
0.53030828E-07	-0.14946683E-10	0.68805375E+05	0.27635468E+02		4				
i-C6H5	H6W/94C	6H	5	0	OG	300.000	3000.000		1
0.22501663E+02	-0.81009977E-02	0.15955695E-04	-0.72310371E-08	0.10310424E-11	2				
0.58473410E+05	-0.91224777E+02	-0.78585434E+00	0.60221825E-01	-0.62890264E-04	3				
0.36310730E-07	-0.87000259E-11	0.64942270E+05	0.28658905E+02		4				
CH3ONO2	103190C	1H	3N	1O	3G	0300.00	4000.00	1500.00	1
0.01436189E+03	0.04112243E-01	-0.05113052E-05	-0.01496436E-08	0.03012156E-12	2				
-0.01972440E+06	-0.05131842E+03	0.07803354E+01	0.03454204E+00	-0.02822328E-03	3				
0.01232324E-06	-0.02302164E-10	-0.01465346E+06	0.02245752E+03		4				
A1	H6W/94C	6H	5	0	OG	300.000	3000.000		1
0.14493439E+02	0.75712688E-02	0.37894542E-05	-0.30769500E-08	0.51347820E-12	2				
0.33189977E+05	-0.54288940E+02	-0.49076147E+01	0.59790771E-01	-0.45639827E-04	3				
0.14964993E-07	-0.91767826E-12	0.38733410E+05	0.46567780E+02		4				
l-C6H6	H6W/94C	6H	6	0	OG	300.000	3000.000		1
0.17584442E+02	0.64486600E-02	0.48933980E-05	-0.34696221E-08	0.56150749E-12	2				
0.34111988E+05	-0.66017838E+02	-0.10170622E+01	0.61794821E-01	-0.59461061E-04	3				
0.31873491E-07	-0.71717693E-11	0.39202707E+05	0.29460373E+02		4				
C4H5C2H	OC	6H	6	0	OG	200.000	5000.000	1100.00	0 1
0.13903605E+02	0.17453182E-01	-0.63026581E-05	0.10316520E-08	-0.63440931E-13	2				
0.35975470E+05	-0.47671401E+02	-0.23220260E+00	0.54092928E-01	-0.36134322E-04	3				
0.69104632E-08	0.13734168E-11	0.39978520E+05	0.25932864E+02		4				

A	H6W/94C	6H	6	0	OG	300.000	3000.000		1
	0.17246994E+02	0.38420164E-02	0.82776232E-05	-0.48961120E-08	0.76064545E-12				2
	0.26646055E+04	-0.71945175E+02	-0.48998680E+01	0.59806932E-01	-0.36710087E-04				3
	0.32740399E-08	0.37600886E-11	0.91824570E+04	0.44095642E+02					4
FC6H6	T03/97C	6H	6	0	G	200.000	6000.000	1000.0	1
	1.19233607E+01	1.98993861E-02	-7.21223888E-06	1.17141499E-09	-7.04278845E-14				2
	2.27199368E+04	-4.13488172E+01	1.25853571E-01	3.04056534E-02	4.01806332E-05				3
	-8.27651456E-08	3.77645005E-11	2.68838408E+04	2.44628931E+01	2.84820633E+04				4
CYC6H7	BURCAT T 6/93C	6H	7	0	G	200.000	6000.000	1000.	1
	0.12801758E+02	0.21924749E-01	-0.79713001E-05	0.12972935E-08	-0.78100416E-13				2
	0.17889539E+05	-0.45804341E+02	-0.10303140E+00	0.34393354E-01	0.39788466E-04				3
	-0.85116612E-07	0.39012224E-10	0.22425515E+05	0.26022350E+02	0.24125213E+05				4
n-C6H7	H6W/94C	6H	7	0	OG	300.000	3000.000		1
	0.22577469E+02	-0.30737517E-02	0.14225234E-04	-0.69880848E-08	0.10232874E-11				2
	0.41228980E+05	-0.91568619E+02	0.13248032E+00	0.57103366E-01	-0.43712644E-04				3
	0.15538603E-07	-0.12976356E-11	0.47730512E+05	0.25339081E+02					4
i-C6H7	H6W/94C	6H	7	0	OG	300.000	3000.000		1
	0.20481506E+02	0.79439697E-03	0.11450761E-04	-0.60991177E-08	0.91756724E-12				2
	0.37728426E+05	-0.81812073E+02	-0.17099094E+01	0.62486034E-01	-0.54290707E-04				3
	0.26959682E-07	-0.58999090E-11	0.44086621E+05	0.33344772E+02					4
C6H8	H6W/94C	6H	8	0	OG	300.000	3000.000		1
	0.28481979E+02	-0.15702948E-01	0.26771697E-04	-0.11780109E-07	0.16573427E-11				2
	0.93346445E+04	-0.12500226E+03	0.15850439E+01	0.40215142E-01	0.78439543E-05				3
	-0.38761325E-07	0.18545207E-10	0.17949613E+05	0.19112625E+02					4
CY13C6H8	BURCAT T 2/90C	6H	8	0	G	200.000	6000.000	1000.	1
	0.11779870E+02	0.25519980E-01	-0.92666947E-05	0.15068122E-08	-0.90658701E-13				2
	0.65486686E+04	-0.41618805E+02	0.17265319E+01	0.14887612E-01	0.94809230E-04				3
	-0.14083394E-06	0.58859873E-10	0.11021297E+05	0.19130886E+02	0.12784878E+05				4
C5H4O	10/00BURCBLYP C	5H	40	1	G	300.000	5000.000	1402.000	1
	1.37907739E+01	1.19738147E-02	-4.11436106E-06	6.40954643E-10	-3.72821366E-14				2
	2.74553951E+02	-5.06296371E+01	-3.01174376E+00	5.82012965E-02	-5.36527132E-05				3
	2.48757306E-08	-4.54630764E-12	5.38127213E+03	3.70844611E+01					4
C5H5O	ZHONG/BOZ1998 C	5H	50	1	G	300.000	5000.000	1395.000	1
	1.49072105E+01	1.36369619E-02	-4.70762207E-06	7.36028654E-10	-4.29314124E-14				2
	1.43724130E+04	-5.69296345E+01	-4.14628450E+00	6.23584874E-02	-5.28374678E-05				3
	2.24628793E-08	-3.80136191E-12	2.04992627E+04	4.37921058E+01					4
C5H4OH	ALZUETA 2000 C	5H	50	1	G	300.000	5000.000	1417.000	1
	1.54616992E+01	1.21543874E-02	-3.97713729E-06	5.99530783E-10	-3.40841280E-14				2
	1.18008962E+03	-5.80092304E+01	-3.36507049E+00	6.65211552E-02	-6.40907012E-05				3
	3.04663074E-08	-5.61147666E-12	6.55733089E+03	3.92124189E+01					4
C6H9	BURCAT T 2/92C	6H	9	0	G	298.150	3000.000	1000.	1
	0.21786938E+02	0.11894129E-01	-0.21209124E-05	0.00000000E+00	0.00000000E+00				2
	0.20013752E+05	-0.89218982E+02	0.20594889E+01	0.46753513E-01	-0.186444505E-04				3
	0.00000000E+00	0.00000000E+00	0.27665639E+05	0.20293525E+02	0.30193000E+05				4
CYC6H9	BURCAT T 2/92C	6H	9	0	G	298.150	3000.000	1000.	1
	0.26295828E+02	0.86828857E-02	-0.15770376E-05	0.00000000E+00	0.00000000E+00				2
	0.20863563E+04	-0.12573825E+03	-0.35714300E+01	0.61696043E-01	-0.26928803E-04				3
	0.00000000E+00	0.00000000E+00	0.13657039E+05	0.39986250E+02	0.15096500E+05				4
CYC6H10	BURCAT T 2/90C	6H	10	0	G	200.000	6000.000	1000.	1
	0.11773904E+02	0.30947360E-01	-0.11234330E-04	0.18262494E-08	-0.10985119E-12				2
	-0.72028376E+04	-0.42658688E+02	0.23662378E+01	0.10681712E-01	0.11822112E-03				3
	-0.16567854E-06	0.67612802E-10	-0.24824973E+04	0.16769357E+02	-0.55324968E+03				4
C6H10	BURCAT T 2/92C	6H	10	0	G	298.150	3000.000	1000.	1
	0.23903966E+02	0.12046216E-01	-0.19588306E-05	0.00000000E+00	0.00000000E+00				2
	-0.43733937E+04	-0.10376594E+03	-0.96299362E+00	0.60880377E-01	-0.28062414E-04				3
	0.00000000E+00	0.00000000E+00	0.45722054E+04	0.32010145E+02	0.67431033E+04				4
CYC6H11	BURCAT 12/98 C	6H	11	0	G	298.150	5000.000	1000.	1
	1.28647309E+01	3.52600147E-02	-1.39450525E-05	2.51808759E-09	-1.70899213E-13				2
	6.15531214E+02	-4.88786148E+01	-3.76580647E+00	5.88838077E-02	1.22955158E-07				3



-3.30729397E-08	1.42142299E-11	6.76556720E+03	4.36106643E+01	8.20243165E+03	4						
C6H11-12	C	6H	110	00	OG	300.00	5000.00	1000.00	1		
0.15903220E+02	0.23659610E-01	-0.67095560E-05	0.94231160E-09	-0.53289920E-13	2						
0.15837710E+05	-0.54096690E+02	0.14245270E+00	0.61529150E-01	-0.39403020E-04	3						
0.13625820E-07	-0.21393720E-11	0.20807860E+05	0.29545670E+02		4						
C6H11-15	C	6H	110	00	OG	300.00	5000.00	1000.00	1		
0.16511810E+02	0.23103710E-01	-0.65196350E-05	0.91279680E-09	-0.51533620E-13	2						
0.11020680E+05	-0.57226020E+02	-0.65185990E+00	0.69069390E-01	-0.55091450E-04	3						
0.26728390E-07	-0.60813550E-11	0.16144180E+05	0.32558910E+02		4						
C6H11-13	C	6H	110	00	OG	300.00	5000.00	1000.00	1		
0.15939530E+02	0.24454600E-01	-0.71328250E-05	0.10237720E-08	-0.58843450E-13	2						
0.27317560E+04	-0.56236800E+02	-0.18343630E+00	0.62924820E-01	-0.39494870E-04	3						
0.12901540E-07	-0.19206490E-11	0.78098810E+04	0.29353710E+02		4						
C6H11-14	C	6H	110	00	OG	300.00	5000.00	1000.00	1		
1.32786E+01	2.79515E-02	-8.47472E-06	1.23752E-09	-7.12640E-14	2						
1.22232E+04	-3.88114E+01	-1.06617E+00	7.16134E-02	-5.85771E-05	3						
2.71262E-08	-5.15786E-12	1.59829E+04	3.43102E+01		4						
C6H11	BURCAT	2/92	C	6H	11	0	G	298.150	3000.000	1000.	1
0.24938654E+02	0.13258801E-01	-0.23302223E-05	0.00000000E+00	0.00000000E+00	2						
0.51145941E+04	-0.10690338E+03	0.63802451E+00	0.56209452E-01	-0.23047424E-04	3						
0.00000000E+00	0.00000000E+00	0.14624427E+05	0.28133981E+02	0.17109367E+05	4						
CYC6H12	BURCAT	2/90	C	6H	12	0	G	200.000	5000.000	1000.	1
0.10209166E+02	0.41894173E-01	-0.17234045E-04	0.32239024E-08	-0.22540929E-12	2						
-0.21742125E+05	-0.38990666E+02	0.40402264E+01	-0.61827997E-02	0.17662080E-03	3						
-0.22300383E-06	0.86393385E-10	-0.16919808E+05	0.85269500E+01	-0.14829497E+05	4						
hexene1	BURCAT	T	6/93C	6H	12	0	G	200.000	6000.000	1000.	1
1.60616093E+01	2.75650562E-02	-9.32973368E-06	1.49349013E-09	-8.98810268E-14	2						
-1.28042951E+04	-5.69925586E+01	7.31509054E+00	3.71150329E-03	1.27250318E-04	3						
-1.71556964E-07	6.89805935E-11	-8.20916507E+03	-5.94354365E-01	-5.04539654E+03	4						
hex1yl	BURCAT	T	6/93C	6H	13	0	G	200.000	6000.000	1000.	1
1.39163141E+01	3.48510892E-02	-1.26898935E-05	2.07144196E-09	-1.24756674E-13	2						
-4.01785625E+03	-4.33071846E+01	8.76348959E+00	2.16244832E-03	1.31674686E-04	3						
-1.73828247E-07	6.92518175E-11	-5.42630596E+02	-5.91729689E+00	3.01881891E+03	4						
hex2yl	BURCAT	T	6/93C	6H	13	0	G	200.000	6000.000	1000.	1
1.41986473E+01	3.46787125E-02	-1.25515738E-05	2.02767674E-09	-1.21224274E-13	2						
-3.68102477E+03	-4.23012097E+01	7.58145549E+00	1.89615514E-02	8.16571755E-05	3						
-1.18091545E-07	4.81236008E-11	-2.27328454E+02	5.28216352E-05	3.38664816E+03	4						
hex3yl	C	6H	130	00	OG	300.00	5000.00	1000.00	1		
0.18621920E+02	0.24911520E-01	-0.68681720E-05	0.94495470E-09	-0.52683770E-13	2						
-0.51170230E+04	-0.69174640E+02	-0.17466440E+01	0.81867340E-01	-0.74301960E-04	3						
0.43594630E-07	-0.11843740E-10	0.94735310E+03	0.37018690E+02		4						
cyCHOCHCHNCH	NL0512H	4C	4N	10	1g	200.00	5000.00	1000.00	1		
1.03705295E+01	1.68075131E-02	-6.61865393E-06	1.19161020E-09	-8.05474290E-14	2						
9.67068671E+03	-3.13371480E+01	3.67481839E-01	2.72420856E-02	2.73087786E-05	3						
-6.12972824E-08	2.80352020E-11	1.31318307E+04	2.41467476E+01		4						
cyOCHCHNCH2	NL0512H	5C	4N	10	1g	200.00	5000.00	1000.00	1		
9.76552055E+00	2.02657471E-02	-7.98168483E-06	1.43674533E-09	-9.70897569E-14	2						
2.84807107E+02	-2.85557941E+01	1.16612804E+00	2.16650486E-02	4.45062449E-05	3						
-7.69829934E-08	3.30130453E-11	3.65457986E+03	2.10458988E+01		4						
cyNCH2CH2OCHCH	NL0512H	6C	4N	10	1g	200.00	5000.00	1000.00	1		
9.97152024E+00	2.28761402E-02	-8.99290464E-06	1.61649943E-09	-1.09121631E-13	2						
1.60990018E+03	-3.00221894E+01	1.66539922E+00	1.95697562E-02	5.65836534E-05	3						
-9.03888845E-08	3.79072249E-11	5.08978152E+03	1.90149637E+01		4						
cyCHCH2OCH2CHN	NL0512H	6C	4N	10	1g	200.00	5000.00	1000.00	1		
1.04023579E+01	2.25422296E-02	-8.88080545E-06	1.59862300E-09	-1.08020089E-13	2						
5.31436341E+03	-3.05589738E+01	1.98370077E+00	2.06090929E-02	5.29123058E-05	3						
-8.64542761E-08	3.64783370E-11	8.77929416E+03	1.88141517E+01		4						
CH2CH2NCHCHO	NL0512H	6C	4N	10	1g	200.00	5000.00	1000.00	1		
1.00065027E+01	2.12590310E-02	-8.31100940E-06	1.48775653E-09	-1.00118748E-13	2						

1.21780377E+04	-1.93320698E+01	4.33376118E+00	1.86085860E-02	3.55081766E-05	3					
-5.83047758E-08	2.41648557E-11	1.46495593E+04	1.44416372E+01		4					
CH2OCHCHNCH2	NL0512H	6C	4N	1O	1g	200.00	5000.00	1000.00	1	
1.03605553E+01	2.06456475E-02	-7.99918574E-06	1.42319844E-09	-9.53626274E-14	2					
1.96067184E+04	-2.13482013E+01	3.72756375E+00	2.38804018E-02	2.39881369E-05	3					
-4.83222462E-08	2.10324917E-11	2.21567964E+04	1.65262174E+01		4					
CH2CHOCH2CHNH	NL0512H	7C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.43983097E+00	2.43022381E-02	-9.41764568E-06	1.67592431E-09	-1.12319107E-13	2					
-4.75041182E+03	-1.64775948E+01	3.72389545E+00	1.38728098E-02	6.19611809E-05	3					
-9.06265414E-08	3.69314827E-11	-1.96325859E+03	1.92328019E+01		4					
OCHCH2NHCHCH2	NL0512H	7C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.51050292E+00	2.42544440E-02	-9.40389507E-06	1.67405636E-09	-1.12220969E-13	2					
-1.05680496E+04	-1.66197033E+01	3.42017416E+00	1.87512420E-02	4.73591100E-05	3					
-7.43155583E-08	3.06779216E-11	-7.82478385E+03	2.01847716E+01		4					
cyOCHCHNHCH2CH2	NL0512H	7C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.96793833E+00	2.53402066E-02	-9.85898966E-06	1.75969237E-09	-1.18197555E-13	2					
-1.16516760E+04	-3.03807434E+01	1.21602259E+00	2.35404585E-02	5.39979642E-05	3					
-8.96195781E-08	3.79292297E-11	-8.06933954E+03	2.08719874E+01		4					
cyOCH2CHNCH2CH2	NL0512H	7C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.33224514E+00	2.64207014E-02	-1.04038145E-05	1.87193808E-09	-1.26439658E-13	2					
-1.23029574E+04	-2.70916446E+01	2.49837851E+00	1.28784770E-02	7.73276547E-05	3					
-1.10046453E-07	4.44047025E-11	-8.88976270E+03	1.59397184E+01		4					
NHCH2CH2OCHCH2	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.68514907E+00	2.63704105E-02	-1.02072196E-05	1.81470963E-09	-1.21528697E-13	2					
7.77400194E+03	-1.57389988E+01	4.66014797E+00	9.74899317E-03	7.73358783E-05	3					
-1.07446350E-07	4.32187645E-11	1.05573351E+04	1.73860355E+01		4					
CH2CH2NHCH2CHO	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.63125770E+00	2.65728138E-02	-1.03260369E-05	1.84083887E-09	-1.23517420E-13	2					
1.11522710E+03	-1.56168502E+01	4.58706944E+00	1.29143845E-02	6.58248031E-05	3					
-9.30880660E-08	3.73253324E-11	3.82891071E+03	1.70693852E+01		4					
OCH2CH2NHCHCH2	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
1.02790961E+01	2.62562858E-02	-1.01579159E-05	1.80548429E-09	-1.20895234E-13	2					
7.62616153E+03	-2.11386698E+01	3.01769742E+00	2.23810637E-02	5.00400721E-05	3					
-8.16538191E-08	3.42477167E-11	1.07319447E+04	2.20035773E+01		4					
CH2CH2OCH2CHNH	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.69346283E+00	2.64566136E-02	-1.02654930E-05	1.82814406E-09	-1.22574898E-13	2					
5.79069027E+03	-1.59166130E+01	5.00481411E+00	1.02546298E-02	7.21573999E-05	3					
-9.95032423E-08	3.96464100E-11	8.46664878E+03	1.52754770E+01		4					
CH2OCH2CH2NCH2	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.19762303E+00	2.70086271E-02	-1.05012971E-05	1.87264019E-09	-1.25671746E-13	2					
7.15236012E+03	-1.35395043E+01	4.90847630E+00	9.21835654E-03	7.37451907E-05	3					
-9.99089152E-08	3.94556163E-11	9.76473253E+03	1.57658288E+01		4					
cyOrthoMorphyl	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
1.00887739E+01	2.82096961E-02	-1.10180966E-05	1.97161497E-09	-1.32664086E-13	2					
-1.23231840E+03	-3.15337889E+01	2.05875485E+00	1.90415609E-02	7.10034306E-05	3					
-1.06937795E-07	4.39210066E-11	2.43624755E+03	1.73572200E+01		4					
cyMetaMorphyl	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
1.01394481E+01	2.81012751E-02	-1.09599640E-05	1.95928556E-09	-1.31743233E-13	2					
-3.46128688E+03	-3.17383673E+01	1.86240736E+00	2.14671652E-02	6.42559456E-05	3					
-9.97807063E-08	4.12699685E-11	1.94265168E+02	1.80014282E+01		4					
cyParaMorphyl	NL0512H	8C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.81857071E+00	2.87092590E-02	-1.12748460E-05	2.02488549E-09	-1.36588144E-13	2					
-2.55902949E+03	-3.03711366E+01	2.49291590E+00	1.36616039E-02	8.52467307E-05	3					
-1.21418965E-07	4.91270481E-11	1.10200123E+03	1.58247257E+01		4					
cyMorph	NL0512H	9C	4N	1O	1g	200.00	5000.00	1000.00	1	
9.31663792E+00	3.18026464E-02	-1.24290335E-05	2.22486836E-09	-1.49735740E-13	2					
-2.42647198E+04	-2.86792745E+01	2.42819448E+00	1.18580482E-02	9.64514708E-05	3					
-1.33245554E-07	5.32368692E-11	-2.05315873E+04	1.61901809E+01		4					
C6H5CH3	5/19/93	thermC	7H	8	0	0g	300.000	5000.000	1389.000	11

1.63091542e+01	2.25331612e-02	-7.84281827e-06	1.23200630e-09	-7.20675043e-14	2	
-2.75804095e+03	-6.66759774e+01	-4.08982289e+00	6.86477374e-02	-4.74716566e-05	3	
1.67001205e-08	-2.39578007e-12	4.49937542e+03	4.34582591e+01		4	
C6H5CH2	5/11/93 thermC	7H 7 0 0g	300.000	5000.000	1380.000	11
1.74066429e+01	1.94934914e-02	-6.89552346e-06	1.09498206e-09	-6.45370306e-14		2
1.52488939e+04	-7.16678643e+01	-3.13104309e+00	6.45512922e-02	-4.39082794e-05		3
1.46756825e-08	-1.95214937e-12	2.26869723e+04	3.96945254e+01			4
C6H4CH3	P 1/93C	7H 7 0 0G	300.000	2500.000		1
0.11615498e+02	0.27431838E-01	-0.10899345E-04	0.18641830E-08	-0.10191607E-12		2
0.31209334e+05	-0.38994637E+02	-0.31415942E+01	0.56723077E-01	-0.86885111E-05		3
-0.34249616e-07	0.19266902E-10	0.35738547E+05	0.39742840E+02			4
C6H5CCH	H6W/94C	8H 6 0 0G	300.000	3000.000		1
0.24090759e+02	0.78232400E-03	0.11453964E-04	-0.61620504E-08	0.93346685E-12		2
0.27429445e+05	-0.10499631E+03	-0.52645016E+01	0.84511042E-01	-0.76597848E-04		3
0.33216978e-07	-0.47673063E-11	0.35566242E+05	0.46378815E+02			4
C6H4CCH	HW /94C	8H 5 0 0G	300.000	3000.000		1
0.28686157e+02	-0.13869863E-01	0.22721186E-04	-0.99882271E-08	0.14085851E-11		2
0.56047309e+05	-0.12750334E+03	-0.29324217E+01	0.66043675E-01	-0.39500475E-04		3
-0.31830381e-08	0.85300387E-11	0.65324043E+05	0.38058685E+02			4
C6H5CHCH	HW /94C	8H 7 0 0G	300.000	3000.000		1
0.30433151e+02	-0.13965182E-01	0.25416972E-04	-0.11354174E-07	0.16092050E-11		2
0.35738719e+05	-0.13416492E+03	-0.44899931E+01	0.78750789E-01	-0.62376959E-04		3
0.21952140e-07	-0.16960955E-11	0.45902949E+05	0.47980759E+02			4
C6H5CHCH2	T12/94C	8H 8 0 0G	298.150	5000.000		1
0.16139277e+02	0.24210847E-01	-0.72678359E-05	0.11392276E-08	-0.72984881E-13		2
0.10249251e+05	-0.61169437E+02	-0.10717708E+02	0.12666725E+00	-0.17762493E-03		3
0.14344049e-06	-0.47616577E-10	0.16597133E+05	0.71526331E+02	0.17723291E+05		4
C6H5CO	2/25/94 thermC	7H 50 1 0g	300.000	5000.000	1382.000	11
1.77196103e+01	1.59990428e-02	-5.54532150e-06	8.69582681e-10	-5.08335220e-14		2
4.57408086e+03	-6.82553109e+01	-1.93001550e+00	6.18799970e-02	-4.60916515e-05		3
1.70133701e-08	-2.49869948e-12	1.13352170e+04	3.71779131e+01			4
C6H5CH2CH2	A11/04C	8H 9 0 0G	200.000	6000.000		1
1.61326962e+01	2.82904273E-02	-1.01801876E-05	1.64176637E-09	-9.81375329E-14		2
2.08791061e+04	-6.00115413E+01	7.33299107E-01	4.59053158E-02	3.78257231E-05		3
-9.12367411e-08	4.25589678E-11	2.61572945E+04	2.50411074E+01	2.85902549E+04		4
C6H5CHO	2/25/94 thermC	7H 60 1 0g	300.000	5000.000	1382.000	11
1.75038056e+01	1.87911370e-02	-6.51897523e-06	1.02244104e-09	-5.97629759e-14		2
-1.31835944e+04	-6.88975598e+01	-2.70517666e+00	6.46821582e-02	-4.57286415e-05		3
1.60322213e-08	-2.23734122e-12	-6.07344750e+03	4.00414090e+01			4
C6H5CH2CH3	A 6/83C	8H 10 0 0G	300.	3000.	1000.00	1
0.3878978E 01	0.5810059E-01	-0.3196380E-04	0.8448993E-08	-0.8694825E-12		2
-0.5024922E 03	0.3837099E 01	-0.7266845E 01	0.1003089E 00	-0.9651715E-04		3
0.5565908E-07	-0.1453370E-10	0.1987290E 04	0.5857746E 02	0.3529492E+04		4
OC6H4CH3	EST/BUR P 1/93C	7H 70 1 0G	300.000	2500.000		1
0.22609371e+02	0.75646150E-02	0.65960894E-05	-0.47150865E-08	0.80409063E-12		2
-0.82025244e+04	-0.97292511E+02	-0.28855777E+00	0.48003536E-01	0.18032993E-04		3
-0.61741488e-07	0.28852587E-10	-0.68945581E+03	0.26720068E+02			4
C6H5CH2O	4/14/94 thermC	7H 70 1 0g	300.000	5000.000	1392.000	11
1.78843033e+01	2.09011735e-02	-7.21832713e-06	1.12839851e-09	-6.57955260e-14		2
4.93182818e+03	-7.01304667e+01	-4.77736690e+00	7.51049308e-02	-5.68532831e-05		3
2.18290029e-08	-3.38134298e-12	1.26234438e+04	5.10429366e+01			4
C6H5OCH2	1/ 1/80 therm C	7H 70 1 0g	300.000	5000.000	1402.000	21
2.21257590e+01	1.63629505e-02	-5.55282773e-06	8.58992521e-10	-4.97570425e-14		2
2.27948250e+03	-9.52304329e+01	-5.69072376e+00	9.13768507e-02	-8.35104568e-05		3
3.76414300e-08	-6.64543995e-12	1.07829618e+04	5.03483382e+01			4
C6H4O2	O=C6H4=O T10/97C	6H 40 200 0G	200.000	6000.000	1000.	1
1.43886174e+01	1.81624210E-02	-6.69934678E-06	1.10097880E-09	-6.67372266E-14		2
-2.12444054e+04	-5.02572901E+01	3.79867882E+00	2.51676569E-02	3.79846917E-05		3
-7.06777516e-08	3.06126573E-11	-1.72429606E+04	9.80455363E+00	-1.478138819-04		4

C6H5OCH3	1/ 1/80 thermC	7H	80	1	0g	300.000	5000.000	1393.000	21
	2.07553992e+01	2.02558450e-02	-6.93113185e-06			1.07748801e-09	-6.26048146e-14		2
	-1.87342907e+04	-8.82873516e+01	-5.18552392e+00			8.57486409e-02	-7.07576026e-05		3
	2.95162383e-08	-4.92530544e-12	-1.03019987e+04			4.91527969e+01			4
HOC6H4CH3	AVG CRESOL6/87C	7H	80	1	0G	200.000	6000.000	1000.00	1
	0.15932987e+02	0.27011160E-01	-0.99448722E-05			0.16296689E-08	-0.98513298E-13		2
	-0.23592065E+05	-0.59732841E+02	0.42258267E+00			0.45551636E-01	0.32012513E-04		3
	-0.81121959E-07	0.37665658E-10	-0.18202621E+05			0.26032903E+02	-0.15911701E+05		4
C6H5CH2OH	4/14/94 thermC	7H	80	1	0g	300.000	5000.000	1393.000	21
	1.83336336e+01	2.24113846e-02	-7.68817710e-06			1.19642445e-09	-6.95416019e-14		2
	-2.13970553e+04	-7.22444987e+01	-4.04500885e+00			7.57965615e-02	-5.64777639e-05		3
	2.15225418e-08	-3.32436586e-12	-1.37783634e+04			4.74803479e+01			4
C6H5C6H5	L12/84C	12H	10	0	0G	300.000	5000.000		1
Burcat 2007									
	0.24289017E 02	0.34006648E-01	-0.11722408E-04			0.17729298E-08	-0.96812532E-13		2
	0.10287000E 05	-0.10802374E 03	-0.40739527E 01			0.86973310E-01	-0.42353613E-05		3
	-0.64564460E-07	0.34150169E-10	0.19405965E 05			0.44741348E 02	0.21905340E 05		4
C7H6f	C	7H	6			300.000	5000.000	1000.000	1
	8.63047626E+00	3.28146569E-02	-1.67463533E-05			4.12422205E-09	-3.97875311E-13		2
	3.78424508E+04	-2.14598163E+01	-4.83808621E+00			7.96144479E-02	-7.75198421E-05		3
	3.84238455E-08	-7.26609427E-12	4.09670495E+04			4.54480924E+01			4
VALS0	C	10H	10		G	300.000	5000.000	1000.000	1
	1.96542923E+01	3.33886286E-02	-1.20413130E-05			1.94963753E-09	-1.16973259E-13		2
	2.53473433E+04	-8.08051980E+01	1.92659259E+00			2.78897531E-02	1.32941165E-04		3
	-2.10257150E-07	9.03339117E-11	3.24585081E+04			2.27839249E+01			4
VALS4	C	10H	9		G	300.000	5000.000	1000.000	1
	1.97227364E+01	3.05121625E-02	-1.10537483E-05			1.79050874E-09	-1.07387763E-13		2
	4.42281159E+04	-7.53736816E+01	2.29508183E+00			4.52323197E-02	5.98076375E-05		3
	-1.21133405E-07	5.46626377E-11	5.04522033E+04			2.21435730E+01			4
VALS3	C	10H	9		G	300.000	5000.000	1000.000	1
	1.97227364E+01	3.05121625E-02	-1.10537483E-05			1.79050874E-09	-1.07387763E-13		2
	4.42281159E+04	-7.53736816E+01	2.29508183E+00			4.52323197E-02	5.98076375E-05		3
	-1.21133405E-07	5.46626377E-11	5.04522033E+04			2.21435730E+01			4
VALS2	C	10H	9		G	300.000	5000.000	1000.000	1
	1.97227364E+01	3.05121625E-02	-1.10537483E-05			1.79050874E-09	-1.07387763E-13		2
	4.42281159E+04	-7.53736816E+01	2.29508183E+00			4.52323197E-02	5.98076375E-05		3
	-1.21133405E-07	5.46626377E-11	5.04522033E+04			2.21435730E+01			4
VALS1	C	10H	9		G	300.000	5000.000	1000.000	1
	1.95200250E+01	3.16330790E-02	-1.06661220E-05			1.69368430E-09	-1.04134560E-13		2
	4.29767700E+04	-7.74975890E+01	-6.56485750E+00			1.06748180E-01	-8.40770010E-05		3
	2.85706730E-08	-2.61119970E-12	4.97565620E+04			5.59485050E+01			4
C10H9b	C	10H	9		G	300.000	5000.000	1000.000	1
	1.97227364E+01	3.05121625E-02	-1.10537483E-05			1.79050874E-09	-1.07387763E-13		2
	4.42281159E+04	-7.53736816E+01	2.29508183E+00			4.52323197E-02	5.98076375E-05		3
	-1.21133405E-07	5.46626377E-11	5.04522033E+04			2.21435730E+01			4
C10H9c	C	10H	9		G	300.000	5000.000	1000.000	1
	2.65244750E+01	2.37225740E-02	-7.49371430E-06			1.13649020E-09	-6.77165710E-14		2
	3.15103200E+04	-1.45784070E+02	-2.17385960E+00			1.03760940E-01	-7.89928160E-05		3
	2.02245010E-08	9.91735660E-13	3.90386090E+04			1.54065250E+00			4
C10H8	C	10H	8		G	300.000	5000.000	1000.000	1
	1.86129884E+01	3.04494175E-02	-1.11224825E-05			1.81615474E-09	-1.09601281E-13		2
	8.91578988E+03	-8.00230396E+01	-1.04919475E+00			4.62970781E-02	7.07591636E-05		3
	-1.38408111E-07	6.20475407E-11	1.59848987E+04			3.02121626E+01			4
C10H7	C	10H	7		G	300.000	5000.000	1000.000	1
	2.00959894E+01	2.63995288E-02	-9.54744190E-06			1.54881511E-09	-9.30556695E-14		2
	6.51277376E+04	-8.23946362E+01	-2.07613880E+00			7.07561989E-02	-2.27951149E-06		3
	-6.32032786E-08	3.52065658E-11	7.18269865E+04			3.55334903E+01			4
C10H7O-1	C	10H	7O	1	G	300.000	5000.000	1000.000	1
	2.55199785E+01	2.25375617E-02	-7.79622686E-06			1.22014387E-09	-7.12043903E-14		2

-9.13287721E+02-1.15169184E+02-7.45889821E+00	1.10408595E-01-9.86444941E-05	3
4.41246608E-08-7.80459565E-12 9.35231821E+03	5.79329757E+01	4
C10H7O-2	C 10H 7O 1 G 300.000 5000.000 1000.000	1
2.55976281E+01 2.24775925E-02-7.77612184E-06	1.21700823E-09-7.10201185E-14	2
9.06605861E+02-1.15554102E+02-7.30371611E+00	1.10120287E-01-9.82564465E-05	3
4.38428145E-08-7.73044601E-12 1.11390084E+04	5.71293774E+01	4
C10H7a	C 10H 7 G 300.000 5000.000 1000.000	1
2.32134837E+01 2.19245132E-02-7.57801031E-06	1.18526564E-09-6.91369406E-14	2
3.75456274E+04-1.03911378E+02-7.74269427E+00	1.04220941E-01-9.25076899E-05	3
4.12403544E-08-7.28199643E-12 4.72057155E+04	5.86484815E+01	4
C10H7*2	C 10H 7 G 300.000 5000.000 1000.000	1
2.32356550E+01 2.19168575E-02-7.57777612E-06	1.18547456E-09-6.91588767E-14	2
3.76662306E+04-1.04074200E+02-7.71898395E+00	1.04275854E-01-9.26741654E-05	3
4.13767346E-08-7.31737931E-12 4.73225871E+04	5.84596982E+01	4
C9H7	C 9H 7 G 300.000 5000.000 1000.000	1
1.85549761E+01 2.50350502E-02-9.14573755E-06	1.49348099E-09-9.01328268E-14	2
2.57211482E+04-7.63004782E+01-2.66986010E+00	6.21770959E-02 1.50674040E-05	3
-7.96461960E-08 4.09191931E-11 3.23869684E+04	3.78611069E+01	4
C9H8	C 9H 8 G 300.000 5000.000 1000.000	1
1.73186757E+01 2.89827586E-02-1.06050551E-05	1.73345448E-09-1.04679146E-13	2
1.11514275E+04-7.15553836E+01-6.81899560E-01	4.16587045E-02 7.07413209E-05	3
-1.34308856E-07 5.99158843E-11 1.77050360E+04	2.97813474E+01	4
A2CH3-1	C 11H 10 G 300.000 5000.000 1000.000	1
2.17939213E+01 3.60214098E-02-1.33228698E-05	2.19304403E-09-1.33071380E-13	2
3.16261439E+03-9.48675403E+01-1.03043715E+00	6.03358177E-02 5.45655719E-05	3
-1.22769251E-07 5.54507327E-11 1.13241014E+04	3.22970611E+01	4
A2CH2-1	C 11H 9 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
A2CH2-2	C 11H 9 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
A2CH2-1f*	C 11H 9 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
A2CH2-2f*	C 11H 9 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
A2CH2-2f	C 11H 8 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
VALC10H9	C 10H 9 G 300.000 5000.000 1000.000	1
1.97227364E+01 3.05121625E-02-1.10537483E-05	1.79050874E-09-1.07387763E-13	2
4.42281159E+04-7.53736816E+01 2.29508183E+00	4.52323197E-02 5.98076375E-05	3
-1.21133405E-07 5.46626377E-11 5.04522033E+04	2.21435730E+01	4
A2CH3-2	C 11H 10 G 300.000 5000.000 1000.000	1
2.17939213E+01 3.60214098E-02-1.33228698E-05	2.19304403E-09-1.33071380E-13	2
3.16261439E+03-9.48675403E+01-1.03043715E+00	6.03358177E-02 5.45655719E-05	3
-1.22769251E-07 5.54507327E-11 1.13241014E+04	3.22970611E+01	4
A2CH2-1f	C 11H 8 G 300.000 5000.000 1000.000	1
2.18977539E+01 3.26102636E-02-1.18401218E-05	1.92574628E-09-1.15903442E-13	2
2.24571098E+04-9.41050741E+01-2.53234304E+00	7.32920338E-02 2.02974707E-05	3
-9.36547823E-08 4.70753594E-11 3.02906705E+04	3.79638513E+01	4
C12H8	C 12H 8 G 300.000 5000.000 1000.000	1

```

2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13 2
3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05 3
-5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4
C12H9 HR 4/99 BLYP00C 12H 9 0 OG 300.000 5000.000 1394.000 11
2.85117985E+01 2.78635355E-02-9.77609837E-06 1.54399902E-09-9.06592229E-14 2
3.81667876E+04-1.31297837E+02-1.01510948E+01 1.32751910E-01-1.21966149E-04 3
5.68823204E-08-1.05361005E-11 5.02094552E+04 7.13031888E+01 4
C6H5C3H2 1/17/ 0 THERMC 9H 7 0 OG 300.000 5000.000 1383.000 11
2.05632118E+01 2.18474960E-02-7.69371038E-06 1.21810939E-09-7.16463859E-14 2
4.65470757E+04-8.26412428E+01-2.26779736E+00 7.34853337E-02-5.21100716E-05 3
1.85954603E-08-2.69498985E-12 5.46642559E+04 4.06118884E+01 4
N2O4 ATcT AN 2O 4 0 OG 200.00 6000.00 1000. 1
!BURCAT
1.15752932E+01 4.01615532E-03-1.57178022E-06 2.68273657E-10-1.66921538E-14 2
!H298 =10.785+/-0.17 kJ/mol [ATcT(BURCAT)]
-2.96184070E+03-3.19488531E+01 3.02002271E+00 2.95904359E-02-3.01342572E-05 3
!S298 =72.76 cal/mol/K
1.42360526E-08-2.44100411E-12-6.79967151E+02 1.18059714E+01 4 !
C6H5O HR 6/99 BLYP C 6H 5O 1 G 300.000 5000.000 1402.000 1
1.63197375E+01 1.49421635E-02-5.14462138E-06 8.02578740E-10-4.67303957E-14 2
-1.19712631E+03-6.52157169E+01-4.17772040E+00 6.95185958E-02-6.15479047E-05 3
2.74342242E-08-4.84615473E-12 5.19007431E+03 4.23910339E+01 4
C6H5OH HR 6/99 BLYP C 6H 6O 1 G 300.000 5000.000 1391.000 1
1.68693795E+01 1.70838426E-02-5.98946836E-06 9.45398420E-10-5.54859198E-14 2
-1.97294434E+04-6.87883562E+01-4.92900267E+00 7.76036830E-02-7.29208148E-05 3
3.51831137E-08-6.74079973E-12-1.29920911E+04 4.50935388E+01 4
C2H4OH T 4/83H 5C 2O 1 OG 300.000 5000. 1000. 1
0.75944014E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-13 2
-0.57727852E+04-0.13955572E+02 0.14019508E+01 0.21543175E-01-0.22326512E-05 3
-0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19148981E+02-0.25154820E+04 4
CH3CHOH T 4/83C 2O 1H 5 OG 300.000 5000. 1000. 1
0.67665424E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-13 2
-0.56092969E+04-0.93980442E+01 0.24813328E+01 0.16790036E-01 0.37755499E-05 3
-0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02-0.25172860E+04 4
!burkat
HOC2H4O2 C 2H 5O 3 OG 300.000 5000.000 1391.000 01
1.00941573E+01 1.23879015E-02-3.73811683E-06 5.46874551E-10-3.09943951E-14 2
-2.37710522E+04-2.00956526E+01 4.44209543E+00 2.52880383E-02-1.51605275E-05 3
5.24921198E-09-7.91470852E-13-2.17507126E+04 1.04122371E+01 4
C2H5OH L 8/88C 2H 6O 1 OG 200.000 6000.000 1000. 1
0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4
CH3OCH3 AK0904C 2H 6O 1 OG 270.000 3000.000 710.00 1
8.30815546E-01 2.69173263E-02-1.38874777E-05 3.47515079E-09-3.41706784E-13 2
-2.34120975E+04 2.02174360E+01 5.68097447E+00-5.39434751E-03 6.49472750E-05 3
-8.05065318E-08 3.27474018E-11-2.39755455E+04-6.36955496E-01 4
CH3OCH2 7/20/98 THERMC 2H 5O 1 OG 300.000 5000.000 1376.000 21
8.17137842E+00 1.10086181E-02-3.82352277E-06 5.99637202E-10-3.50317513E-14 2
-3.41941605E+03-1.78650856E+01 2.91327415E+00 2.03364659E-02-9.59712342E-06 3
2.07478525E-09-1.71343362E-13-1.18844240E+03 1.16066817E+01 4
CH3OCH2O 2/ 9/96 THERMC 2H 5O 2 OG 300.000 5000.000 2012.000 21
8.60261845E+00 1.35772195E-02-4.84661602E-06 7.77766193E-10-4.62633624E-14 2
-2.13762444E+04-1.75775023E+01 3.25889339E+00 2.22146359E-02-7.78556340E-06 3
-2.41484158E-10 4.51914496E-13-1.92377212E+04 1.23680069E+01 4
CH3OCHO 4/20/99 THERMC 2H 4O 2 OG 300.000 5000.000 1686.000 21
8.69123518E+00 1.15503122E-02-4.27782486E-06 7.02533059E-10-4.24333552E-14 2
-4.64364769E+04-1.89301478E+01 3.08839783E+00 2.03760048E-02-6.84777040E-06 3
-7.28186203E-10 5.62130216E-13-4.41855167E+04 1.25364719E+01 4

```

CH3OCO	4/20/99	THERMC	2H	30	2	OG	300.000	5000.000	1362.000	21
1.30877600E+01	4.53544950E-03	-1.65096364E-06	2.67197277E-10	-1.59576863E-14						2
-2.46616400E+04	-3.27914051E+01	3.94199159E+00	2.43434884E-02	-1.65595560E-05						3
4.58537411E-09	-3.31795708E-13	-2.14404829E+04	1.66954362E+01							4
OCHO	2/14/95	THERMC	1H	10	2	OG	300.000	5000.000	1690.000	01
6.12628782E+00	3.75602932E-03	-1.42010352E-06	2.36429200E-10	-1.44167651E-14						2
-2.17698466E+04	-8.01574694E+00	1.35213452E+00	1.50082004E-02	-1.09896141E-05						3
3.73679840E-09	-4.81014498E-13	-2.02253647E+04	1.74373147E+01							4
CH2NCH2	1104	C	2H	4N	10	OG	298.150	3000.000	1000.00	1
3.32004739E+00	1.85256567E-02	-9.56913297E-06	2.33791748E-09	-2.22816553E-13						2
2.51357839E+04	6.51880960E+00	8.69061323E-01	2.52857715E-02	-1.51435611E-05						3
3.01037347E-09	3.70026806E-13	2.57781726E+04	1.91043579E+01							4
CH3CH2OCH2CHNH	NL0512H	9C	4N	10	1g	200.00	5000.00	1000.00		1
8.36000200E+00	3.06389215E-02	-1.19217691E-05	2.12710396E-09	-1.42805755E-13						2
-1.92820605E+04	-9.98252697E+00	6.10346035E+00	-3.66483343E-03	1.12168585E-04						3
-1.38733317E-07	5.31527398E-11	-1.67028344E+04	1.14681226E+01							4
CH3OCH2CH2NCH2	NL0512H	9C	4N	10	1g	200.00	5000.00	1000.00		1
8.05415179E+00	3.11255928E-02	-1.21622491E-05	2.17616891E-09	-1.46388264E-13						2
-1.55439366E+04	-8.60414956E+00	6.20974625E+00	-5.18178680E-03	1.14720181E-04						3
-1.39910256E-07	5.31704738E-11	-1.30042686E+04	1.10095350E+01							4
OHCH2CH2NHCHCH2	NL0512H	9C	4N	10	1g	200.00	5000.00	1000.00		1
9.59411279E+00	2.87385506E-02	-1.09953106E-05	1.93953570E-09	-1.29179308E-13						2
-1.92057654E+04	-1.58976491E+01	4.33461015E+00	1.22408435E-02	7.74855054E-05						3
-1.08614992E-07	4.36754430E-11	-1.63320526E+04	1.85695490E+01							4
CH3CH2NHCH2CHO	NL0512H	9C	4N	10	1g	200.00	5000.00	1000.00		1
8.37917027E+00	3.06041482E-02	-1.19039388E-05	2.12339984E-09	-1.42532279E-13						2
-2.35334995E+04	-1.01585630E+01	5.60458654E+00	5.92374408E-04	1.01275767E-04						3
-1.27517982E-07	4.90685747E-11	-2.09329223E+04	1.33156783E+01							4
NH2CH2CH2OCHCH2	NL0512H	9C	4N	10	1g	200.00	5000.00	1000.00		1
9.24017968E+00	2.92252711E-02	-1.12209141E-05	1.98384906E-09	-1.32333667E-13						2
-1.72651475E+04	-1.35100265E+01	4.73403778E+00	8.03702900E-03	8.77461142E-05						3
-1.18729852E-07	4.72834190E-11	-1.44781450E+04	1.76832014E+01							4
CH2CHOH	NL0512H	4C	2O	1	0g	200.00	5000.00	1000.00		1
5.42272094E+00	1.15933167E-02	-4.33696384E-06	7.52881119E-10	-4.95662269E-14						2
-1.69295063E+04	-2.60547080E+00	3.06992485E+00	6.70489764E-03	2.86649911E-05						3
-4.28687590E-08	1.78068027E-11	-1.58054191E+04	1.21037066E+01							4
C2	ATCT/AC	2.	0.	0.	0.G	200.000	6000.000	1000.		1
4.12492246E+00	1.08348338E-04	1.57252585E-07	-4.24046828E-11	3.25059373E-15						2
9.81882961E+04	7.97432262E-01	-1.96261001E+00	5.76822247E-02	-1.58039636E-04						3
1.72462711E-07	-6.57913199E-11	9.82538219E+04	2.33201223E+01	9.91459509E+04						4
C2O	110203C	2O	1	0	OG	300.000	4000.000	1000.00	0	1 !
Melius 2003; see WIL/FLE07										
0.50266479E+01	0.28918227E-02	-0.13913841E-05	0.30703546E-09	-0.25567905E-13						2 !
0.44888900E+05	-0.17853398E+01	0.29665556E+01	0.10513229E-01	-0.13516489E-04						3
0.99333965E-08	-0.30881376E-11	0.45385915E+05	0.84432753E+01							4
OCHCHO	SAND	120596H	2C	2O	2	OG	300.00	3000.00	1000.00	1
0.49087462E+01	0.13182673E-01	-0.71416730E-05	0.18461316E-08	-0.18525858E-12						2
-0.27116386E+05	0.59148768E+00	0.25068862E+01	0.18899139E-01	-0.10302623E-04						3
0.62607508E-09	0.88114253E-12	-0.26427374E+05	0.13187043E+02							4
CHCNH	1107	C	2H	2N	10	OG	298.150	3000.000	1000.00	1
5.54662620E+00	7.65157744E-03	-3.57997666E-06	8.31108900E-10	-7.71666875E-14						2
4.53945633E+04	-3.17646312E+00	2.87300918E+00	1.98561384E-02	-2.41519574E-05						3
1.60558556E-08	-4.26087659E-12	4.58537821E+04	9.34467032E+00							4
CH2CN	BUR0302	T01/03C	2.H	2.N	1.	0.G	200.000	6000.000	1000.	1
6.14873620E+00	6.06600240E-03	-2.17174620E-06	3.49750387E-10	-2.09004207E-14						2
2.86491222E+04	-6.59235995E+00	2.63064017E+00	1.73644377E-02	-1.70284117E-05						3
9.86551140E-09	-2.46033517E-12	2.95791691E+04	1.12776223E+01	3.10031788E+04						4
CH2CHN	1110	C	2H	3N	10	OG	298.150	3000.000	1000.00	1
4.14453572E+00	1.31731672E-02	-6.28186453E-06	1.43989655E-09	-1.30842159E-13						2

4.10389141E+04	3.75755189E+00	3.85114887E-01	2.63155652E-02	-2.31525336E-05	3					
1.07917240E-08	-1.99497769E-12	4.18855625E+04	2.23684056E+01		4					
CH2CHN(S)	1110	C	2H	3N	1O	OG	298.150	3000.000	1000.00	1
4.14453572E+00	1.31731672E-02	-6.28186453E-06	1.43989655E-09	-1.30842159E-13	2					
4.85873563E+04	3.75755189E+00	3.85114887E-01	2.63155652E-02	-2.31525336E-05	3					
1.07917240E-08	-1.99497769E-12	4.94340048E+04	2.23684056E+01		4					
CHCNH2	1107	C	2H	3N	1O	OG	298.150	3000.000	1000.00	1
4.67245309E+00	1.04989910E-02	-4.62630454E-06	1.01345924E-09	-8.92616681E-14	2					
2.60712723E+04	-5.77430843E-01	1.34809615E+00	2.60893264E-02	-3.14511691E-05	3					
2.11896099E-08	-5.70652625E-12	2.66214983E+04	1.48874428E+01		4					
CH3CN	BUR0302	T01/03C	2.H	3.N	1.	O.G	200.000	6000.000	1000.	1
5.09921882E+00	9.69585649E-03	-3.48051966E-06	5.61420173E-10	-3.35835856E-14	2					
6.60967324E+03	-3.36087178E+00	3.82392803E+00	4.08201943E-03	2.16209537E-05	3					
-2.89807789E-08	1.12962700E-11	7.44430382E+03	5.52656156E+00	8.90492212E+03	4					
c-C2H3N	1110	C	2H	3N	1O	OG	298.150	3000.000	1000.00	1
2.80979324E+00	1.50201816E-02	-7.58141908E-06	1.85246807E-09	-1.77642437E-13	2					
3.06581771E+04	8.95343001E+00	8.28524446E-02	2.20080656E-02	-1.21834261E-05	3					
1.00059353E-09	1.01529601E-12	3.13995593E+04	2.30893128E+01		4					
CH3NCH	1106	C	2H	4N	1O	OG	298.150	3000.000	1000.00	1
3.29670257E+00	1.69750507E-02	-8.65108533E-06	2.12635860E-09	-2.04492818E-13	2					
2.51028107E+04	8.60277030E+00	2.23655533E+00	1.58044545E-02	1.22158661E-06	3					
-9.86660781E-09	4.14654507E-12	2.55853994E+04	1.50701642E+01		4					
CH3CNH	1106	C	2H	4N	1O	OG	298.150	3000.000	1000.00	1
3.29670257E+00	1.69750507E-02	-8.65108533E-06	2.12635860E-09	-2.04492818E-13	2					
2.51028107E+04	8.60277030E+00	2.23655533E+00	1.58044545E-02	1.22158661E-06	3					
-9.86660781E-09	4.14654507E-12	2.55853994E+04	1.50701642E+01		4					
CH3CHN	1106	C	2H	4N	1O	OG	298.150	3000.000	1000.00	1
2.67758316E+00	1.76421637E-02	-8.68916543E-06	2.06973359E-09	-1.93574323E-13	2					
2.23928599E+04	1.20240438E+01	2.81409484E+00	1.32950847E-02	3.53300166E-06	3					
-9.87941013E-09	3.74396969E-12	2.25556092E+04	1.23157119E+01		4					
CH2CNH2	1107	C	2H	4N	1O	OG	298.150	3000.000	1000.00	1
4.21874005E+00	1.56980617E-02	-7.75730038E-06	1.84326074E-09	-1.71837565E-13	2					
3.03905504E+04	4.69611801E+00	2.01233456E+00	2.56068048E-02	-2.42450966E-05	3					
1.39182460E-08	-3.46136416E-12	3.07776754E+04	1.50699688E+01		4					
CHCHNH2	1104	C	2H	4N	1O	OG	298.150	3000.000	1000.00	1
4.77534564E+00	1.46041683E-02	-6.78153232E-06	1.55237043E-09	-1.41604244E-13	2					
3.54379126E+04	3.02319529E-01	5.83297823E-01	3.10085354E-02	-3.08423467E-05	3					
1.72290892E-08	-3.96982789E-12	3.62945134E+04	2.06174831E+01		4					
CH3CHNH	1104	C	2H	5N	1O	OG	298.150	3000.000	1000.00	1
1.99419246E+00	2.12775413E-02	-1.02686597E-05	2.40039260E-09	-2.20647891E-13	2					
4.56273305E+03	1.43228859E+01	2.24230513E+00	1.46071399E-02	8.25386853E-06	3					
-1.56259103E-08	5.70541553E-12	4.79700805E+03	1.45453734E+01		4					
CH3NCH2	1104	C	2H	5N	1O	OG	298.150	3000.000	1000.00	1
1.74096270E+00	2.20935014E-02	-1.09102093E-05	2.60523608E-09	-2.44224882E-13	2					
7.19229187E+03	1.52596427E+01	2.12431227E+00	1.61641640E-02	4.57770566E-06	3					
-1.21159798E-08	4.53506389E-12	7.33541892E+03	1.45091874E+01		4					
CH2CHNH2	1104	C	2H	5N	1O	OG	298.150	3000.000	1000.00	1
4.59217082E+00	1.72595719E-02	-7.93920737E-06	1.79644782E-09	-1.61748720E-13	2					
2.46743039E+03	-8.63800108E-02	-7.10306111E-01	3.74245041E-02	-3.66191425E-05	3					
1.98714291E-08	-4.41925018E-12	3.58017455E+03	2.57562499E+01		4					
CH3CH2NH	1104	C	2H	6N	1O	OG	298.150	3000.000	1000.00	1
3.09795233E+00	2.24757903E-02	-1.07197166E-05	2.48313682E-09	-2.26728211E-13	2					
1.65130465E+04	1.02924690E+01	1.92365746E+00	2.38729244E-02	-7.86534966E-06	3					
-2.71981984E-09	1.89902230E-12	1.69129077E+04	1.67827743E+01		4					
CH3CHNH2	1104	C	2H	6N	1O	OG	298.150	3000.000	1000.00	1
4.08789216E+00	2.05227724E-02	-9.45003681E-06	2.12694610E-09	-1.89705755E-13	2					
1.19396821E+04	5.24987703E+00	1.64074549E+00	2.85826810E-02	-1.89468825E-05	3					
6.72949839E-09	-9.08174290E-13	1.25155453E+04	1.74881147E+01		4					
CH2CH2NH2	1104	C	2H	6N	1O	OG	298.150	3000.000	1000.00	1



4.10302792E+00	2.03084588E-02-9.25456057E-06	2.06112265E-09-1.81949714E-13	2
1.70234069E+04	5.55411391E+00 1.25928611E+00	3.01867188E-02-2.18268895E-05	3
8.94596797E-09-1.52898422E-12	1.76669906E+04	1.96477011E+01	4
CH3CH2NH2	1104 C 2H 7N 1O 0G	298.150 3000.000 1000.00	1
2.82804839E+00	2.53750154E-02-1.18740298E-05	2.70990740E-09-2.44590811E-13	2
-8.03920733E+03	1.01771802E+01 6.44080211E-01	3.14866800E-02-1.71052145E-05	3
3.57315578E-09	1.95649123E-13-7.47120329E+03	2.13696162E+01	4
H2NCO	T09/96H 2N 1C 1O 1G	200.000 6000.000 1000.00	1 !
Burcat			
0.57886741D+01	0.60938325D-02-0.21165797D-05	0.33404486D-09-0.19684582D-13	2
-0.50210948D+04-0.44063740D+01	0.35677914D+01	0.10193381D-01-0.15289951D-05	3
-0.47571551D-08	0.26052647D-11-0.42980380D+04	0.75824281D+01-0.28029168D+04	4
H2NCHO	T12/92N 1C 1H 3O 1G	200.000 6000.000 1000.00	1 !
Burcat			
0.50996641E+01	0.96197778E-02-0.33675100E-05	0.52625772E-09-0.30639100E-13	2
-0.25835964E+05-0.22514334E+01	0.31136723E+01	0.29491209E-02 0.32396676E-04	3
-0.44756760E-07	0.18144841E-10-0.24750380E+05	0.10806345E+02-0.23484619E+05	4
CH3NHCH2	1104 C 2H 6N 1O 0G	298.150 3000.000 1000.00	1
3.95751097E+00	2.09452232E-02-9.75570653E-06	2.21626118E-09-1.99156129E-13	2
1.60587518E+04	4.96297406E+00 1.71401860E+00	2.75573004E-02-1.61309839E-05	3
4.10455384E-09-8.07562261E-14	1.66255449E+04	1.63770009E+01	4
CH3NCH3	1104 C 2H 6N 1O 0G	298.150 3000.000 1000.00	1
1.54968373E+00	2.47836253E-02-1.20302906E-05	2.81641066E-09-2.58540173E-13	2
1.73453147E+04	1.93447983E+01 3.61164557E+00	9.06653308E-03 2.27492150E-05	3
-2.78391712E-08	9.27266651E-12 1.73063845E+04	1.12643356E+01	4
CH3NHCH3	1104 C 2H 7N 1O 0G	298.150 3000.000 1000.00	1
2.13913083E+00	2.68643078E-02-1.28763453E-05	2.99663495E-09-2.74772023E-13	2
-4.17331872E+03	1.29759199E+01 1.22882380E+00	2.60430675E-02-4.95078244E-06	3
-6.74954202E-09	3.27738931E-12-3.76813390E+03	1.84832422E+01	4
NCCN	C 2N 2O 0O 0G	300.00 5000.00 1000.00	1
0.65480000E+01	0.39847100E-02-0.16342200E-05	0.30386000E-09-0.21110000E-13	2
0.34907200E+05-0.97360000E+01	0.42654600E+01	0.11922570E-01-0.13420140E-04	3
0.91923000E-08-0.27789400E-11	0.35478900E+05	0.17130000E+01	4
CH2NN H2C=N=N	T09/09C 1.H 2.N 2. 0.G	200.000 6000.000 1000.	1
5.48509574E+00	6.47548090E-03-2.27700420E-06	3.62251938E-10-2.14627058E-14	2
3.01582071E+04-4.44806421E+00	2.70017481E+00	1.53945741E-02-1.42688481E-05	3
8.44885976E-09-2.25039897E-12	3.09049980E+04	9.72801485E+00 3.22838652E+04	4
CH2NO H2C=N-O*	T06/08C 1.H 2.N 1.O 1.G	200.000 6000.000 1000.	1
5.41478025E+00	6.68230119E-03-2.38625695E-06	3.83764001E-10-2.29149657E-14	2
1.63459530E+04-3.03719498E+00	3.00389272E+00	6.88209471E-03 1.26563213E-05	3
-2.17579528E-08	9.28731765E-12 1.73161337E+04	1.09485576E+01 1.85908365E+04	4
CH3N	NL0512H 3C 1N 1 0g	200.00 5000.00 1000.00	1
3.47435316E+00	8.90511141E-03-3.45265524E-06	6.14249201E-10-4.11440888E-14	2
3.58953250E+04	4.68744026E+00 4.05938864E+00	-6.37703777E-03 4.24396060E-05	3
-4.91579210E-08	1.85297277E-11 3.63766007E+04	4.92297238E+00	4
CH2NHNH2	NL0512H 5C 1N 2 0g	200.00 5000.00 1000.00	1
5.38918485E+00	1.36677756E-02-5.06038159E-06	8.71303083E-10-5.69969006E-14	2
2.88735149E+04	3.79464404E-01 3.56810411E+00	7.39883066E-03 2.89039288E-05	3
-4.26008614E-08	1.75343624E-11 2.98509598E+04	1.23314054E+01	4
CH2NNH2	NL0512H 4C 1N 2 0g	200.00 5000.00 1000.00	1
5.03931713E+00	1.20256813E-02-4.52114259E-06	7.87423335E-10-5.19552431E-14	2
1.65652364E+04-2.48661011E-01	3.07990856E+00	7.44662359E-03 2.37048127E-05	3
-3.55412708E-08	1.45796497E-11 1.75548321E+04	1.21966403E+01	4
CH3NHNH	NL0512H 5C 1N 2 0g	200.00 5000.00 1000.00	1
4.63174083E+00	1.47871383E-02-5.60045843E-06	9.80256309E-10-6.49014119E-14	2
2.23321958E+04	3.18439809E+00 5.04587002E+00	-3.20775711E-03 4.93020757E-05	3
-5.82273135E-08	2.18060409E-11 2.30346875E+04	5.12706947E+00	4
CH2CHOOH	4/25/ 6 thermC 2H 4O 2 0g	300.000 5000.000 1397.000	21
1.15749951e+01	8.09909174e-03-2.81808668e-06	4.42697954e-10-2.58998042e-14	2

-8.85355935e+03-3.43859117e+01 1.35644398e+00 3.37002447e-02-2.75988500e-05	3
1.14222854e-08-1.89488886e-12-5.50499964e+03 1.98354466e+01	4
CHCHOOH 4/25/ 6 thermC 2H 3O 2 0g 300.000 5000.000 1398.000	21
1.14545496e+01 5.70488492e-03-2.00315570e-06 3.16596832e-10-1.86008264e-14	2
2.12557351e+04-3.18525958e+01 2.29523631e+00 3.00886042e-02-2.72416044e-05	3
1.22702909e-08-2.18203315e-12 2.41142608e+04 1.62401413e+01	4
CH*CH2NHCH2CHO NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.30164816e+01 2.80109857e-02-1.08741014E-05 1.93802554E-09-1.30043635E-13	2
-1.16546837E+04-2.48070328E+01 5.42040565E+00 1.88068691E-02 6.82656239E-05	3
-1.02615169E-07 4.20518143E-11-8.15501883E+03 2.15806945E+01	4
CH2CH*NCH2 NL0512 H 6C 3N 1O 2g 200.00 5000.00 1000.00	1
1.10263776E+01 1.92266713E-02-7.36564355E-06 1.30050347E-09-8.66782140E-14	2
1.48722617E+04-2.21910608E+01 3.35068539E+00 2.94352732E-02 1.01622407E-05	3
-3.60568146E-08 1.71869326E-11 1.74736591E+04 1.99785496E+01	4
CH2CH*NHCH2CHO NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.40465661E+01 2.66858117E-02-1.02641634E-05 1.81759017E-09-1.21404761E-13	2
-1.27783905E+04-3.12450536E+01 4.01476630E+00 3.63117104E-02 2.38107787E-05	3
-5.84599747E-08 2.64529437E-11-9.18082726E+03 2.48175037E+01	4
CH2CH*OCH2CHNH NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.40062755E+01 2.67439268E-02-1.02921034E-05 1.82323617E-09-1.21815680E-13	2
-1.00990260E+04-3.11807636E+01 4.33637567E+00 3.12375346E-02 3.92601547E-05	3
-7.58887531E-08 3.31854325E-11-6.44480528E+03 2.39032338E+01	4
CH2CH2N*CH2CHO NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.43298921E+01 2.66279222E-02-1.02932659E-05 1.82885000E-09-1.22439348E-13	2
-7.56828280E+02-3.22917241E+01 4.34641135E+00 3.58416230E-02 2.48370467E-05	3
-5.96169809E-08 2.69284262E-11 2.84302255E+03 2.35913156E+01	4
CH2CH2NCH* NL0512 H 6C 3N 1O 2g 200.00 5000.00 1000.00	1
1.07415634E+01 1.96049391E-02-7.54215785E-06 1.33561647E-09-8.92082500E-14	2
1.17770921E+04-2.02938447E+01 4.55218264E+00 2.10948298E-02 2.80592757E-05	3
-5.21784900E-08 2.24998609E-11 1.42023644E+04 1.53464850E+01	4
CH2CH2NHCH*CHO NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.39177909E+01 2.69352936E-02-1.03947453E-05 1.84498100E-09-1.23437476E-13	2
-1.21139348E+04-3.08542226E+01 4.31928289E+00 3.27643759E-02 3.32594468E-05	3
-6.81791196E-08 2.99826668E-11-8.51476305E+03 2.35875495E+01	4
CH2CH2OCH*CHNH NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.39841286E+01 2.68473912E-02-1.03540469E-05 1.83694761E-09-1.22862498E-13	2
-7.49192309E+03-3.12875790E+01 4.93155036E+00 2.80235738E-02 4.55169594E-05	3
-8.10850759E-08 3.47748839E-11-3.91850160E+03 2.10288051E+01	4
CH2CH2OCH2CHN* NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.38305676E+01 2.72323278E-02-1.05645345E-05 1.88172948E-09-1.26204325E-13	2
4.68495732E+03-2.99185206E+01 5.33303875E+00 2.57673014E-02 4.93770536E-05	3
-8.35210041E-08 3.52644673E-11 8.18787198E+03 1.98723445E+01	4
CH2CHCHhO NL0512 H 5C 3O 3 0g 200.00 5000.00 1000.00	1
1.13317066E+01 1.67319420E-02-6.43469628E-06 1.13960394E-09-7.61353298E-14	2
-6.25190487E+03-2.51050816E+01 3.08845462E+00 2.74265239E-02 1.45812538E-05	3
-4.25715682E-08 2.01523137E-11-3.49086614E+03 2.01343963E+01	4
N*CH2CH2OCHCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.31127368E+01 2.78836158E-02-1.08125627E-05 1.92537665E-09-1.29108102E-13	2
2.83867075E+01-2.47108351E+01 5.65560427E+00 1.63244277E-02 7.64947642E-05	3
-1.12744930E-07 4.62242315E-11 3.53914880E+03 2.13180178E+01	4
CH2NOOH NL0512 H 3C 1N 1O 2g 200.00 5000.00 1000.00	1
7.17582349E+00 9.79263705E-03-3.71946961E-06 6.52992770E-10-4.33523400E-14	2
6.82963103E+03-7.13181609E+00 3.15036645E+00 1.35715816E-02 1.15310867E-05	3
-2.65245945E-08 1.21229787E-11 8.23708842E+03 1.52814276E+01	4
CH2OCH*CH2NCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1
1.35820823E+01 2.73236615E-02-1.05637153E-05 1.87720255E-09-1.25695193E-13	2
-8.81756260E+03-2.94341643E+01 4.47710974E+00 2.88018273E-02 4.41123322E-05	3
-7.93251300E-08 3.39947812E-11-5.21935493E+03 2.31601299E+01	4
CH2OCH2CH*NCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00	1

1.34620945E+01	2.74988677E-02	-1.06479392E-05	1.89416533E-09	-1.26924720E-13	2
-6.99738127E+03	-2.87092643E+01	4.97554314E+00	2.60642602E-02	4.88869557E-05	3
-8.27593539E-08	3.48786455E-11	-3.49531052E+03	2.10252758E+01		4
CH2OCH2CH2NCH*	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.30784904E+01	2.78970237E-02	-1.08131229E-05	1.92491950E-09	-1.29051131E-13	2
-9.00870949E+03	-2.61182406E+01	6.02328824E+00	1.85725386E-02	6.44918395E-05	3
-9.64751511E-08	3.93113397E-11	-5.70056608E+03	1.72066346E+01		4
CH2OCHCH*	NL0512	H 5C 3O 3 0g	200.00	5000.00 1000.00	1
1.12483668E+01	1.61273413E-02	-6.14165814E-06	1.08005797E-09	-7.17860356E-14	2
-2.66635615E+03	-2.21385221E+01	3.92166702E+00	2.81579238E-02	3.49502879E-06	3
-2.69389309E-08	1.35880864E-11	-3.04097256E+02	1.75373003E+01		4
CHNOOH	NL0512	H 2C 1N 1O 2g	200.00	5000.00 1000.00	1
7.80042897E+00	6.40552192E-03	-2.40515771E-06	4.18901008E-10	-2.76544439E-14	2
3.39008772E+04	-9.43082516E+00	2.60123962E+00	2.34626502E-02	-2.31820252E-05	3
1.10678507E-08	-1.76655034E-12	3.51793443E+04	1.66965104E+01		4
cyMeta*Morph2yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.44936260E+01	2.84174553E-02	-1.10130662E-05	1.96075052E-09	-1.31481905E-13	2
-1.75139579E+04	-4.61749827E+01	2.85460413E+00	3.47108929E-02	4.58139450E-05	3
-8.84256420E-08	3.87426690E-11	-1.31631576E+04	1.99033209E+01		4
cyMeta*Morph4yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.40033433E+01	2.92910380E-02	-1.14606805E-05	2.05376880E-09	-1.38349845E-13	2
-1.79211949E+04	-4.49087515E+01	3.48965388E+00	2.51688611E-02	7.13937282E-05	3
-1.14226316E-07	4.78915530E-11	-1.35236855E+04	1.71376235E+01		4
cyMeta*Morph5yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.44092626E+01	2.85603054E-02	-1.10876144E-05	1.97658231E-09	-1.32672377E-13	2
-1.80920027E+04	-4.64954956E+01	3.05337416E+00	3.22718540E-02	5.17972652E-05	3
-9.39861692E-08	4.05573759E-11	-1.37222731E+04	1.85841574E+01		4
cyMeta*Morph6yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.42811521E+01	2.87517833E-02	-1.11807730E-05	1.99549274E-09	-1.34050797E-13	2
-1.55544397E+04	-4.59761819E+01	3.31230094E+00	2.89368322E-02	6.08024541E-05	3
-1.03344033E-07	4.39751277E-11	-1.11814296E+04	1.76774595E+01		4
cyMetaOOMorphyl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.34256646E+01	3.05058652E-02	-1.19859435E-05	2.15387694E-09	-1.45372407E-13	2
-2.02548603E+04	-4.43498328E+01	3.19764079E+00	2.28944790E-02	7.92420820E-05	3
-1.21708190E-07	5.02915820E-11	-1.57771252E+04	1.69491455E+01		4
cyOrtho*Morph3yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.43813934E+01	2.85914794E-02	-1.11005523E-05	1.97894351E-09	-1.32831719E-13	2
-1.95955185E+04	-4.60547527E+01	2.77886114E+00	3.42731564E-02	4.67991048E-05	3
-8.88417849E-08	3.86756711E-11	-1.52115669E+04	2.00076157E+01		4
cyOrtho*Morph4yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.40670573E+01	2.92187586E-02	-1.14295978E-05	2.04788683E-09	-1.37939904E-13	2
-1.85486652E+04	-4.48488250E+01	3.70708125E+00	2.43215815E-02	7.30279111E-05	3
-1.15752226E-07	4.84308955E-11	-1.41794651E+04	1.64811958E+01		4
cyOrtho*Morph5yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.43585773E+01	2.86262145E-02	-1.11175743E-05	1.98241316E-09	-1.33085330E-13	2
-1.97719027E+04	-4.64166304E+01	2.87434461E+00	3.32590726E-02	4.94614281E-05	3
-9.15756165E-08	3.96642141E-11	-1.53885119E+04	1.92027980E+01		4
cyOrtho*Morph6yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.43413148E+01	2.87036271E-02	-1.11638036E-05	1.99264499E-09	-1.33866837E-13	2
-1.73152303E+04	-4.62804717E+01	2.87622151E+00	3.20463318E-02	5.36776820E-05	3
-9.64406960E-08	4.15481657E-11	-1.28852074E+04	1.95191682E+01		4
cyOrthoOOMorphyl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.34466865E+01	3.04892931E-02	-1.19806733E-05	2.15311303E-09	-1.45330662E-13	2
-2.11677212E+04	-4.48218647E+01	2.95386103E+00	2.44607933E-02	7.56095403E-05	3
-1.18042498E-07	4.89435730E-11	-1.66509885E+04	1.76572080E+01		4
cyPara*Morph2yl	NL0512	H 8C 4N 1O 3g	200.00	5000.00 1000.00	1
1.47102177E+01	2.83961643E-02	-1.10519010E-05	1.97340093E-09	-1.32600818E-13	2
-3.64746991E+03	-4.78982998E+01	2.55437348E+00	3.78704072E-02	3.80416173E-05	3
-8.02865143E-08	3.56803063E-11	7.87841849E+02	2.04920295E+01		4

cyParaOOMorphyl	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.36300476E+01	3.04519141E-02	-1.19984403E-05	2.15997110E-09	-1.45956292E-13						2
-8.87940963E+03	-4.56742592E+01	2.79542102E+00	2.73891189E-02	6.79938461E-05						3
-1.10279161E-07	4.61586986E-11	-4.35342225E+03	1.81096207E+01							4
NCHOOH	NL0512	H	2C	1N	1O	2g	200.00	5000.00	1000.00	1
7.10570171E+00	7.19161595E-03	-2.74797378E-06	4.84767950E-10	-3.23061095E-14						2
1.51061797E+04	-6.07644452E+00	3.74118310E+00	1.03240545E-02	9.72734050E-06						3
-2.15309443E-08	9.73393078E-12	1.62918435E+04	1.26861875E+01							4
NHCH*CH2OCHCH2	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.40550909E+01	2.66804501E-02	-1.02631256E-05	1.81757914E-09	-1.21414362E-13						2
-6.55580797E+03	-3.17317087E+01	3.32439456E+00	3.39748652E-02	3.85084033E-05						3
-7.87538466E-08	3.50903365E-11	-2.64736165E+03	2.87460439E+01							4
NHCH*CHO	NL0512	H	4C	2N	1O	3g	200.00	5000.00	1000.00	1
1.08834987E+01	1.39364479E-02	-5.36548409E-06	9.51136725E-10	-6.35927285E-14						2
-7.61189374E+03	-1.96122436E+01	4.44731671E+00	2.09870104E-02	1.46881216E-05						3
-3.66476905E-08	1.68526989E-11	-5.37874098E+03	1.60627465E+01							4
NHCH2CH*OCHCH2	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.41215687E+01	2.66566036E-02	-1.02636180E-05	1.81883384E-09	-1.21552853E-13						2
-9.73098248E+03	-3.18788658E+01	4.28533096E+00	2.91580811E-02	4.81909202E-05						3
-8.74330598E-08	3.79872753E-11	-5.95766516E+03	2.45406587E+01							4
NHCH2CH2OCHCH*	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.37181650E+01	2.71811666E-02	-1.05059024E-05	1.86673563E-09	-1.24990383E-13						2
-3.96420344E+03	-2.97215086E+01	4.69972662E+00	2.61459466E-02	5.25333871E-05						3
-8.91156072E-08	3.78427651E-11	-3.08411468E+02	2.29044430E+01							4
NHCHCHO	NL0512	H	3C	2N	1O	1g	200.00	5000.00	1000.00	1
6.06110214E+00	1.17315660E-02	-4.58245457E-06	8.20065433E-10	-5.51835208E-14						2
-6.71499719E+03	-3.93068633E+00	3.66909704E+00	5.30244554E-03	3.07387433E-05						3
-4.26415871E-08	1.68900909E-11	-5.41456528E+03	1.16018000E+01							4
NHCHOOH	NL0512	H	3C	1N	1O	2g	200.00	5000.00	1000.00	1
6.97204150E+00	9.85204326E-03	-3.71095118E-06	6.47859126E-10	-4.28456257E-14						2
-8.50754478E+03	-6.04757205E+00	3.58188558E+00	9.23867044E-03	2.18529170E-05						3
-3.66413746E-08	1.56809911E-11	-7.16056328E+03	1.36940577E+01							4
OCH*CH2NHCHCH2	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.44473084E+01	2.66987605E-02	-1.02498668E-05	1.81283474E-09	-1.20987251E-13						2
-9.81285088E+03	-3.58238308E+01	2.28019125E+00	4.30569383E-02	1.78101658E-05						3
-5.83943085E-08	2.78060133E-11	-5.72981492E+03	3.09016390E+01							4
OCH*CHNH	NL0512	H	4C	2N	1O	3g	200.00	5000.00	1000.00	1
1.11063015E+01	1.42173081E-02	-5.48184513E-06	9.72926411E-10	-6.51105684E-14						2
-4.83909000E+03	-2.36269923E+01	2.97333270E+00	2.66600442E-02	8.98499815E-06						3
-3.50419505E-08	1.71598540E-11	-2.20140198E+03	2.05640924E+01							4
OCH2CH*NHCHCH2	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.45742148E+01	2.66561292E-02	-1.02535445E-05	1.81599074E-09	-1.21318258E-13						2
-8.57671485E+03	-3.64424404E+01	3.02570077E+00	4.00653041E-02	2.30154756E-05						3
-6.24782673E-08	2.90138138E-11	-4.59418218E+03	2.74144568E+01							4
OCH2CH2N*CHCH2	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.48058721E+01	2.66024711E-02	-1.02732732E-05	1.82428256E-09	-1.22094157E-13						2
6.45678993E+03	-3.74286417E+01	3.00050291E+00	4.05458330E-02	2.31961795E-05						3
-6.35628437E-08	2.96284231E-11	1.05119923E+04	2.77780948E+01							4
OCH2CH2NHCHCH*	NL0512	H	8C	4N	1O	3g	200.00	5000.00	1000.00	1
1.43367527E+01	2.70324643E-02	-1.04397282E-05	1.85404209E-09	-1.24100858E-13						2
-3.52196182E+03	-3.44009184E+01	4.05664603E+00	3.38473722E-02	3.48119332E-05						3
-7.17391346E-08	3.16499012E-11	2.91335126E+02	2.37361430E+01							4
OCH2CHN*	NL0512	H	4C	2N	1O	3g	200.00	5000.00	1000.00	1
1.10300682E+01	1.45184852E-02	-5.65716043E-06	1.01114507E-09	-6.79990668E-14						2
1.01731294E+04	-2.27953442E+01	3.54243352E+00	2.46766429E-02	1.07538024E-05						3
-3.45468820E-08	1.63904561E-11	1.26981966E+04	1.82890149E+01							4
N*CH2CHO	NL0512	H	4C	2N	1O	3g	200.00	5000.00	1000.00	1
1.00051943E+01	1.50715838E-02	-5.88652810E-06	1.05364933E-09	-7.09219581E-14						2
-9.84274147E+02	-1.43535163E+01	4.86607433E+00	1.37414053E-02	3.16707895E-05						3

```

-5.18684616E-08 2.17445312E-11 1.15680407E+03 1.58712857E+01 4
OCHOOH NL0512 H 2C 1O 3 0g 200.00 5000.00 1000.00 1
6.59570455E+00 7.71138318E-03-2.96087667E-06 5.24049901E-10-3.50043803E-14 2
-3.67925907E+04-3.36287842E+00 4.12675703E+00 6.35427459E-03 1.75788334E-05 3
-2.77785835E-08 1.15459444E-11-3.57375164E+04 1.13121420E+01 4
cyPara*Morph3yl NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.54166324E+01 2.81691005E-02-1.10840504E-05 1.99450306E-09-1.34769408E-13 2
2.26750237E+04-5.28862611E+01 2.84806241E+00 3.18532543E-02 5.91337653E-05 3
-1.04088922E-07 4.45800368E-11 2.75500178E+04 1.92961907E+01 4
CH*CH2OCH2CHNH NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.43927498E+01 2.74549524E-02-1.08625213E-05 1.96219978E-09-1.32955189E-13 2
6.87350101E+03-3.27794818E+01 7.29744474E+00 1.12182087E-03 1.19723674E-04 3
-1.57232030E-07 6.18725468E-11 1.09797900E+04 1.48081111E+01 4
CH2NHCHCH* NL0512 H 6C 3N 1O 2g 200.00 5000.00 1000.00 1
1.13162338E+01 1.85103901E-02-6.97320497E-06 1.21677780E-09-8.04147624E-14 2
1.37277095E+04-2.32257879E+01 3.59085639E+00 3.15936836E-02 2.11982510E-06 3
-2.73622171E-08 1.40277919E-11 1.61934065E+04 1.84972072E+01 4
CH*CH2NCH2 NL0512 H 6C 3N 1O 2g 200.00 5000.00 1000.00 1
1.16785871E+01 1.96070016E-02-7.78699082E-06 1.41045208E-09-9.57580059E-14 2
2.48851949E+04-2.65236022E+01 4.63740383E+00 8.84713781E-03 7.22066789E-05 3
-1.01983568E-07 4.10812971E-11 2.82370817E+04 1.70278372E+01 4
CH*OCH2CH2NCH2 NL0512 H 8C 4N 1O 3g 200.00 5000.00 1000.00 1
1.35296823E+01 2.80081240E-02-1.10036466E-05 1.97765559E-09-1.33507372E-13 2
1.18128499E+04-2.88704692E+01 5.85599616E+00 1.07507540E-02 9.43258839E-05 3
-1.31148909E-07 5.25622949E-11 1.57249325E+04 1.99048334E+01 4
CH*OCHCH2 NL0512 H 5C 3O 3 0g 200.00 5000.00 1000.00 1
1.14821134E+01 1.64350154E-02-6.40711507E-06 1.14601429E-09-7.71243035E-14 2
1.08000752E+04-2.46800638E+01 3.19973238E+00 2.05901841E-02 3.59399245E-05 3
-6.59932095E-08 2.88282279E-11 1.38796089E+04 2.23418535E+01 4
CH*NHCHCH2 NL0512 H 6C 3N 1O 2g 200.00 5000.00 1000.00 1
1.16713205E+01 1.87336990E-02-7.21354447E-06 1.27919413E-09-8.55599211E-14 2
2.44423797E+04-2.59814895E+01 2.88962207E+00 2.47255506E-02 3.25458850E-05 3
-6.42362362E-08 2.84441742E-11 2.76341655E+04 2.34988397E+01 4
END

```

### Transport parameters in CHEMKIN format

```

HE 0 10.200 2.576 0.000 0.000 0.000 !(*)
AR 0 136.500 3.330 0.000 0.000 0.000 !
NE 0 32.800 2.820 0.000 0.000 0.000 !ReidApp

H 0 145.000 2.050 0.000 0.000 0.000 !
H2 1 38.000 2.920 0.000 0.790 280.000 !

C 0 71.400 3.298 0.000 0.000 0.000 !(*)
CH 1 80.000 2.750 0.000 0.000 0.000 !
CH2 1 144.000 3.800 0.000 0.000 0.000 !
CH2SING 1 144.000 3.800 0.000 0.000 0.000 !
CH2(S) 1 144.000 3.800 0.000 0.000 0.000 !
CH3 1 144.000 3.800 0.000 0.000 0.000 !
CH4 2 141.400 3.746 0.000 2.600 13.000 !

O 0 80.000 2.750 0.000 0.000 0.000 !
OSING 0 80.000 2.750 0.000 0.000 0.000 !
OH 1 80.000 2.750 0.000 0.000 0.000 !
H2O 2 572.400 2.605 1.844 0.000 4.000 !

C2H 1 209.000 4.100 0.000 0.000 2.500 !
C2H2 1 209.000 4.100 0.000 0.000 2.500 !
C2H3 2 209.000 4.100 0.000 0.000 1.000 !(*)

```

C2H4	2	280.800	3.971	0.000	0.000	1.500	!
C2H5	2	252.300	4.302	0.000	0.000	1.500	!
C2H6	2	252.300	4.302	0.000	0.000	1.500	!
CO	1	98.100	3.650	0.000	1.950	1.800	!
HCO	2	498.000	3.590	0.000	0.000	0.000	!
CHO	2	498.000	3.590	0.000	0.000	0.000	!
CH:O	2	498.000	3.590	0.000	0.000	0.000	!
HCO+	1	498.000	3.590	0.000	0.000	0.000	!
CH2O	2	498.000	3.590	0.000	0.000	2.000	!
CH2:O	2	498.000	3.590	0.000	0.000	2.000	!
CH3O	2	417.000	3.690	1.700	0.000	2.000	!
CH2OH	2	417.000	3.690	1.700	0.000	2.000	!
CH3OH	2	481.800	3.626	0.000	0.000	1.000	!(SVE)
CH4O	2	417.000	3.690	1.700	0.000	2.000	!
O2	1	107.400	3.458	0.000	1.600	3.800	!
O3	1	107.400	3.458	0.000	1.600	3.800	!
HO2	2	107.400	3.458	0.000	0.000	1.000	!(* )
H2O2	2	107.400	3.458	0.000	0.000	3.800	!
C3H	1	252.000	4.760	0.000	0.000	1.000	!same as C3H3
C3H2	2	209.000	4.100	0.000	0.000	1.000	!(* )
C3H3	2	252.000	4.760	0.000	0.000	1.000	!(JAM)
H2CCCH	2	252.000	4.760	0.000	0.000	1.000	!(JAM)
CH3CC	2	252.000	4.760	0.000	0.000	1.000	!(JAM)
C3H4	1	252.000	4.760	0.000	0.000	1.000	!
C3H4P	2	252.000	4.760	0.000	0.000	1.000	!(JAM)
AC3H4	2	252.000	4.760	0.000	0.000	1.000	!
PC3H4	2	252.000	4.760	0.000	0.000	1.000	!
H2CCCH2	2	252.000	4.760	0.000	0.000	1.000	!
CH3CCH	2	252.000	4.760	0.000	0.000	1.000	!
cC3H4	2	252.000	4.760	0.000	0.000	1.000	!
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000	!
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000	!
CH3CHCHE	2	260.000	4.850	0.000	0.000	1.000	!
CH3CHCHZ	2	260.000	4.850	0.000	0.000	1.000	!
C3H5	2	260.000	4.850	0.000	0.000	1.000	!(JAM)
SC3H5	2	260.000	4.850	0.000	0.000	1.000	!(JAM)
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000	!(JAM)
TC3H5	2	260.000	4.850	0.000	0.000	1.000	!(JAM)
AC3H5	2	260.000	4.850	0.000	0.000	1.000	!(JAM)
C3H6	2	266.800	4.982	0.000	0.000	1.000	!
C3H7	2	266.800	4.982	0.000	0.000	1.000	!
I*C3H7	2	266.800	4.982	0.000	0.000	1.000	!
nC3H7	2	266.800	4.982	0.000	0.000	1.000	!
NC3H7	2	266.800	4.982	0.000	0.000	1.000	!
iC3H7	2	266.800	4.982	0.000	0.000	1.000	!
IC3H7	2	266.800	4.982	0.000	0.000	1.000	!
C3H8	2	266.800	4.982	0.000	0.000	1.000	!
HCCO	2	150.000	2.500	0.000	0.000	1.000	!(* )
CH2CO	2	436.000	3.970	0.000	0.000	2.000	!
HCCOH	2	436.000	3.970	0.000	0.000	2.000	!
CH2CHO	2	436.000	3.970	0.000	0.000	2.000	!est.
CH2HCO	2	436.000	3.970	0.000	0.000	2.000	!est.
CH3CO	2	436.000	3.970	0.000	0.000	2.000	!
C2H3OO	2	556.000	4.610	0.000	0.000	0.000	!(Hennessy?)
C2H2OH	2	224.700	4.162	0.000	0.000	1.000	!(* )
CH3CHO	2	436.000	3.970	0.000	0.000	2.000	!
CH3HCO	2	436.000	3.970	0.000	0.000	2.000	!
CO2	1	244.000	3.763	0.000	2.650	2.100	!
C2H4O	2	436.000	3.970	0.000	0.000	2.000	!guess
C2H5O	2	436.000	3.970	0.000	0.000	2.000	!est
CH3OO	2	436.000	3.970	0.000	0.000	2.000	!est

CH300H	2	436.000	3.970	0.000	0.000	2.000	!est
CH302	2	436.000	3.970	0.000	0.000	2.000	!est
CH302H	2	436.000	3.970	0.000	0.000	2.000	!est
O3	2	180.000	4.100	0.000	0.000	2.000	!
C4H	1	357.000	5.180	0.000	0.000	1.000	!
C4H2	1	357.000	5.180	0.000	0.000	1.000	!
H2C4O	2	357.521	4.459	0.000	0.000	1.000	! LJcjp
nC4H3	2	357.000	5.180	0.000	0.000	1.000	!guess
ic4H3	2	357.000	5.180	0.000	0.000	1.000	!TC from Wang
C4H3	2	357.000	5.180	0.000	0.000	1.000	!guess
HCCHCCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
H2CCCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H4	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
H2CCCH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H5	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCCH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H6	2	357.000	5.176	0.000	0.000	1.000	
C4H6-13	2	357.000	5.176	0.000	0.000	1.000	
C4H6-1	2	357.000	5.176	0.000	0.000	1.000	
!GEO added following two species iiC4H6=1,2butadiene;iiiC4H6=1,3butadiene							
!done on 10/14/98							
iiC4H6	2	357.000	5.176	0.000	0.000	1.000	
iiiC4H6	2	357.000	5.176	0.000	0.000	1.000	
C2H5C2H	2	357.000	5.176	0.000	0.000	1.000	
C4H7	2	357.000	5.176	0.000	0.000	1.000	
C4H8	2	357.000	5.176	0.000	0.000	1.000	!
cC4H8	2	357.000	5.176	0.000	0.000	1.000	
tC4H8	2	357.000	5.176	0.000	0.000	1.000	
nC4H8-1	2	357.000	5.176	0.000	0.000	1.000	
IC4H8	2	357.000	5.176	0.000	0.000	1.000	
IIC4H8	2	357.000	5.176	0.000	0.000	1.000	
UC4H8	2	357.000	5.176	0.000	0.000	1.000	
nC4H9	2	357.000	5.176	0.000	0.000	1.000	!
S*C4H9	2	357.000	5.176	0.000	0.000	1.000	!
I*C4H9	2	357.000	5.176	0.000	0.000	1.000	!
C4H10	2	357.000	5.176	0.000	0.000	1.000	
NC4H10	2	357.000	5.176	0.000	0.000	1.000	
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	!(* )
HCCCHO	2	429.000	4.999	2.9	0.	1.	!est
CH2CCO	2	429.000	4.999	2.9	0.	1.	!est
HCCCH2O	2	429.000	4.999	2.9	0.	1.	!est
OCYCCCH	2	429.000	4.999	2.9	0.	1.	!est
CH2CHCO	2	429.000	4.999	2.9	0.	1.	!est
CH3CCO	2	429.000	4.999	2.9	0.	1.	!est
CH2CCHO	2	429.000	4.999	2.9	0.	1.	!est
CH3CHCO	2	429.000	4.999	2.9	0.	1.	!est
CH3CHOH	2	470.600	4.410	0.000	0.000	1.500	!From LLNL Marinov set
C2H4OH	2	470.600	4.410	0.000	0.000	1.500	!From LLNL Marinov set
CH3CH2O	2	470.600	4.410	0.000	0.000	1.500	! nmm !From LLNL
Marinov set							
C2H5OH	2	470.600	4.410	0.000	0.000	1.500	! nmm!From LLNL
Marinov set							
HOC2H4O2	2	470.600	4.410	0.000	0.000	1.500	!7/01 same as c2h5oh,
wjp!From LLNL Marinov set							
C2H3CO	2	429.000	4.999	2.9	0.	1.	!est
C2H3CHO	2	429.000	4.999	2.9	0.	1.	!PRW2/93
C2H3CH2O	2	429.000	4.999	2.9	0.	1.	!PRW5/93
CH3CHCHO	2	429.000	4.999	2.9	0.	1.	!est
cC3H5O	2	357.000	5.176	0.000	0.000	1.000	!est
CH2COCH3	2	357.000	5.176	0.000	0.000	1.000	
CH3COCH3	2	357.000	5.176	0.000	0.000	1.000	

C3H6O	2	357.000	5.176	0.000	0.000	1.000	
CH2CHOCH2	2	357.000	5.176	0.000	0.000	1.000	!est
Propox	2	357.000	5.176	0.000	0.000	1.000	
C3H6OH	2	576.7	4.549	0.000	0.000	1.000	!est.
nC3H7O	2	576.7	4.549	0.000	0.000	1.000	!est.
iC3H7O	2	576.7	4.549	0.000	0.000	1.000	!est.
CH3CO2	2	576.7	4.549	0.000	0.000	1.000	!est.
CH3CO2H	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H5OO	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H5O2	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H5OOH	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H5O2H	2	576.7	4.549	0.000	0.000	1.000	!est.
CH3OOCH3	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H3CO2	2	576.7	4.549	0.000	0.000	1.000	!est.
C3H5OO	2	576.7	4.549	0.000	0.000	1.000	!est.
C3H5OOH	2	576.7	4.549	0.000	0.000	1.000	!est.
nC3H7OO	2	576.7	4.549	0.000	0.000	1.000	!est.
iC3H7OO	2	576.7	4.549	0.000	0.000	1.000	!est.
nC3H7OOH	2	576.7	4.549	0.000	0.000	1.000	!est.
iC3H7OOH	2	576.7	4.549	0.000	0.000	1.000	!est.
CH3CO3	2	576.7	4.549	0.000	0.000	1.000	!est.
CH3CO3H	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H3CO3	2	576.7	4.549	0.000	0.000	1.000	!est.
C2H3CO3H	2	576.7	4.549	0.000	0.000	1.000	!est.
O2C3H6OH	2	576.7	4.549	0.000	0.000	1.000	!est.
!C5H2	1	357.000	5.180	0.000	0.000	1.000	! Deleted by Wenjun
using Miller							
!C5H3	1	357.000	5.180	0.000	0.000	1.000	! Deleted by Wenjun
using Miller							
C5H4O	2	450.000	5.500	0.000	0.000	1.000	! !
C5H4OH	2	450.000	5.500	0.000	0.000	1.000	! !
pn2en4yny1	1	357.000	5.180	0.000	0.000	1.000	! same as C5H3
C5H5	1	357.000	5.180	0.000	0.000	1.000	! same as C5H3
!							
C5H2	1	386.805	4.852	0.000	0.000	1.000	! LJcjp
H2CCCCCH	2	389.341	5.055	0.000	0.000	1.000	! LJcjp
HCCCCHCCH	2	378.067	5.021	0.000	0.000	1.000	! LJcjp
C5H4	1	357.000	5.180	0.000	0.000	1.000	!HR,10/00
!							
C5H5O	2	450.000	5.500	0.000	0.000	1.000	! !
C5H5OH	2	450.000	5.500	0.000	0.000	1.000	!(JAM)
C5H6	2	354.700	5.13	0.000	0.000	1.000	!ab
C5H7	2	393.700	5.26	0.000	0.000	1.000	!ab
C5H8	2	393.700	5.26	0.000	0.000	1.000	!ab
C5H4	2	441.700	5.00	0.000	0.000	1.000	!ab
cypentenyl	2	354.700	5.13	0.000	0.000	1.000	!After ab C5H6
cypnt3enyl	2	354.700	5.13	0.000	0.000	1.000	!After ab C5H6
cypentene	2	354.700	5.13	0.000	0.000	1.000	!After ab C5H6
pentdienyl	2	393.700	5.26	0.000	0.000	1.000	!After ab C5H7
pentdienal	2	450.000	5.500	0.000	0.000	1.000	!After (JAM) C5H5OH
C5H4CH3	2	412.300	5.349	0.000	0.000	1.000	!like other C6H7's
C6H	1	412.300	5.349	0.000	0.000	1.000	!ab/97
C6H3	2	412.300	5.349	0.000	0.000	1.000	!ab/97
n-C6H5	2	412.300	5.349	0.000	0.000	1.000	!ab/97
i-C6H5	2	412.300	5.349	0.000	0.000	1.000	!ab/97
l-C6H6	2	412.300	5.349	0.000	0.000	1.000	!ab/97
C4H5C2H	2	412.3	5.349	0.00	0.00	1.00	! JAM(12/02)
n-C6H7	2	412.300	5.349	0.000	0.000	1.000	!ab/97
c-C6H7	2	412.300	5.349	0.000	0.000	1.000	!ab/97
i-C6H7	2	412.300	5.349	0.000	0.000	1.000	!ab/97
A1	2	412.300	5.349	0.000	0.000	1.000	!ab/97
A	2	412.300	5.349	0.000	0.000	1.000	!ab/97
l-C6H4	2	367.700	5.36	0.000	0.000	1.000	!ab/97
c-C6H4	2	367.700	5.36	0.000	0.000	1.000	!ab/97



C6H8	2	412.300	5.349	0.000	0.000	1.000	!ab/97
n-C4H5	2	357.000	5.180	0.000	0.000	1.000	!AB/97
i-C4H5	2	357.000	5.180	0.000	0.000	1.000	!AB/97
FC6H6	2	412.300	5.349	0.000	0.000	1.000	!ab/97
C6H2	1	357.000	5.180	0.000	0.000	1.000	!
C6H5	2	412.300	5.349	0.000	0.000	1.000	!(JAM)
C6H5 (L)	2	412.300	5.349	0.000	0.000	1.000	!(JAM)
C6H6	2	412.300	5.349	0.000	0.000	1.000	!(SVE)
C6H7	2	412.300	5.349	0.000	0.000	1.000	!(JAM)
C6H10	2	399.3	5.949	0.000	0.000	1.000	!est
C6H14	2	399.3	5.949	0.000	0.000	1.000	!
C6H5O	2	450.000	5.500	0.000	0.000	1.000	!(JAM)
C6H5OH	2	450.000	5.500	0.000	0.000	1.000	! !
CYC6H12	2	324.	6.093	0.000	0.000	1.000	! BSL60
CYC6H11	2	324.	6.093	0.000	0.000	1.000	! BSL60
C6H11	2	412.300	5.349	0.000	0.000	1.000	!mel/04 same as
benzene							
C6H11-13	2	412.300	5.349	0.000	0.000	1.000	!Wenjun/20080824 same
as benzene							
C6H11-12	2	399.3	5.949	0.000	0.000	1.000	!est from C6H10
C6H11-14	2	399.3	5.949	0.000	0.000	1.000	!est from C6H10
C6H11-15	2	399.3	5.949	0.000	0.000	1.000	!est from C6H10
CYC6H10	2	324.	6.093	0.000	0.000	1.000	! BSL60
CYC6H9	2	324.	6.093	0.000	0.000	1.000	! BSL60
C6H9	2	324.	6.093	0.000	0.000	1.000	!ab/97
CY13C6H8	2	412.300	5.349	0.000	0.000	1.000	!mel/04 same as
benzene							
CYC6H7	2	412.300	5.349	0.000	0.000	1.000	!mel/04 same as
benzene							
hexene1	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
hexene3	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
hex1yl	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
hex2yl	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
hex3yl	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
hex2enyl	2	413.	5.909	0.000	0.000	1.000	! BSL60 for nC6H14
C4H6O	2	442.700	4.85	0.000	0.000	1.000	!ab
C4H8O	2	426.200	5.21	0.000	0.000	1.000	!ab
C6H4	2	367.700	5.36	0.000	0.000	1.000	!ab
C8H2	1	357.000	5.180	0.000	0.000	1.000	! same as C6H2
N	0	71.400	3.298	0.000	0.000	0.000	! (*)
N2	1	97.530	3.621	0.000	1.760	4.000	!
N2H2	2	71.400	3.798	0.000	0.000	1.000	! (*)
N2H3	2	200.000	3.900	0.000	0.000	1.000	! (*)
N2H4	2	205.000	4.230	0.000	4.260	1.500	!
N2O	1	232.400	3.828	0.000	0.000	1.000	! (*)
NCN	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
NCO	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
NH	1	80.000	2.650	0.000	0.000	4.000	!
NH2	2	80.000	2.650	0.000	2.260	4.000	!
NH3	2	481.000	2.920	1.470	0.000	10.000	!
NNH	2	71.400	3.798	0.000	0.000	1.000	! (*)
NO	1	97.530	3.621	0.000	1.760	4.000	!
NCNO	2	232.400	3.828	0.000	0.000	1.000	! (OIS)
NO2	2	200.000	3.500	0.000	0.000	1.000	! (*)
NOO	2	200.000	3.500	0.000	0.000	1.000	!
NO3	2	200.000	3.500	0.000	0.000	1.000	!
HCN	1	569.000	3.630	0.000	0.000	1.000	! (OIS)
CN	1	75.000	3.856	0.000	0.000	1.000	! (OIS)
CNC	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
CNN	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
CN2	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
C2N	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
C2N2	1	349.000	4.361	0.000	0.000	1.000	! (OIS)

H2CN	1	569.000	3.630	0.000	0.000	1.000	!(os/jm)
HC2N2	1	349.000	4.361	0.000	0.000	1.000	!(OIS)
HCNO	2	232.400	3.828	0.000	0.000	1.000	!(JAM)
HOCN	2	232.400	3.828	0.000	0.000	1.000	!(JAM)
HNCO	2	232.400	3.828	0.000	0.000	1.000	!(OIS)
HCOOH	2	232.400	3.828	0.000	0.000	1.000	!(TC,guess)
C2O	2	232.400	3.828	0.000	0.000	1.000	!(TC,no data)
HOCO	2	232.400	3.828	0.000	0.000	1.000	!
COOH	2	232.400	3.828	0.000	0.000	1.000	!dummy
HONO	2	232.400	3.828	0.000	0.000	1.000	!
HNO3	2	232.400	3.828	0.000	0.000	1.000	!
HOONO	2	232.400	3.828	0.000	0.000	1.000	!
HNO	2	116.700	3.492	0.000	0.000	1.000	!(* )
HNNO	2	232.400	3.828	0.000	0.000	1.000	!(* )
S	0	847.000	3.839	0.000	0.000	0.000	!(OIS)
S2	1	847.000	3.900	0.000	0.000	1.000	!(OIS)
SH	1	847.000	3.900	0.000	0.000	1.000	!(OIS)
H2S	2	301.000	3.600	0.000	0.000	1.000	!(OIS)
HSO2	2	252.000	4.290	0.000	0.000	1.000	!(OIS)
SO	1	301.000	3.993	0.000	0.000	1.000	!(OIS)
SO2	2	252.000	4.290	0.000	0.000	1.000	!(OIS)
SO3	2	378.400	4.175	0.000	0.000	1.000	!(OIS)
SIH4	2	207.6	4.084	0.000	0.000	1.000	!(mec)
SIH3	2	170.3	3.943	0.000	0.000	1.000	!(mec)
SIH2	2	133.1	3.803	0.000	0.000	1.000	!(mec)
SIH	1	95.8	3.662	0.000	0.000	1.000	!(mec)
SI	0	3036.	2.910	0.000	0.000	0.000	!(mec)
SI2H6	2	301.3	4.828	0.000	0.000	1.000	!(mec)
SI2H5	2	306.9	4.717	0.000	0.000	1.000	!(mec)
SI2H4	2	312.6	4.601	0.000	0.000	1.000	!(mec)
SI2H3	2	318.2	4.494	0.000	0.000	1.000	!(mec)
SI2H2	2	323.8	4.383	0.000	0.000	1.000	!(mec)
SI2	1	3036.	3.280	0.000	0.000	1.000	!(mec)
SI3	2	3036.	3.550	0.000	0.000	1.000	!(mec)
SIF4	2	171.9	4.880	0.000	0.000	1.000	!(sve)
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000	!(mec)
H3SISIH	2	312.6	4.601	0.000	0.000	1.000	!(mec)
SI3H8	2	331.2	5.562	0.000	0.000	1.000	!(mec)
ASH3	2	259.8	4.145	0.000	0.000	1.000	!(mec)
AS2	1	1045.5	5.510	0.000	0.000	1.000	!(mec)
GAME3	2	378.2	5.52	0.000	0.000	1.000	!(mec)
GAME2	2	675.8	5.22	0.000	0.000	1.000	!(mec)
GAME	2	972.7	4.92	0.000	0.000	1.000	!(mec)
GA	0	2961.8	4.62	0.000	0.000	0.000	!(mec)
K	0	850.	4.25	0.000	0.000	1.000	!(singh)
KOH	2	1213.	4.52	0.000	0.000	1.000	!(singh)
KO2	2	1213.	4.69	0.000	0.000	1.000	!(singh)
KO	1	383.0	3.812	0.000	0.000	1.000	!(singh)
KH	1	93.3	3.542	0.000	0.000	1.000	!(singh)
K+	0	850.	4.25	0.000	0.000	1.000	!(singh)
KCL	1	1989.	4.186	0.000	0.000	1.000	!(singh)
CL	0	130.8	3.613	0.000	0.000	1.000	!(singh)
CL-	0	130.8	3.613	0.000	0.000	1.000	!(singh)
HCL	1	344.7	3.339	1.084	0.000	1.000	!(singh)
CH2CL	2	858.000	3.400	0.000	0.000	0.000	! (**ois)
C2HCL3	2	280.000	3.971	0.000	0.000	0.000	! (**ois)
CCL	1	98.100	3.650	0.000	1.950	1.800	! (**ois)
CHOCL	2	498.000	3.590	0.000	0.000	0.000	! (**ois)
HOCL	2	107.400	3.458	0.000	0.000	0.000	! (**ois)
COCL	2	860.000	4.000	0.000	0.000	0.000	! (**ois)

CLO	2	110.000	3.590	0.000	0.000	0.000	! (**ois)
CL2O	2	356.000	2.649	0.000	0.000	0.000	! (**ois)
CLO2	2	107.400	3.458	0.000	0.000	0.000	! (**ois)
CH3CL	2	855.000	3.375	0.000	0.000	0.000	! (**ois)
F	0	80.000	2.750	0.000	0.000	0.000	!
F2	1	125.700	3.301	0.000	1.600	3.800	!
HF	1	330.000	3.148	1.920	2.460	1.000	! (sv/mec)
HF0	1	352.000	2.490	1.730	0.000	5.000	!
HF1	1	352.000	2.490	1.730	0.000	5.000	!
HF2	1	352.000	2.490	1.730	0.000	5.000	!
HF3	1	352.000	2.490	1.730	0.000	5.000	!
HF4	1	352.000	2.490	1.730	0.000	5.000	!
HF5	1	352.000	2.490	1.730	0.000	5.000	!
HF6	1	352.000	2.490	1.730	0.000	5.000	!
HF7	1	352.000	2.490	1.730	0.000	5.000	!
HF8	1	352.000	2.490	1.730	0.000	5.000	!
HOF	2	107.400	3.458	0.000	0.000	0.000	! (ois)
F2O	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO	1	109.600	3.412	0.000	0.000	0.000	! (ois)
HOOF	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
F2O2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
CH3F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CH2F2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF3	2	262.	4.123	1.8	0.000	0.000	!ReidPRW
CF4	2	134.0	4.662	0.000	0.000	0.000	!ReidPra
CH2F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF3	2	121.000	4.320	0.000	0.000	0.000	! (ois)
CHF	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF2	2	108.000	3.977	0.000	0.000	0.000	! (ois)
CF	1	94.200	3.635	0.000	0.000	0.000	! (Svehla)
CF3OH	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3OF	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CH2FO	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF2O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF:O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF2:O	2	350.500	4.906	0.000	0.000	0.000	! (ois)
CF:O	2	860.000	4.000	0.000	0.000	0.000	! (ois)
CH3-CH2F	2	312.2	4.583	2.0	0.000	0.000	!ReidPRW
CH3-CHF2	2	323.4	4.798	2.3	0.000	0.000	!ReidPRW
CH2F-CH2F	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF3	2	289.1	4.911	2.3	0.000	0.000	!ReidPRW
CH2F-CHF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF3	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CHF2-CHF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CHF2-CF3	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CF3-CF3	2	231.8	4.969	0.0	0.000	0.000	!PRW2/93
CH3-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH2F-CH2	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CHF2-CH2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CHF	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CF3-CH2	2	289.1	4.911	2.3	0.000	0.000	!PRW2/93
CF3-CHF	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CF3-CF2	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CH2:CHF	2	272.2	4.322	1.4	0.000	0.000	!ReidPRW
CH2:CF2	2	251.5	4.442	1.4	0.000	0.000	!ReidPRW
CHF:CHF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CHF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF2	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93

CF2:CF2	2	254.2	4.647	0.0	0.000	0.000	!ReidPRW
CH2:CF	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-E	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-Z	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CH	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CF	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
C2HF	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
C2F2	1	240.	4.4	0.	0.000	0.000	!PRW2/93
C2F	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
CHFCO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF2CO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
FCCO-E	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF2CL2	2	253.000	5.250	0.000	0.000	0.000	!(ois)
CF2CLBR	2	253.000	5.250	0.000	0.000	0.000	!(ois)
CF2CL	2	121.000	4.320	0.000	0.000	0.000	!(ois)
C6H5CH2	2	495.300	5.680	0.000	0.000	1.000	! NMM
C6H5CH3	2	495.300	5.680	0.430	12.30	1.000	! NMM
C6H5OCH3	2	495.300	5.680	0.430	12.30	1.000	! Est by Wenjun from
C6H5CH3							
C6H5OCH2	2	495.300	5.680	0.430	12.30	1.000	! Est by Wenjun from
C6H5CH3							
C6H4CH3	2	495.300	5.680	0.000	0.000	1.000	! NMM
C6H5CO	2	622.400	5.530	0.000	0.000	1.000	! NMM
C6H5CHO	2	622.400	5.530	0.000	0.000	1.000	! NMM
C6H5CH2OH	2	622.400	5.530	0.000	0.000	1.000	! Est from above
C6H5CH2O	2	622.400	5.530	0.000	0.000	1.000	! NMM
C6H5CH2OO	2	622.400	5.530	0.000	0.000	1.000	! EST by Wenjun as
C6H5CH2OH							
OC6H4CH3	2	621.100	5.640	0.000	0.000	1.000	! NMM
C6H4O2	2	621.100	5.640	0.000	0.000	1.000	! Est by Wenjun
HOC6H4CH3	2	621.100	5.640	0.000	0.000	1.000	! NMM
C6H5CH2CH3	2	523.600	5.960	0.000	0.000	1.000	! NMM
C6H5CH2CH2	2	523.600	5.960	0.000	0.000	1.000	! Est by Wenjun
C6H5CHCH2	2	546.200	6.000	0.130	15.00	1.000	! NMM
C6H5CHCH	2	546.200	6.000	0.000	0.000	1.000	! NMM
C6H5CCH2	2	546.200	6.000	0.000	0.000	1.000	
C6H5CCH	2	534.300	5.710	0.770	0.000	1.000	! NMM
C6H4CCH	2	534.300	5.710	0.000	0.000	1.000	! NMM
BiBenzyl	2	783.800	6.640	0.000	0.000	1.000	! NMM
C6H5C5H5	2	783.800	6.640	0.000	0.000	1.000	
C6H5C5H4	2	783.800	6.640	0.000	0.000	1.000	
C6H5C6H5	2	783.800	6.640	0.000	0.000	1.000	! Est by wenjun as
above species							
!							
! C3H2 isomers are From Miller 2008 email							
H2CCC(S)	1	290.616	4.368	0.000	0.000	1.000	!JAM 7/10/02
C3H2(S)	1	290.616	4.368	0.000	0.000	1.000	!JAM 7/10/02
C3H2C	1	290.616	4.368	0.000	0.000	1.000	! JAM 10/22/02
C3H	1	290.616	4.368	0.000	0.000	1.000	! LJcjp?
PC6H4O2	2	450.000	5.500	0.000	0.000	1.000	! HR
OC6H4O2	2	450.000	5.500	0.000	0.000	1.000	! HR
C6H3O2	2	450.000	5.500	0.000	0.000	1.000	! HR
C6H3O3	2	450.000	5.500	0.000	0.000	1.000	! "
!							
!							
!							
!-----Added by Wenjun on 20091117-----							
A2	2	630.4	6.18	0.00	16.50	1.000	! naphthalene
A2-	2	630.4	6.18	0.00	16.50	1.000	!

P2	2	676.5	6.31	0.00	20.00	1.000	!	biphe
!C6H5C6H5	2	783.800	6.640	0.000	0.000	1.000	!	Est by wenjun as
above species								
C6H5C6H5	2	676.5	6.31	0.00	20.00	1.000	!	biphe
!								
P2-	2	676.5	6.31	0.00	20.00	1.000	!	
INDENYL	2	402.9	6.744	0.000	0.000	1.000	!	MIT2b
INDENE	2	402.9	6.744	0.000	0.000	1.000	!	MIT2b
A2CH3	2	658.602	6.335	0.000	0.000	0.000	!	from Marina, from
Pitsch								
A2CH2	2	655.890	6.320	0.000	0.000	0.000	!	from Marina, from
Pitsch								
A2R5	2	693.1	6.47	0.00	18.00	1.000	!	acena
A2R5-	2	693.1	6.47	0.00	18.00	1.000	!	
A2C2H	2	693.1	6.47	0.00	18.00	1.000	!	
A2C2H*	2	693.1	6.47	0.00	18.00	1.000	!	
A3	2	772.0	6.96	0.00	38.80	1.000	!	phenanthrene
A3-	2	837.500	7.275	0.000	0.000	0.000		
A3C2H	2	879.600	7.561	0.000	0.000	0.000	!	MIT2b
A3C2H*	2	879.600	7.561	0.000	0.000	0.000	!	as A3C2H from
MIT2b								
A3CH3	2	879.600	7.561	0.000	0.000	0.000	!	MIT2b
A3CH2	2	879.600	7.561	0.000	0.000	0.000	!	as A3C2H MIT2b
A4	2	834.9	7.24	0.00	45.00	1.000	!	pyrene
A4R5	2	879.600	7.561	0.000	0.000	0.000		
A4-	2	834.9	7.24	0.00	45.00	1.000	!	pyrene
A4C2H	2	776.2	7.407	0.000	0.000	1.000	!	"PYRYNEP MIT2b
A4C2H*	2	776.2	7.407	0.000	0.000	1.000	!	" PYRYNEP*S
MIT2b								
C18H12	2	879.600	7.561	0.000	0.000	0.000	!	C18H10 from MIT2b
C18H11	2	879.600	7.561	0.000	0.000	0.000	!	C18H10 from MIT2b
BAPYR	2	833.062	8.087	0.000	0.000	1.000	!	MIT2b
BAPYR*S	2	833.062	8.087	0.000	0.000	1.000	!	+MIT2b
BGHIF	2	870.7	7.559	0.000	0.000	1.000	!	b[ghi] from
MIT2b								
C4H	1	357.000	5.180	0.000	0.000	1.000		
C6H	1	357.000	5.180	0.000	0.000	1.000		
C8H	1	357.000	5.180	0.000	0.000	1.000	!	C6H
C8H2	1	357.000	5.180	0.000	0.000	1.000	!	C6H2
C10H	1	357.000	5.180	0.000	0.000	1.000	!	C6H
C10H2	1	357.000	5.180	0.000	0.000	1.000	!	C6H2
C12H	1	357.000	5.180	0.000	0.000	1.000	!	C6H
C12H2	1	357.000	5.180	0.000	0.000	1.000	!	C6H2
C6H4CHCH2	2	546.2	6.00	0.13	15.00	1.000	!	
H2CC	2	238.	4.07	0.0	0.0	2.5	!	JAM(1/02)
c-C4H5	2	330.	5.09	0.0	0.0	1.	!	JAM 10/02
!								
! Below are from Detillex 09 JPCA								
!-----								
!C12H8	2	450.000	6.463	0.000	0.000	1.000	!	
cp !								
A2CH3-1	2	450.000	6.090	0.000	0.000	1.000	!	
cp !								
A2CH3-2	2	450.000	6.090	0.000	0.000	1.000	!	
cp !								
A2CH2-1	2	450.000	6.090	0.000	0.000	1.000	!	
cp !								
A2CH2-2	2	450.000	6.090	0.000	0.000	1.000	!	
cp !								
A2CH2-1f	2	450.000	6.090	0.000	0.000	1.000	!	
cp !								

A2CH2-2f	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
A2CH2-1f*	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
A2CH2-2f*	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C9H7	2	402.900	6.744	0.000	0.000	1.000 !
A2 (HR)						
C9H7a	2	402.900	6.744	0.000	0.000	1.000 !
A2 (HR)						
C9H7b	2	402.900	6.744	0.000	0.000	1.000 !
A2 (HR)						
C9H8	2	402.900	6.744	0.000	0.000	1.000 !
A2 (HR)						
C10H7O-1	2	402.900	6.744	0.000	0.000	1.000 !
"						
C10H7O-2	2	402.900	6.744	0.000	0.000	1.000 !
"						
A1C2H*2	2	450.000	5.646	0.000	0.000	1.000 !
HR						
C10H7	2	450.000	6.090	0.000	0.000	1.000 !
cp, HR						
C10H7a	2	450.000	6.090	0.000	0.000	1.000 !
cp, HR						
C10H7*2	2	450.000	6.090	0.000	0.000	1.000 !
cp, HR						
C6H5C3H2	2	450.000	5.719	0.000	0.000	1.000 !
HR						
!C12H9	2	450.000	6.463	0.000	0.000	1.000 !
cp !						
!BICPD*	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALS0	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALC10H10	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALC10H9	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALS1	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALS2	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALS3	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
VALS4	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9a	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9b	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9c	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9d	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H9e	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C10H8	2	450.000	6.090	0.000	0.000	1.000 !
cp !						
C7H6f	2	357.000	5.176	0.000	0.000	1.000
C12H8	2	450.000	6.463	0.000	0.000	1.000 !
cp !						
CH2CHCH2CCH	2	357.000	5.176	0.000	0.000	1.000
CH2CHCHCCH2	2	357.000	5.176	0.000	0.000	1.000
C6H5C3H2	2	450.000	5.719	0.000	0.000	1.000 !HR



CH3ONO	2	232.400	3.828	0.000	0.000	1.000	! same as HOONO
CH3ONO2	2	232.400	3.828	0.000	0.000	1.000	! same as HOONO
CH3NO	2	436.000	3.970	0.000	0.000	2.000	! same as CH3OO est
CH3NO2	2	576.7	4.549	0.000	0.000	1.000	! Same as CH3CO2 est
HCNN	2	232.400	3.828	0.000	0.000	1.000	! Same as HCNO
CH2CN	2	436.000	3.970	0.000	0.000	2.000	!same as CH2CO
CH3CN	2	436.000	3.970	0.000	0.000	2.000	!same as CH3CO
CH3NH2	1	569.000	3.630	0.000	0.000	1.000	! same as H2CN(os/jm)
CH2NH2	1	569.000	3.630	0.000	0.000	1.000	! same as H2CN(os/jm)
!c7h16-2	2	546.85	5.99	0	13.61	1	!calc SMS 2010
TMEDA	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-1	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-3	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-2	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
!iC3H7	2	266.800	4.982	0.000	0.000	1	
CH3NCH3	2	266.800	4.982	0.000	0.000	1	!same as iC3H7
!dc5h11	2	523.2	5.664	1.7	0.0	1	! wjp
N(CH3)2CH2CH2	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
!ic4h10	2	295.8	5.392	0.1	0.0	1	! !L-J from Mourits 1977
(Mani 2010)							
N(CH3)2CH2	2	295.8	5.392	0.1	0.0	1	!same as ic4h10
!AC3H5	2	260.000	4.850	0.000	0.000	1	! (JAM)
CH3NCH2	2	260.000	4.850	0.000	0.000	1	!same as AC3H5
TMEDA-0-5	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
N(CH3)2CHCH2	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
TMEDA-0-4	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-0-3	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-1-3	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-1-4	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-1-5	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
TMEDA-3-5	2	546.85	5.99	0	0	1	!same as c7h16-2 with 0
polarizability							
N(CH3)2CHCH	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
!C4H7	2	357.000	5.176	0.000	0.000	1	
CH2CHNCH3	2	357.000	5.176	0.000	0.000	1	!same as C4H7
CH2CH2NCH2	2	357.000	5.176	0.000	0.000	1	!same as C4H7
!C3H5	2	260.000	4.850	0.000	0.000	1	! (JAM)
CH2NCH2	2	260.000	4.850	0.000	0.000	1	!same as AC3H5
N(CH3+CH2)CHCH2	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
N(CH3)2CCH2	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
!C4H6-13	2	357.000	5.176	0.000	0.000	1	
CH2CHNCH2	2	357.000	5.176	0.000	0.000	1	!same as C4H6-13
N(CH3)2CCH	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
!CH2CHCHCH	2	357.000	5.180	0.000	0.000	1	! (JAM)
CHCHNCH2	2	357.000	5.180	0.000	0.000	1	!same as CH2CHCHCH
CH2CHNCH	2	357.000	5.180	0.000	0.000	1	!same as CH2CHCHCH
CH3NCH	2	260.000	4.850	0.000	0.000	1	!same as AC3H5
N(CH3+CH2)CH2CH3	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
!nC4H8-1	2	357.000	5.176	0.000	0.000	1	
CH3CH2NCH2	2	357.000	5.176	0.000	0.000	1	!same as nC4H8-1
CH3CHNCH2	2	357.000	5.176	0.000	0.000	1	!same as C4H7
!PC3H4	1	252.000	4.760	0.000	0.000	1	
CH2NCH	2	252.000	4.760	0.000	0.000	1	!same as PC3H4
CH3N(NH2)NO2	2	523.2	5.664	1.7	0.0	1	!same as dc5h11



CH3N (NH2) ONO	2	523.2	5.664	1.7	0.0	1	!same as dc5h11
H2NN	2	71.400	3.798	0.000	0.000	1.000	! same as N2H2
HON	2	116.700	3.492	0.000	0.000	1.000	! same as HNO
HNNNH2	2	252.000	4.760	0.000	0.000	1.000	! same as H2CCCH (JAM)
HNOO	2	232.400	3.828	0.000	0.000	1.000	! same as HONO
HONHO	2	232.400	3.828	0.000	0.000	1.000	! same as HONO
NH2NO2	2	232.400	3.828	0.000	0.000	1.000	! same as HNO3
NCH2	1	569.000	3.630	0.000	0.000	1.000	!(os/jm)
NH2NO	2	232.400	3.828	0.000	0.000	1.000	! same as HNNO (*)
NHNHO	2	232.400	3.828	0.000	0.000	1.000	! same as HNNO (*)
NH2NHO	2	232.400	3.828	0.000	0.000	1.000	! same as HNNO (*)
NH2OH	2	116.700	3.492	0.000	0.000	1.000	! same as HNO (*)
CH3OCH3	2	329.400	4.624	0.000	0.000	1.000	!loc_est
CH3OCH2	2	329.400	4.624	0.000	0.000	1.000	!=CH3OCH3
CH3OCH2O	2	470.900	4.862	0.000	0.000	1.000	!loc_est
CH3OCHO	2	406.500	4.709	0.000	0.000	1.000	!loc_est
CH3OCO	2	406.500	4.709	0.000	0.000	1.000	!=CH3OCH
OCHO	2	485.400	4.410	0.000	0.000	1.000	!loc_est
C2	1	97.530	3.621	0.000	1.760	4.000	
CHCNH	1	252.000	4.760	0.000	0.000	1.000	! = c3h4
CH3CH2NH2	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH3NHCH3	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH2CH2NH2	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH3NCH3	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH3NHCH2	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH3CHNH2	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH3CH2NH	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
CH2CHNH2	2	303.400	4.810	0.000	0.000	1.000	! = c3h7
CH3CHNH	2	303.400	4.810	0.000	0.000	1.000	! = c3h7
CH3NCH2	2	303.400	4.810	0.000	0.000	1.000	! = c3h7
CH2CHNH	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CHCHNH2	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH2NCH2	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH3CHN	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH3NCH	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH3CNH	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH2CNH2	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
CH2CNH	2	260.000	4.850	0.000	0.000	1.000	! = c3h5
CH2CHN	2	260.000	4.850	0.000	0.000	1.000	! = c3h5
CH2CHN (S)	2	260.000	4.850	0.000	0.000	1.000	! = c3h5
c-C2H3N	2	260.000	4.850	0.000	0.000	1.000	! = c3h5
CHCNH2	2	260.000	4.850	0.000	0.000	1.000	! = c3h5
H2NCHO	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
H2NCO	2	307.800	4.140	0.000	0.000	1.000	! = c3h6
NCCN	1	349.000	4.361	0.000	0.000	1.000	!(OIS)
CH2CHOH	2	436.000	3.970	0.000	0.000	2.000	! = CH3CHO
OCHCHO	2	406.937	4.823	0.000	0.000	2.000	! LJcjp
CH3N	2	569.000	3.630	0.000	0.000	1.000	! same as H2CN (os/jm)
CH2NN	2	232.400	3.828	0.000	0.000	1.000	! same as CNN (OIS)
CH2NNH2	2	260.000	4.850	0.000	0.000	1.000	! same as C3H5 (JAM)
CH2NO	2	232.400	3.828	0.000	0.000	1.000	! same as HCNO (JAM)
CH2NHNH2	2	260.000	4.850	0.000	0.000	1.000	! same as C3H5 (JAM)
CH3NHNH	2	260.000	4.850	0.000	0.000	1.000	! same as C3H5 (JAM)
CH3CH2NHCH2CHO	2	413.	5.909	0.000	0.000	1.000	! same as 1hexene:
BSL60 for nC6H14							
NH2CH2CH2OCHCH2	2	413.	5.909	0.000	0.000	1.000	! same as 1hexene:
BSL60 for nC6H14							
CH3CH2OCH2CHNH	2	413.	5.909	0.000	0.000	1.000	! same as 1hexene:
BSL60 for nC6H14							
OHCH2CH2NHCHCH2	2	413.	5.909	0.000	0.000	1.000	! same as 1hexene:
BSL60 for nC6H14							
CH3OCH2CH2NCH2	2	413.	5.909	0.000	0.000	1.000	! same as 1hexene:
BSL60 for nC6H14							

cyOrthoOOMorphyl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyMetaOOMorphyl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyParaOOMorphyl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyOrtho*Morph3yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyOrtho*Morph4yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyOrtho*Morph5yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyOrtho*Morph6yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyMeta*Morph2yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyMeta*Morph4yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyMeta*Morph5yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyMeta*Morph6yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyPara*Morph2yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
cyPara*Morph3yl	2	475.7	5.916	0.0	0.0	1.0	!	same as
methylcyclohexane	from Westbrook mechanisms							
CH2CH2OCH*CHNH	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH2NHCH*CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2OCH2CH*NCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCH2CH2N*CHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCH2CH2NHCHCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
NHCH2CH2OCHCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2OCH2CH2NCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH2OCH2CHN*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2OCH*CH2NCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
NHCH2CH*OCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCH2CH*NHCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH2N*CH2CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*OCH2CH2NCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*CH2NHCH2CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*CH2OCH2CHNH	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
N*CH2CH2OCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH*OCH2CHNH	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCH*CH2NHCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH*NHCH2CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
NHCH*CH2OCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								

OCH*CHNH	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
NHCH*CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH*NCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2N*CHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2NHCHCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2OCHCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH2CH2NCH*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCH2CHN*	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*CH2NCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*OCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
CH*NHCHCH2	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
N*CH2CHO	2	413.	5.909	0.000	0.000	1.000	!	same as 1hexene:
BSL60 for nC6H14								
OCHOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
CH2CHOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
CH2NOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
NHCHOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
CHCHOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
NCHOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
CHNOOH	2	428.8	4.958	2.9	0.0	1.0	!	WJP: C2H3CHO
NHCHCHO	2	429.000	4.999	2.9	0.	1.	!	same as CH3CHCHO

### A.1.1 Full Labbe Model

#### Kinetic parameters in CHEMKIN format

```

=====
REACTIONS
=====
!= Acetylene Mechanism Subset =
=====
!Reaction                A          n      Ea      ref.
!-----
!-----H2/O2 chemistry-----
2O+M=O2+M                6.16E+15  -0.50    0.    ! (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.0/
2O+AR=O2+AR              1.89E+13   0.00   -1790. ! (1) TSA/HAM 86
O+H+M=OH+M               4.71E+18  -1.00    0.    ! (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.75/
H2+M=2H+M                4.58E+19  -1.40   104380. ! (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.0/
H2+AR=2H+AR              5.84E+18  -1.10   104380. ! (1) TSA/HAM 86
H+OH+M=H2O+M            2.21E+22  -2.00    0.    ! (45) Baulch 92
  H2O/12.0/ H2/2.5/ AR/0/
H+OH+AR=H2O+AR          8.41E+21  -2.00    0.    ! (1) TSA/HAM 86
H2O2 (+M)=2OH (+M)      2.95E+14   0.00   48400. ! (2) BRO/COB 87
  LOW
  H2O/12.00/ H2/2.5/ AR/0.16/
  /1.20E+17   0.00   45500./ ! (3) Warnatz 84

```

```

H2O+O=OH+OH                2.97E+06  2.02  13400.  ! (4) Sutherland 91
O+H2=H+OH                   5.08E+04  2.67   6290.  ! (5) Sutherland 86
OH+H2=H+H2O                 2.16E+08  1.51   3430.  ! (6) Michael/Sutherland
88
H+O2 (+M)=HO2 (+M)          1.48E+12  0.60    0.  ! (7) Cobos 85
  LOW                        /3.50E+16 -0.41 -1120./ ! (8) Mueller 99
  H2O/12.0/ H2/2.5/ AR/0.05/
H+O2=O+OH                   4.489E+08  1.257  16191.  ! (9) Miller/Pilling 05
  DUPLICATE
H+O2=O+OH                   2.076E+16 -0.673  16191.  ! (9) Miller/Pilling 05
  DUPLICATE
O+HO2=OH+O2                 3.25E+13  0.00    0.  ! (10) Baulch 94
H+HO2=O2+H2                 1.66E+13  0.00   820.  ! (8) Mueller 99
H+HO2=2OH                   7.08E+13  0.00   300.  ! (8) Mueller 99
OH+HO2=O2+H2O              4.64E+13  0.00  -500.  ! (11) GRI 1.2
2HO2=O2+H2O                1.30E+11  0.00 -1630.  ! (12) HIP/TRO 90
  DUPLICATE
2HO2=O2+H2O                4.20E+14  0.00  11980.  ! (12) HIP/TRO 90
  DUPLICATE
O+H2O2=OH+HO2              9.55E+06  2.00   3970.  ! (1) TSA/HAM 86
H+H2O2=HO2+H2              4.82E+13  0.00   7950.  ! (1) TSA/HAM 86
H+H2O2=OH+H2O              2.41E+13  0.00   3970.  ! (1) TSA/HAM 86
OH+H2O2=HO2+H2O           1.00E+12  0.00    0.  ! (13) HIP/TRO 92
  DUPLICATE
OH+H2O2=HO2+H2O           5.80E+14  0.00   9560.  ! (13) HIP/TRO 92
  DUPLICATE
!-----CO chemistry-----
!
O+CO (+M)=CO2 (+M)          1.80E+10  0.00   2385.  ! (1) TSA/HAM 86
  LOW                        /6.02E+14  0.00  3000./
  H2/2./ O2/6./ H2O/6./ CH4/2./ CO/1.5/ CO2/3.5/ C2H6/3.0/ AR/0.5/
O2+CO=O+CO2                2.50E+12  0.00  47800.  ! (3) Warnatz 84
H2+CO (+M)=CH2O (+M)       4.30E+07  1.50  79600.  ! (14) GRI-Mech 1.2
  LOW                        /5.07E+27 -3.42  84350./
  TROE /0.932 197 1540 10300/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+CO=H+CO2                4.10E+04  2.11 -1578.  ! (15) Carriere 04
! Miller
! CO+OH=CO2+H              2.1370E05  1.9000 -1064.0 ! JPS,SJK,&JAM 30th symp
! PLOG/ 0.01315 2.1370E05 1.9000 -1064.0/
! PLOG/ 0.1315 2.4537E05 1.8800 -1042.6/
! PLOG/ 1.315 8.7059E05 1.7300 -685.32/
! PLOG/ 13.158 6.7579E06 1.4800 48.483/
! PLOG/ 131.58 2.3432E07 1.3500 974.42/
! CO+OH=HOCO 1.6589E15 -2.6800 859.18 ! JPS,SJK,&JAM 30th Symp
! PLOG/ 0.013158 1.6589E15 -2.6800 859.18/
! PLOG/ 0.13158 5.8859E18 -3.3500 887.00/
! PLOG/ 1.3158 2.5693E20 -3.5000 1309.0/
! PLOG/ 13.158 7.0764E20 -3.3200 1762.9/
! PLOG/ 131.58 1.1215E20 -2.7800 2055.6/
HO2+CO=OH+CO2              1.50E+14  0.00  23600.  ! (16) Baulch 76
O+HCO=OH+CO                3.00E+13  0.00    0.  ! (1) TSA/HAM 86
O+HCO=H+CO2                3.00E+13  0.00    0.  ! (1) TSA/HAM 86
H+HCO (+M)=CH2O (+M)       1.09E+12  0.48  -260.  ! (17) Eiteneer 98
  LOW                        /2.47E+24 -2.57  425./
  TROE /0.7824 271 2755 6570/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H+HCO=H2+CO                7.30E+13  0.00    0.  ! (18) TIMONEN 87a
OH+HCO=H2O+CO              3.00E+13  0.00    0.  ! (1) TSA/HAM 86
HCO+M=H+CO+M               1.87E+17 -1.00  17000.  ! (19) TIMONEN 87b
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
HCO+O2=HO2+CO              4.22E+12  0.00    0.  ! (20) TIMONEN 88
HCO+HO2=CO2+OH+H          3.00E+13  0.00    0.  ! (1) TSA/HAM 86
!
!-----CHxO chemistry-----
!

```

O+CH2O=OH+HCO	1.81E+13	0.00	3078.	!	(1)	TSA/HAM 86
O2+CH2O=HO2+HCO	2.05E+13	0.00	38920.	!	(1)	TSA/HAM 86
!Miller						
!CH2O+O2=HCO+HO2	2.44E5	2.5	36461.	!		Baulch 2004
H+CH2O=HCO+H2	5.18E+7	1.66	1834.	!	(21)	Hochgreb 92
H+CH2O(+M)=CH2OH(+M)	5.40E+11	0.45	3600.	!	(22)	GRI 3.0
LOW	/1.27E+32	-4.82	6530./			
TROE /0.7187 103 1291 4160/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/						
H+CH2O(+M)=CH3O(+M)	5.40E+11	0.45	2600.	!	(14)	GRI-Mech 1.2
LOW	/2.20E+30	-4.80	5560./			
TROE /0.758 94 1555 4200/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/						
OH+CH2O=HCO+H2O	3.43E+09	1.18	-447.	!	(1)	TSA/HAM 86
HO2+CH2O=HCO+H2O2	1.47E+13	0.00	15200.	!	(21)	Hochgreb 92
! Miller						
! CH2O+HO2=HCO+H2O2	3.0E12	0.0	13000.	!		CEC 1994
O+CH2OH=OH+CH2O	4.20E+13	0.00	0.	!	(23)	Tsang 87
H+CH2OH=H2+CH2O	6.00E+12	0.00	0.	!	(23)	Tsang 87
H+CH2OH=OH+CH3	9.63E+13	0.00	0.	!	(1)	TSA/HAM 86
OH+CH2OH=H2O+CH2O	2.40E+13	0.00	0.	!	(23)	Tsang 87
CH2OH+O2=HO2+CH2O	2.41E+14	0.00	5017.	!	(24)	Grotheer 88
DUPLICATE						
CH2OH+O2=HO2+CH2O	1.51E+15	-1.00	0.	!	(24)	Grotheer 88
DUPLICATE						
CH2OH+HO2=CH2O+H2O2	1.20E+13	0.00	0.	!	(23)	Tsang 87
CH2OH+HCO=CH3OH+CO	1.20E+14	0.00	0.	!	(23)	Tsang 87
CH2OH+HCO=CH2O+CH2O	1.80E+14	0.00	0.	!	(23)	Tsang 87
2CH2OH=CH3OH+CH2O	3.00E+12	0.00	0.	!	(23)	Tsang 87
CH2OH+CH3O=CH3OH+CH2O	2.40E+13	0.00	0.	!	(23)	Tsang 87
O+CH3O=OH+CH2O	6.00E+12	0.00	0.	!	(1)	TSA/HAM 86
H+CH3O=H2+CH2O	2.00E+13	0.00	0.	!	(3)	Warnatz 84
H+CH3O=OH+CH3	3.20E+13	0.00	0.	!	(14)	GRI-Mech 1.2
OH+CH3O=H2O+CH2O	1.80E+13	0.00	0.	!	(23)	Tsang 87
CH3O+O2=HO2+CH2O	9.03E+13	0.00	11980.	!	(26)	Wantuck 87
DUPLICATE						
CH3O+O2=HO2+CH2O	2.20E+10	0.00	1748.	!	(26)	Wantuck 87
DUPLICATE						
CH3O+HO2=CH2O+H2O2	3.00E+11	0.00	0.	!	(23)	Tsang 87
CH3O+CO=CH3+CO2	1.57E+13	0.00	11800.	!	(23)	Tsang 87
CH3O+HCO=CH3OH+CO	9.00E+13	0.00	0.	!	(23)	Tsang 87
2CH3O=CH3OH+CH2O	6.00E+13	0.00	0.	!	(23)	Tsang 87
O+CH3OH=OH+CH2OH	3.88E+05	2.50	3080.	!	(23)	Tsang 87
H+CH3OH=CH2OH+H2	1.44E+13	0.00	6095.	!	(25)	Held 98
H+CH3OH=CH3O+H2	3.60E+12	0.00	6095.	!	(25)	Held 98
OH+CH3OH=CH2OH+H2O	7.10E+06	1.80	-596.	!	(27)	Bott 91
OH+CH3OH=CH3O+H2O	1.00E+06	2.10	496.5	!	(27)	Bott 91
CH3+CH3OH=CH2OH+CH4	3.19E+01	3.17	7172.	!	(23)	Tsang 87
O2+CH3OH=CH2OH+HO2	2.05E+13	0.00	44900.	!	(23)	Tsang 87
HCO+CH3OH=CH2OH+CH2O	9.63E+03	2.90	13110.	!	(23)	Tsang 87
HO2+CH3OH=CH2OH+H2O2	3.98E+13	0.00	19400.	!	(28)	Cathonnet 82
CH3O+CH3OH=CH2OH+CH3OH	3.00E+11	0.00	4060.	!	(23)	Tsang 87
CH3OH(+M)=CH3+OH(+M)	1.90E+16	0.00	91730.	!	(25)	Held 98
LOW	/2.95E+44	-7.35	95460./			
TROE /0.414 279 5459 /						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/						
! Miller						
! OH+CH3(+M)=CH3OH(+M)	4.34E15	-0.79	0.0	!		BAULCH ET AL 2004
LOW/3.85E37 -6.21 1333/						
TROE/0.25 210 1434/						
! N2/1.43/ H2O/8.58/ CO2/3/ CO/2/ H2/2/						
CH3OH(+M)=CH2OH+H(+M)	2.69E+16	-0.08	98940.	!	(25)	Held 98

```

LOW /2.34E+40 -6.33 103100.0/
TROE /0.773 693 5333 /
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!
!-----CH4 (CHx) chemistry-----
!
O+CH4=OH+CH3 1.02E+09 1.50 8600. ! (1) TSA/HAM 86
H+CH4=CH3+H2 6.60E+08 1.62 10840. ! (22) GRI 3.0
OH+CH4=CH3+H2O 1.00E+08 1.60 3120. ! (30) Cohen 91
CH+CH4=H+C2H4 6.00E+13 0.00 0. ! (31) Butler 80
CH2SING+CH4=2CH3 1.60E+13 0.00 -570. ! (22) GRI 3.0
CH2+CH4=2CH3 2.46E+06 2.00 8270. ! (32) Bohland 85
O+CH3=H+CH2O 5.06E+13 0.00 0. ! (22) GRI 3.0
O+CH3=H+H2+CO 3.37E+13 0.00 0. ! (22) GRI 3.0
! Used by Miller
!CH3+O=CH2O+H 7.14E13 0.0 0.0 !Baulch 2004
!CH3+O=CO+H2+H 1.26E13 0.0 0.0 ! JAM ( 15% branching)

H+CH3 (+M)=CH4 (+M) 1.39E+16 -0.53 536. ! (22) GRI 3.0
LOW /2.62E+33 -4.76 2440. /
TROE /0.783 74 2941 6964/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+CH3=CH2+H2O 5.60E+07 1.60 5420. ! (22) GRI 3.0
OH+CH3=CH2SING+H2O 6.44E+17 -1.34 1417. ! (22) GRI 3.0
! Miller
! OH+CH3 (+M)=CH2SING+H2O (+M) 6.4E-8 5.8 -964. ! BAULCH ET AL 2004
! LOW/1.08E16 -0.91 546. /
! TROE/0.336 3569. 108. 3240. /
!OH+CH3=CH2OH+H 7.23E11 0.0 5484. ! BAULCH ET AL 2004
!OH+CH3=CH3O+H 1.2E10 0.0 13889. ! BAULCH ET AL 2004
!OH+CH3=CH2O+H2 3.19E9 0.0 5027. ! BAULCH ET AL 2004
!OH+CH3 (+M)=HCOH+H2 (+M) 1.14E-17 8.0 -2464. ! BAULCH ET AL 2004
! LOW/2.29E10 -0.12 -415. /
! TROE/0.705 3704. 312. 1238. /

HO2+CH3=O2+CH4 1.00E+12 0.00 0. ! (33) Reid 84
HO2+CH3=OH+CH3O 2.00E+13 0.00 0. ! (1) TSA/HAM 86
CH+CH3=H+C2H3 3.00E+13 0.00 0. ! (34) Miller 89
CH2SING+CH3=H+C2H4 1.20E+13 0.00 -570. ! (14) GRI-Mech 1.2
CH3+O2=O+CH3O 3.56E+13 0.00 30480. ! (22) GRI 3.0
CH3+O2=OH+CH2O 2.31E+12 0.00 20315. ! (22) GRI 3.0
! Miller
!CH3+O2=CH3O+O 6.08E7 1.54 27957. ! Herbon,etal (30th Symp)
!CH3+O2=CH2O+OH 68.6 2.86 9474. ! Herbon,etal (30th Symp)
CH3+H2O2=HO2+CH4 2.45E+04 2.47 5180. ! (22) GRI 3.0
2CH3 (+M)=C2H6 (+M) 6.77E+16 -1.18 654. ! (22) GRI 3.0
LOW /3.40E+41 -7.03 2763./
TROE /0.619 73.2 1180 9999/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Below from Miller
! CH3+CH3 (+M)=C2H6 (+M) 9.22E16 -1.174 635.8 ! PILL,WAG 23RD
! LOW/1.135E36 -5.246 1704.8/
! TROE/0.405 1120. 69.6/
! H2/2/ CO/2/ CO2/3/ H2O/5/

2CH3=H+C2H5 6.84E+12 0.10 10600. ! (22) GRI 3.0
! Miller
! C2H5+H=CH3+CH3 3.47E13 0.205 -41.38 ! SJK theory*0.9(recrossing)

CH3+HCO=CH4+CO 1.21E+14 0.00 0. ! (1) TSA/HAM 86
CH3+CH2O=HCO+CH4 3.32E+03 2.81 5860. ! (22) GRI 3.0
! Miller
! CH2O+CH3=HCO+CH4 7.8E-8 6.1 1967. ! CEC 1994

CH2+CH3=H+C2H4 4.00E+13 0.00 0. ! (3) Warnatz 84

```

O+CH2=H+HCO	8.00E+13	0.00	0.	!	(35)	Herron 88
O+CH2SING=H2+CO	1.50E+13	0.00	0.	!	(1)	TSA/HAM 86
O+CH2SING=H+HCO	1.50E+13	0.00	0.	!	(1)	TSA/HAM 86
H+CH2 (+M)=CH3 (+M)	6.00E+14	0.00	0.	!	(22)	GRI 3.0
LOW	/1.04E+26	-2.76	1600./			
TROE /0.562 91 5836 8552/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/						
H+CH2SING=CH+H2	3.00E+13	0.00	0.	!	(1)	TSA/HAM 86
OH+CH2=H+CH2O	2.00E+13	0.00	0.	!	(1)	TSA/HAM 86
OH+CH2=CH+H2O	1.13E+07	2.00	3000.	!	(1)	TSA/HAM 86
OH+CH2SING=H+CH2O	3.00E+13	0.00	0.	!	(1)	TSA/HAM 86
HO2+CH2=OH+CH2O	2.00E+13	0.00	0.	!	(1)	TSA/HAM 86
CH+CH2=H+C2H2	4.00E+13	0.00	0.	!	(36)	Braun 81
CH2+O2=OH+H+CO	5.00E+12	0.00	1500.	!	(37)	Vinckier 79
CH2+O2=CO2+2H	5.80E+12	0.00	1500.	!	(37)	Vinckier 79
CH2+O2=O+CH2O	2.40E+12	0.00	1500.	!	(37)	Vinckier 79
CH2+H2=H+CH3	5.00E+05	2.00	7230.	!	(22)	GRI 3.0
2CH2=H2+C2H2	1.60E+15	0.00	11944.	!	(38)	Bauerle 95
2CH2=H+H+C2H2	2.00E+14	0.00	10989.	!	(38)	Bauerle 95
CH2SING+CO=CH2+CO	9.00E+12	0.00	0.	!	(22)	GRI 3.0
CH2SING+AR=CH2+AR	9.00E+12	0.00	600.	!	(22)	GRI 3.0
CH2SING+CO2=CH2+CO2	7.00E+12	0.00	0.	!	(39)	Koch 90
CH2SING+CO2=CO+CH2O	1.40E+13	0.00	0.	!	(39)	Koch 90
CH2+CO (+M)=CH2CO (+M)	8.10E+11	0.50	4510.	!	(22)	GRI 3.0
LOW	/2.69E+33	-5.11	7095./			
TROE /0.5907 275 1226 5185/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.00/ C2H6/3.00/						
CH2SING+O2=H+OH+CO	2.80E+13	0.00	0.	!	(40)	Langford 83
CH2SING+O2=CO+H2O	1.20E+13	0.00	0.	!	(40)	Langford 83
CH2SING+H2=CH3+H	7.00E+13	0.00	0.	!	(22)	GRI 3.0
CH2SING+H2O (+M)=CH3OH (+M)	4.82E+17	-1.16	1145.	!	(22)	GRI 3.0
LOW	/1.88E+38	-6.36	5040./			
TROE /0.6027 208 3922 10180/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/						
CH2SING+H2O=CH2+H2O	3.00E+13	0.00	0.	!	(41)	Hack 88
CH2SING+H2O=H2+CH2O	6.82E+10	0.25	-935.	!	(22)	GRI 3.0
O+CH=H+CO	5.70E+13	0.00	0.	!	(42)	MESSING 80
OH+CH=H+HCO	3.00E+13	0.00	0.	!	(43)	Glarborg 86
CH+O2=O+HCO	6.71E+13	0.00	0.	!	(22)	GRI 3.0
CH+H2=H+CH2	1.08E+14	0.00	3110.	!	(22)	GRI 3.0
CH+H2O=H+CH2O	5.71E+12	0.00	-755.	!	(10)	Baulch 94
CH+CO (+M)=HCCO (+M)	5.00E+13	0.00	0.	!	(14)	GRI-Mech 1.2
LOW	/2.69E+28	-3.74	1936./			
TROE /0.5757 237 1652 5069/						
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/						
CH+CO2=HCO+CO	1.90E+14	0.00	15792.	!	(44)	Markus 96
CH+CH2O=H+CH2CO	9.46E+13	0.00	-515.	!	(45)	Baulch 92
CH+HCCO=CO+C2H2	5.00E+13	0.00	0.	!	(34)	Miller 89
!						
!-----C2H6 chemistry-----						
!						
O+C2H6=OH+C2H5	3.00E+07	2.00	5115.	!	(46)	Miller 92
H+C2H6=C2H5+H2	5.40E+02	3.50	5210.	!	(46)	Miller 92
OH+C2H6=C2H5+H2O	7.26E+06	2.00	864.	!	(45)	Baulch 92
CH3+C2H6=C2H5+CH4	5.50E-01	4.00	8300.	!	(46)	Miller 92
CH2SING+C2H6=CH3+C2H5	4.00E+13	0.00	-550.	!	(47)	Wegener 90
C2H6+O2=C2H5+HO2	4.04E+13	0.00	50872.	!	(1)	TSA/HAM 86
C2H6+CH2OH=CH3OH+C2H5	1.99E+02	3.00	13976.	!	(23)	Tsang 87
C2H6+CH3O=CH3OH+C2H5	2.41E+11	0.00	7094.	!	(1)	TSA/HAM 86
C2H6+C2H=C2H2+C2H5	3.61E+12	0.00	0.	!	(1)	TSA/HAM 86
C2H6+C2H3=C2H4+C2H5	6.01E+02	3.30	10502.	!	(1)	TSA/HAM 86
C2H6+CH3CO=CH3CHO+C2H5	1.81E+4	2.75	17527.	!	(1)	TSA/HAM 86
C2H6+HCO=CH2O+C2H5	4.70E+04	2.72	18235.	!	(1)	TSA/HAM 86
!						
!-----C2H5 chemistry-----						
!						

```

O+C2H5=CH3+CH2O          2.24E+13   0.00           0.   ! (22) GRI 3.0
! Miller
! C2H5+O=CH3+CH2O        4.2E13   0.0   0.0   !JAM&PG rbn (Slagle 1988)

O+C2H5=H+CH3CHO          1.10E+14   0.00           0.   ! (22) GRI 3.0
H+C2H5=H2+C2H4           2.00E+12   0.00           0.   ! (22) GRI 3.0
H+C2H5(+M)=C2H6(+M)      5.21E+17  -0.99          1580. ! (22) GRI 3.0
  LOW                      /1.99E+41  -7.080        6685./
  TROE /0.8422 125 2219 6882/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H5+O2=HO2+C2H4        1.92E+07   1.02          -2035. ! (48) Miller 00
! Miller
! C2H5+O2(+M)= C2H4+HO2(+M) 1.41E7 1.09 -1975.
! HIGH/6.85E-12 6.53 -834./
! TROE/0.45 1.E-10 1.E10/
! H2/2/ CO/2/ CO2/3/ H2O/5/   ! not sure what this does
! C2H5+O2=C2H4+HO2        5.81E6   1.57 20578. ! Miller&Klipp 28th(abs)

C2H5+HO2=C2H5O+OH        3.00E+13   0.00           0.   ! (49) Bozzelli 90
C2H5+HO2=C2H4+H2O2       3.01E+11   0.00           0.   ! (1) TSA/HAM 86
C2H5+OH=C2H4+H2O         2.41E+13   0.00           0.   ! (1) TSA/HAM 86
C2H5+CH3=CH4+C2H4        1.13E+12  -0.50           0.   ! (1) TSA/HAM 86
CH3+C2H5(+M)=C3H8(+M)    9.60E+14  -0.50           0.   ! (50) Qin/Wan 00
  LOW                      /6.80E+61  -13.42        6000./
  TROE /1.00 1000 1433.9 5328.8/
C2H5+CH2OH=C2H4+CH3OH    2.41E+12   0.00           0.   ! (23) Tsang 87
C2H5+CH2OH=C2H6+CH2O     2.41E+12   0.00           0.   ! (23) Tsang 87
C2H5+CH3O=C2H6+CH2O      2.41E+13   0.00           0.   ! (1) TSA/HAM 86
C2H5+C2H=C2H2+C2H4       1.81E+12   0.00           0.   ! (1) TSA/HAM 86
CH2+C2H5=C2H4+CH3        1.81E+13   0.00           0.   ! (1) TSA/HAM 86
CH2SING+C2H5=C2H4+CH3    9.00E+12   0.00           0.   ! (1) TSA/HAM 86
C2H5+CH2SING=C3H6+H      9.00E+12   0.00           0.   ! (1) TSA/HAM 86
C2H5+H2O2=C2H6+HO2       8.73E+09   0.00           974.  ! (1) TSA/HAM 86
!
!-----C2H4 chemistry-----
!
!H+C2H4(+M)=C2H5(+M)      5.40E+11   0.45          1820. ! (22) GRI 3.0
! LOW                      /6.00E+41  -7.62          6970./
! TROE /0.9753 210 984 4374/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
H+C2H4(+M)=C2H5(+M)      1.367E9   1.463 1355.   ! Miller&Klipp.
  LOW/2.026E39 -6.642 5769./
TROE/-0.569 299. -9147. 152.4/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! N2/1.2/ CO/1.5/ H2/2/ CO2/3/ H2O/10./

H+C2H4=C2H3+H2           1.12E+07   2.12          13366. ! (51) Bhargava 98
!OH+C2H4=C2H3+H2O        5.53E+05   2.31          2900.  ! (51) Bhargava 98
OH+C2H4=C2H3+H2O         1.31E-01   4.20          -860   ! JPCA 110 6960-6970 (2006)
OH+C2H4=CH3+CH2O         3.19E+01   2.71          -1172. ! JPCA 110 6960-6970 (2006)
OH+C2H4=CH3CHO+H         8.73E-05   4.57          -618.  ! JPCA 110 6960-6970 (2006)
! Miller OH+C2H4=H2O+C2H3 1.31E-01 4.20 -860 ! JPCA 110 6960-6970 (2006)
! OH+C2H4=CH3+CH2O 5.35E+00 2.92 -1733 ! JPCA 110 6960-6970 (2006)
! this reaction is in line 792-798
! 0 1.60E-01 3.34 -2776
! PLOG /0.01 5.35E+00 2.92 -1733./
! PLOG /0.025 3.19E+01 2.71 -1172./
! PLOG /0.1 5.55E+02 2.36 -181./
! PLOG /1. 1.78E+05 1.68 2061./
! PLOG /10. 2.37E+09 0.56 6007./
! PLOG /100. 2.76E+13 -0.50 11455./
! OH+C2H4=CH3CHO+H 2.37E-07 5.30 -2051 ! JPCA 110 6960-6970 (2006)
! this reaction is in line 799-805

```



```

! 0      8.91E-09      5.69      -3209
! PLOG /0.01      2.37E-07      5.30      -2051./
! PLOG /0.025      8.73E-05      4.57      -618./
! PLOG /0.1      4.03E-01      3.54      1882./
! PLOG /1.      2.38E-02      3.91      1723./
! PLOG /10.      8.25E+08      1.01      10507./
! PLOG /100.      6.80E+09      0.81      13867./

CH3+C2H4=C2H3+CH4      2.27E+05      2.00      9200. ! (22) GRI 3.0
CH3+C2H4 (+M) <=>nC3H7 (+M)      2.55E+06      1.600      5700. ! (52) Tsang 88
  LOW      /3.00E+63      -14.6      18170./
  TROE /0.1894 277. 8748. 7891./
  H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
C2H4 (+M)=H2+C2H2 (+M)      8.00E+12      0.44      88770. ! (22) GRI 3.0
  LOW      /1.58E+51      -9.30      97800./
  TROE /0.7345 180 1035 5417/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! C2H4+CH2SING=C3H6      9.03E+13      0.00      0. ! (1) TSA/HAM 86
C2H4+CH2SING=AC3H5+H      4.53E+13      0.00      -556. ! Baulch 2004
! Miller CH2SING+C2H4=CH2CHCH2+H      4.53E13      0.0      -556. ! Baulch 2004
C2H4+HO2=C2H4O+OH      6.03E+09      0.00      7949. ! (1) TSA/HAM 86
C2H4+O=H+CH2CHO      7.33E+07      1.60      1260. ! (53) Westmoreland PC
C2H4+O=CH3+HCO      1.13E+08      1.60      1020. ! (53) Westmoreland PC
! Miller
! C2H4+O=CH3+HCO      8.16E6      1.88      182.8 ! BAULCH 2004 similar to CEC 94

C2H4+O=C2H3+OH      2.15E+06      2.55      11900. ! (53) Westmoreland PC
C2H4+O2=C2H3+HO2      4.22E+13      0.00      60800. ! (54) Wang 97
! Miller
! C2H4+O2=CH2HCO+OH      2.0E8      1.5      39000 ! JAM /SWB 1996

C2H4+CO=C2H3+HCO      1.51E+14      0.00      90616. ! (1) TSA/HAM 86
C2H4+C2H=C4H4+H      1.21E+13      0.00      0. ! (1) TSA/HAM 86
C2H4+C2H2=C2H3+C2H3      2.41E+13      0.00      68360. ! (1) TSA/HAM 86
C2H4+C2H4=C2H5+C2H3      4.82E+14      0.00      71539. ! (1) TSA/HAM 86
!
!-----C2H3 chemistry-----
!
H+C2H3 (+M)=C2H4 (+M)      6.08E+12      0.27      280. ! (22) GRI 3.0
  LOW      /1.40E+30      -3.86      3320./
  TROE /0.782 207.5 2663 6095/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! C2H3 (+M)=C2H2+H (+M)      3.86E+08      1.62      37058. ! (55) Knyazev 96
! LOW      /2.56E27      -3.40      35789.7/
! TROE /0.2134 36.643 7794.56 4007.66/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
H+C2H2 (+M)=C2H3 (+M)      1.713E10      1.266      2709. ! Miller & Klipp.
  LOW/6.348E31      -4.6639      3780./
  TROE/ 0,78784      -1.021E4      1.0E-30 /
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! N2/1.2/ CO/1.5/ H2/2/ CO2/3/ H2O/10./

H+C2H3=H2+C2H2      9.64E+13      0.00      0. ! (1) TSA/HAM 86
OH+C2H3=H2O+C2H2      5.00E+12      0.00      0. ! (56) Lutz 88
C2H3+O2=C2H2+HO2      1.34E+06      1.61      -383. ! (58) Mebel96
  DUPLICATE
C2H3+O2=C2H2+HO2      1.37E+02      3.37      3663. ! (53) Westmoreland PC
  DUPLICATE
! C2H3+O2=HCO+CH2O      1.57E+08      1.32      -1953.9 ! (15) Carriere 04
20Torr
! C2H3+O2=C2H3OO      5.61E+19      -3.30      165.4 ! (15) Carriere 04
20Torr
! C2H3+O2=O+CH2CHO      1.31E+01      3.55      2311.5 ! (15) Carriere 04
20Torr

```

```

! Miller
C2H3+O2=HCO+CH2O          9.33E13   -0.653  268.7 ! Klipp.& Miller
C2H3+O2=H+CO+CH2O         2.19E14   -0.653  268.7 ! Klipp. & Miller
C2H3+O2=CH2CHO+O          7.52E8    0.965  -137.4 ! Klipp.& Miller
!C2H3+O2=CH2HCO+O        7.52E8    0.965  -137.4 ! Klipp.& Miller

C2H3+HO2=OH+CH2CO+H      3.01E+13   0.00      0. ! (1) TSA/HAM 86
C2H3+CH3=C2H2+CH4        3.92E+11   0.00      0. ! (1) TSA/HAM 86
! C2H3+O=CH2CO+H          3.00E+13   0.00      0. ! (57) Heinemann 86
! Miller
C2H3+O=CH2CO+H           1.0E14    0.0      0.0 ! Harding&Klippenstein 2003

C2H3OO+H=CH2CHO+OH       1.00E+14   0.00      0. ! (15) Carriere 04 20Torr
C2H3OO+CH2=CH2CHO+CH2O   2.00E+13   0.00      0. ! (15) Carriere 04 20Torr
C2H3OO+OH=CH2CHO+HO2    2.00E+13   0.00      0. ! (15) Carriere 04 20Torr
C2H3OO+O=CH2CHO+O2      2.00E+13   0.00      0. ! (15) Carriere 04 20Torr
C2H3+CH2OH=C2H4+CH2O    3.01E+13   0.00      0. ! (1) TSA/HAM 86
C2H3+CH3O=C2H4+CH2O    2.41E+13   0.00      0. ! (1) TSA/HAM 86
C2H3+CH3OH=C2H4+CH3O    1.44E+01   3.10     6935. ! (1) TSA/HAM 86
C2H3+CH3OH=C2H4+CH2OH   3.19E+01   3.20     7172. ! (1) TSA/HAM 86
C2H3+CO=C2H3CO          1.51E+11   0.00     4809. ! (1) TSA/HAM 86
C2H3+C2H=C4H4           1.00E+14   0.00      0. ! (59) Duran 88
C2H3+C2H=C2H2+C2H2      9.64E+11   0.00      0. ! (1) TSA/HAM 86
C2H3+CH3CO=C2H3CO+CH3   1.81E+13   0.00      0. ! (1) TSA/HAM 86
C2H5+C2H3=AC3H5+CH3     8.00E+25  -3.46    11775. ! (1) TSA/HAM 86 0.1 atm
C2H3+C2H5 (+M)=IC4H8 (+M) 1.50E+13   0.00      0. ! (60) Wang/Laskin 99
    LOW /1.55E+56 -11.79      8984.5/
    TROE /0.198 2277.9 60000 5723.2/
C2H3+C2H5=C2H2+C2H6     4.82E+11   0.00      0. ! (1) TSA/HAM 86
C2H3+CH2SING=C2H2+CH3   1.81E+13   0.00      0. ! (1) TSA/HAM 86
C2H3+CH2=C2H2+CH3       1.81E+13   0.00      0. ! (1) TSA/HAM 86
C2H3+H2O2=C2H4+HO2     1.21E+10   0.00     -596. ! (1) TSA/HAM 86
C2H3+CH2O=C2H4+HCO     5.43E+03   2.81     5862. ! (1) TSA/HAM 86
C2H3+CH2=AC3H4+H       3.00E+13   0.00      0. ! (61) Pauwels 95
C2H3+C2H3=i-C4H5+H     1.50E+30  -4.95    13000. ! (54) Wang 97 20Torr
C2H3+C2H3=n-C4H5+H     1.10E+24  -3.28    12400. ! (54) Wang 97 20Torr
!
!-----C2H2 chemistry-----
!
!-----H2CC chemistry-----
!-----
H2CC+C2H2 (+M)=C4H4 (+M) 3.50E+05   2.055  -2400. ! (141) Laskin/Wang 00
    LOW /1.40E+60 -12.599  7417./
    TROE /0.98 56.0 580.0 4164.0/
    H2/2.0/ CH4/2.0/ H2O/6.0/ C2H2/3.0/ CO/1.5/ C2H4/3.0/ C2H6/3.0/ CO2/2.0/
!H2CC=C2H2              1.0E7     0.00      0. !JAM(10/02) Miller Est
! USC_II
C2H2 (+M)=H2CC (+M)      8.000E+14  -0.520  50750.00 !99LAS/WAN
    LOW / 2.450E+15 -0.640  49700.00 /
    H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/C2H2/2.5/ C2H4/2.5/

H2CC+C2H4=iiiC4H6       1.0E12     0.00      0. ! (141) Laskin/Wang 00
H2CC+O2=CH2+CO2         1.00E+13   0.00      0. ! (141) Laskin/Wang 00
H2CC+H=C2H2+H           1.00E+14   0.00      0. ! (141) Laskin/Wang 00
H2CC+OH=CH2CO+H        2.00E+13   0.00      0. ! (141) Laskin/Wang 00
!-----
!
!O+C2H2=H+HCCO          1.35E+07   2.00     1900. ! (22) GRI 3.0
!O+C2H2=CO+CH2          6.94E+06   2.00     1900. ! (22) GRI 3.0
!O+C2H2=OH+C2H          4.60E+19  -1.41    28950. ! (22) GRI 3.0
!Replaced by USC II as below
C2H2+O=C2H+OH           4.600E+19  -1.410  28950.00 !GRI

```

!C2H2+O=CH2+CO	4.080E+06	2.000	1900.00	!GRI (0.2 branching ratio)
!C2H2+O=HCCO+H	1.632E+07	2.000	1900.00	!GRI (0.8 branching ratio)
!O+C2H2=H+HCCO	5.79E+06	2.09	1560.0	! Lindstedt 97
!O+C2H2=CO+CH2	1.45E+06	2.09	1560.0	! Lindstedt 97
!O+C2H2=OH+C2H	3.16E+15	-0.60	15000.	! MMSK
!C2H2+O=CH2+CO	4.08E6	2.000	1900.000	! JAM, FONT, PEETERS
!C2H2+O=HCCO+H	1.632E7	2.000	1900.000	! JAM, FONT, PEETERS
!C2H2+O=C2H+OH	0.316E+16	-0.600	15000.000	!MMSK
C2H2+O=CH2+CO	2.350E+08	1.4	2204.50	!(0.2 branching ratio)
2005 Baulch Evaluation				
C2H2+O=HCCO+H	9.400E+08	1.4	2204.50	!(0.8 branching ratio)
2005 Baulch Evaluation				

!OH+C2H2=C2H+H2O	3.37E+07	2.00	14000.	! (62) Miller 86
!OH+C2H2=H+CH2CO	2.18E-04	4.50	-1000.	! (62) Miller 86
!OH+C2H2=CH3+CO	4.83E-04	4.00	-2000.	! (62) Miller 86
OH+C2H2=C2H+H2O	2.63E6	2.14	17060.	! SENOSIAIN, KLIPP., & MILLER 2005
OH+C2H2=H+CH2CO	1.52E4	2.28	-292.	! SENOSIAIN, KLIPP., & MILLER 2005
OH+C2H2=CH3+CO	4.37E6	1.40	227.	! SENOSIAIN, KLIPP., & MILLER 2005
! Miller				
! OH+C2H2=C2H+H2O	2.63E6	2.14	17060.	! SENOSIAIN, KLIPP., & MILLER 2005
! OH+C2H2=HCCOH+H	2.77E5	2.28	12419.	! SENOSIAIN, KLIPP., & MILLER 2005
! PLOG / .01	2.77E5	2.28	12419./	
! PLOG / .025	7.47E5	2.16	12547./	
! PLOG / .1	1.78E6	2.04	12669./	
! PLOG / 1.0	2.415E6	2.0	12713./	
! PLOG / 10.	3.21E6	1.97	12810./	
! PLOG / 100.	7.35E6	1.89	13603./	
! OH+C2H2=CH2CO+H	1.578E3	2.56	-844.	! SENOSIAIN, KLIPP., & MILLER 2005
! PLOG / .01	1.578E3	2.56	-844./	
! PLOG / .025	1.52E4	2.28	-292./	
! PLOG / 0.1	3.02E5	1.92	598./	
! PLOG / 1.0	7.53E6	1.55	2106./	
! PLOG / 10.0	5.10E6	1.65	3400./	
! PLOG / 100.	1.46E4	2.45	4477./	
! OH+C2H2=CH3+CO	4.76E5	1.68	-330.	! SENOSIAIN, KLIPP., & MILLER 2005
! PLOG / .01	4.76E5	1.68	-330./	
! PLOG / .025	4.37E6	1.40	227./	
! PLOG / 0.1	7.65E7	1.05	1115./	
! PLOG / 1.0	1.28E9	0.73	2579./	
! PLOG / 10.0	4.31E8	0.92	3736./	
! PLOG / 100.	8.25E5	1.77	4697./	
! OH+C2H2=C2H2OH	2.87E64	-18.57	10009	! SENOSIAIN, KLIPP., & MILLER 2005
! PLOG / .01	2.87E64	-18.57	10009./	
! PLOG / .01	2.64E33	-7.36	6392./	
! PLOG / .025	4.69E59	-16.87	9087./	
! PLOG / .025	4.38E32	-7.02	5933./	
! PLOG / 0.1	1.24E28	-5.56	3724./	
! PLOG / 0.1	6.38E42	-9.96	11737./	
! PLOG / 1.0	1.90E44	-11.38	6299./	
! PLOG / 1.0	3.49E31	-6.20	6635./	
! PLOG / 10.0	1.49E24	-4.06	3261./	
! PLOG / 10.0	4.51E31	-5.92	8761./	
! PLOG / 100.	6.20E20	-2.80	2831./	
! PLOG / 100.	1.60E29	-4.91	9734./	

```

C2H2+CH=C3H2+H          1.10E+13    0.00      0.    ! (63) Warnatz 82
C2H2+CH2=C3H3+H          1.20E+13    0.000    6620. ! (64) Bohland 88
C2H2+CH3=C2H+CH4          1.81E+11    0.00    17289. ! (1) TSA/HAM 86
C2H2+O2=2HCO              1.00E+12    0.00    28000. ! (65) Hidaka 96
C2H2+CH2OH=C2H3+CH2O      7.23E+11    0.00    9004.  ! (23) Tsang 87
C2H2+CO=C2H+HCO           4.82E+14    0.00    106713. ! (1) TSA/HAM 86
C2H2+C2H=C4H2+H           3.00E+13    0.00      0.    ! (10) Baulch94
uncertainty 3.16
C2H2+C2H(+M)=nC4H3(+M)    8.30E+10    0.90    -363.  ! (60) Wang/Laskin 99
  LOW /1.24E+31 -4.72 1871./
  TROE /1.0 100. 5613. 13387./
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
C2H2+C2H(+M)=iC4H3(+M)    8.30E+10    0.90    -363.0 ! (60) Wang/Laskin 99
  LOW /1.24E+31 -4.72 1871./
  TROE /1.0 100. 5613. 13387./
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
C2H2+CH2SING=C3H3+H        3.42E15    -0.624   -230.7 ! (66) Hansen/Miller 08
C2H2+CH2SING=CH2+C2H2      8.55E14    -0.624   -230.7 ! (66) Hansen/Miller 08
HCCO+C2H2=C3H3+CO          1.00E+11    0.00    3000.  ! (46) Miller 92
C2H2+C2H3=n-C4H5           1.10E+32   -7.33    6200.  ! (54) Wang 97 20Torr
C2H2+C2H3=i-C4H5           2.10E+36   -8.78    9100.  ! (54) Wang 97 20Torr
C2H3+C2H2=C4H4+H           5.00E+14   -0.71    6700.  ! (54) Wang 97 20Torr
!Miller These are fits from JAM&SJK 2002 30 Torr
!C2H3+C2H2=CH2CHCHCH 1.01E51 -12.778 15608.
!C2H3+C2H2=CH2CHCCH+H 1.54E16 -1.069 9566.
!
!-----C2H chemistry-----
!
O+C2H=CH+CO                1.00E+13    0.00      0.    ! (3) Warnatz84
H+C2H(+M)=C2H2(+M)         1.000E+17   -1.00      0.    ! (22) GRI3.0
  LOW /3.750E+33 -4.80 1900./
  TROE /0.6464 132 1315 5566/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
! C2H2+M=C2H+H+M           9.08E30    -3.7 127138. !TSANG&HAMP(TAN&GARD)
! H2/2/ CO/2/ CO2/3/ H2O/5/
OH+C2H=H+HCCO              2.00E+13    0.00      0.    ! (67) Frenklach 92
C2H+O2=HCO+CO              1.00E+13    0.00    -775.  ! (22) GRI 3.0
C2H+H2=H+C2H2              5.68E+10    0.90    1993.  ! (68) Farhat 93
! Miller
! H2+C2H=C2H2+H            0.409E+06  2.390    864.300 ! HARDING,SHATZ,CHILE

C2H+HO2=HCCO+OH            1.81E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+CH3=C3H3+H              2.41E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+O2=HCCO+O               6.03E+11    0.00      0.    ! (1) TSA/HAM 86
C2H+CH2OH=C2H2+CH2O        3.61E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+CH2OH=C3H3+OH           1.21E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+CH3OH=C2H2+CH2OH        6.03E+12    0.00      0.    ! (1) TSA/HAM 86
C2H+CH3O=CH2O+C2H2          2.41E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+CH3OH=C2H2+CH3O         1.21E+12    0.00      0.    ! (23) Tsang 87
C2H+CH2=CH+C2H2             1.81E+13    0.00      0.    ! (1) TSA/HAM 86
C2H+CH2SING=C2H2+CH         1.81E+13    0.00      0.    ! (1) TSA/HAM 86
!
!-----C2HxOy chemistry-----
!
O+HCCO=H+2CO                1.00E+14    0.00      0.    ! (69) Frank 88
H+HCCO=CH2SING+CO           5.00E13     0.00      0.    ! (3) Warnatz 84
CH2+HCCO=C2H3+CO            3.00E+13    0.00      0.    ! (62) Miller86
HCCO+O2=CO2+CO+H            4.78E+12   -0.142    1150.  ! (70) Klippenstain 02
HCCO+O2=CO+CO+OH            1.91E+11   -0.02    1023.  ! (70) Klippenstain 02
HCCO+O2=O+CO+HCO            2.18E2     2.69    3541.  ! (70)
Klippenstain 02
! Miller
! HCCO+O2=CO2+CO+H          4.78E12   -0.142    1150.  ! Klipp&JAM 29th
! HCCO+O2=CO +CO +OH        1.91E11   -0.02    1023.
! HCCO+O2=O+CO+HCO          2.18E2    2.69    3541.

```

2HCCO=2CO+C2H2 1.00E+13 0.00 0. ! (34) Miller 89  
 HCCO+CH3=C2H4+CO 5.00E+13 0.00 0. ! (54) Wang 97  
 O+CH2CO=OH+HCCO 1.00E+13 0.00 8000. ! (34) Miller 89  
 O+CH2CO=CH2+CO2 1.75E+12 0.00 1350. ! (71) Cvetanovic 87  
 H+CH2CO=HCCO+H2 5.00E+13 0.00 8000. ! (34) Miller 89  
 ! H+CH2CO=CH3+CO 3.28E+10 0.85 2839. ! (72) Hranislavljevic 98  
 ! Miller  
 CH2CO+H=CH3+CO 7.77E8 1.45 2780. ! SENOSIAN,  
 KLIPP., & MILLER 2005  
  
 !H+CH2CO(+M)=CH2CHO(+M) 4.86E+11 0.42 -1755. ! (22) GRI 3.0  
 ! LOW /1.01E+42 -7.63 3854./  
 ! TROE /0.465 201 1773 5333.0/  
 ! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/  
 CH2CHO=H+CH2CO 2.48E+27 -5.23 44304. ! JPCA 110 5772 (2006)  
 CH2CHO=CH3+CO 1.54E+31 -6.27 42478. ! JPCA 110 5772 (2006)  
 ! Miller  
 ! CH2HCO=H+CH2CO 2.39E+25 -4.8 43424. ! JPCA 110 5772 (2006)  
 ! PLOG /0.01 2.39E+25 -4.80 43424./  
 ! PLOG /0.025 2.48E+27 -5.23 44304./  
 ! PLOG /0.1 2.37E+30 -5.86 46114./  
 ! PLOG /1. 1.32E+34 -6.57 49454./  
 ! PLOG /10. 3.46E+36 -6.92 52979./  
 ! PLOG /100. 1.18E+36 -6.48 55171./  
 ! ! inf 1.43E+15 -0.15 45606  
 ! CH2HCO=CH3+CO 1.16E+30 -6.07 41332. ! JPCA 110 5772 (2006)  
 ! this reaction is in line 976-977  
 ! PLOG /0.01 1.16E+30 -6.07 41332./  
 ! PLOG /0.025 1.54E+31 -6.27 42478./  
 ! PLOG /0.1 6.37E+32 -6.57 44282./  
 ! PLOG /1. 6.51E+34 -6.87 47191./  
 ! PLOG /10. 2.15E+35 -6.76 49548./  
 ! PLOG /100. 2.23E+33 -5.97 50448./  
 ! ! inf 2.93E+12 0.29 40326.  
  
 OH+CH2CO=HCCO+H2O 7.50E+12 0.00 2000. ! (34) Miller 89  
 CH2CO+OH=CH2OH+CO 1.00E+13 0.00 0. ! (45) Baulch 92  
 !CH3CO+M=CH3+CO+M 8.74E+42 -8.62 22410. ! (1) TSA/HAM 86  
 CH3CO=CH3+CO 2.40E+15 -2.00 14805. ! JPCA 110 5772  
 (2006)  
 ! Miller  
 ! CH3CO=CH3+CO 6.88E+14 -1.97 14585. ! JPCA 110 5772 (2006)  
 ! PLOG /0.01 6.88E+14 -1.97 14585./  
 ! PLOG /0.025 2.40E+15 -2.00 14805./  
 ! PLOG /0.1 1.96E+16 -2.09 15197./  
 ! PLOG /1. 6.45E+18 -2.52 16436./  
 ! PLOG /10. 8.18E+19 -2.55 17263./  
 ! PLOG /100. 1.26E+20 -2.32 18012./  
 ! ! inf 1.07E+12 0.63 16895.  
  
 CH2CHO+H=CH3CHO 6.40E35 -7.60 5215. ! (73) Hennessy 94  
 CH2CHO+H=CH3+HCO 4.99E14 -0.32 912. ! (73) Hennessy 94  
 CH2CHO+O=CH2O+HCO 5.00E13 0.00 0. ! (73) Hennessy 94  
 CH2CHO+OH=H2O+CH2CO 1.20E+13 0.00 0. ! (22) GRI 3.0  
 CH2CHO+OH=HCO+CH2OH 3.01E+13 0.00 0. ! (22) GRI 3.0  
 CH2CHO+O2=CH2CO+HO2 1.57E11 0.00 0. ! (45) Baulch 92  
 CH3CHO=CH3+HCO 9.59E+14 0.00 74180. ! (74) Dagaut 95  
 CH3CHO+O2=CH3CO+HO2 2.00E+13 0.50 42200. ! (10) Baulch 94  
 CH3CHO+H=CH2CHO+H2 4.10E+09 1.16 2405. ! (10) Baulch 94  
 CH3CHO+OH=CH3CO+H2O 2.35E+10 0.73 -1113. ! (10) Baulch 94  
 CH3CHO+O=CH2CHO+OH 5.85E+12 0.00 1808. ! (10) Baulch 94  
 CH3CHO+HO2=CH3CO+H2O2 1.70E+12 0.00 10700. ! (75) Colket 77  
 CH3CHO+CH3=CH3CO+CH4 1.70E+12 0.00 8440. ! (76) Wilk 89  
 CH3CHO+HCO=CH3CO+CH2O 7.80E+13 0.00 8440. ! (74) Dagaut 95

```

! C2H5+O2=C2H5OO          2.24E+10    0.77    -568. ! (77) Wagner 90
! Miller
C2H5+O2 (+M)=C2H5OO (+M)  2.02E10 0.98 -63.6 ! Miller&Klipp IJCK 33,654 (2001)
LOW/8.49E29 -4.29 220./
TROE/0.103 601. 1.0E-10/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! H2/2/ CO/2/ CO2/3/ H2O/5/
C2H5OO (+M)=C2H4+HO2 (+M) 7.14E4 2.32 27955.
LOW/8.31E21 -0.651 22890./
TROE/0.0 106. 106./
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! H2/2/ CO/2/ CO2/3/ H2O/5/

C2H5OO+HO2=C2H5O+OH+O2    1.75E+10    0.00    -3275. ! (78) Fischer 00
C2H5O=CH3+CH2O            1.00E+15    0.00    21523. ! (79) Heicklen 88
C2H5O=CH3CHO+H           2.00E+14    0.00    23215. ! (79) Heicklen 88
C2H5O+O2=CH3CHO+HO2     6.03E+10    0.00    1643. ! (45) Baulch 92
C2H4O+O2=CH2CHO+HO2     4.00E+13    0.00    61500. ! (80) Dagaut 96
C2H4O+H=CH2CHO+H2       2.00E13    0.00    8300. ! (81) Lifshitz 83
C2H4O+H=C2H3+H2O        5.00E+09    0.00    5000. ! (81) Lifshitz 83
C2H4O+H=C2H4+OH         9.51E+10    0.00    5000. ! (81) Lifshitz 83
C2H4O+OH=CH2CHO+H2O     4.79E+13    0.00    5955. ! (76) Wilk 89
C2H4O+O=CH2CHO+OH       1.91E+12    0.00    5250. ! (82) Bogan 78
C2H4O+HO2=CH2CHO+H2O2   4.00E+12    0.00    17000. ! (80) Dagaut 96
C2H4O=CH3CHO            6.00E+13    0.00    57167. ! (80) Dagaut 96
C2H4O=CH3+HCO           4.90E+13    0.00    57167. ! (80) Dagaut 96
C2H4O=CH4+CO            1.21E+13    0.00    57167. ! (80) Dagaut 96
!
!-----C3H8 chemistry-----
!
C3H8+H=nC3H7+H2          1.30E+06    2.54    6756. ! (52) Tsang 88
C3H8+H=iC3H7+H2          1.30E+06    2.40    4471. ! (52) Tsang 88
C3H8+O=nC3H7+OH          1.90E+05    2.68    3716. ! (52) Tsang 88
C3H8+O=iC3H7+OH          4.76E+04    2.71    2106. ! (52) Tsang 88
C3H8+OH=iC3H7+H2O        1.40E+03    2.80    -310. ! (52) Tsang 88
C3H8+OH=nC3H7+H2O        1.37E+03    2.70    580. ! (52) Tsang 88
C3H8+O2=nC3H7+HO2        3.97E+13    0.00    50872. ! (52) Tsang 88
C3H8+O2=iC3H7+HO2        3.97E+13    0.00    47693. ! (52) Tsang 88
C3H8+HO2=nC3H7+H2O2      4.76E+04    2.55    16494. ! (52) Tsang 88
C3H8+HO2=iC3H7+H2O2      9.64E+03    2.60    13910. ! (52) Tsang 88
C3H8+CH3=nC3H7+CH4       9.04E-01    3.65    7154. ! (52) Tsang 88
C3H8+CH3=iC3H7+CH4       1.51E+00    3.46    5481. ! (52) Tsang 88
C3H8+CH2OH=nC3H7+CH3OH   1.99E+02    2.95    3976. ! (52) Tsang 88
C3H8+CH3O=nC3H7+CH3OH    4.34E+11    0.00    6458. ! (52) Tsang 88
C3H8+CH2SING=nC3H7+CH3   9.04E-01    3.65    7154. ! (52) Tsang 88
C3H8+C2H3=nC3H7+C2H4     6.03E+02    3.30    10502. ! (52) Tsang 88
C3H8+C2H=nC3H7+C2H2      3.61E+12    0.00    0. ! (52) Tsang 88
C3H8+C2H5=nC3H7+C2H6     9.04E-02    3.65    9141. ! (52) Tsang 88
C3H8+HCO=nC3H7+CH2O      2.05E+05    2.50    18431. ! (52) Tsang 88
C3H8+iC3H7=nC3H7+C3H8    8.40E-03    4.20    8716. ! (52) Tsang 88
C3H8+CH3CO=nC3H7+CH3CHO  4.22E+04    2.60    17658. ! (52) Tsang 88
C3H8+CH2=nC3H7+CH3       9.03E-01    3.65    7154. ! (52) Tsang 88
C3H8+CH2OH=iC3H7+CH3OH   6.03E+01    2.95    11989. ! (52) Tsang 88
C3H8+CH3O=iC3H7+CH3OH    1.45E+11    0.00    4571. ! (52) Tsang 88
C3H8+CH2SING=iC3H7+CH3   1.51E+00    3.46    7472. ! (52) Tsang 88
C3H8+C2H3=iC3H7+C2H4     1.02E+03    3.10    8829. ! (52) Tsang 88
C3H8+C2H=iC3H7+C2H2      1.21E+12    0.00    0. ! (52) Tsang 88
C3H8+C2H5=iC3H7+C2H6     1.21E+00    3.46    7468. ! (52) Tsang 88
C3H8+HCO=iC3H7+CH2O      1.08E+07    1.90    17006. ! (52) Tsang 88
C3H8+CH3CO=iC3H7+CH3CHO  5.30E+06    2.00    16241. ! (52) Tsang 88
C3H8+CH2=iC3H7+CH3       1.51E+00    3.46    7472. ! (52) Tsang 88
!
!-----C3H7 chemistry-----
!
nC3H7+H=C3H6+H2          1.81E+12    0.00    0. ! (52) Tsang 88
nC3H7+H (+M)=C3H8 (+M)  3.60E+13    0.00    0. ! (52) Tsang 88

```

```

LOW /3.01E+58 -9.32 5833.6/
TROE /0.498 1314 1314 50000/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/ 0.7/
nC3H7+H = C2H5+CH3 3.40E+18 -1.33 5386. ! (52) Tsang 88 0.1 atm
nC3H7+O=C2H5+CH2O 9.60E+13 0.00 0. ! (52) Tsang 88
nC3H7+O2=C3H6+HO2 9.04E+10 0.00 0. ! (52) Tsang 88
nC3H7+HO2=C2H5+OH+CH2O 2.41E+13 0.00 0. ! (52) Tsang 88
nC3H7+OH=C3H6+H2O 2.41E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH3=CH4+C3H6 1.14E+13 -0.32 0. ! (52) Tsang 88
nC3H7+C2H5=C3H6+C2H6 1.45E+12 0.00 0. ! (52) Tsang 88
nC3H7+C2H5=C3H8+C2H4 1.15E+12 0.00 0. ! (52) Tsang 88
nC3H7+C2H3=C3H8+C2H2 1.21E+12 0.00 0. ! (52) Tsang 88
nC3H7+C2H2=AC3H5+C2H4 7.23E11 0.00 9004. ! (52) Tsang 88
nC3H7+C2H=C3H3+C2H5 1.21E+13 0.00 0. ! (52) Tsang 88
nC3H7+C2H=C3H6+C2H2 6.03E+12 0.00 0. ! (52) Tsang 88
nC3H7+iC3H7=C3H8+C3H6 5.13E+13 -0.35 0. ! (52) Tsang 88
nC3H7+HCO=CO+C3H8 6.03E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH3O=C3H8+CH2O 2.41E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH2SING=C2H5+C2H4 2.58E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH2SING=C3H6+CH3 1.03E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH2=C2H4+C2H5 1.81E+13 0.00 0. ! (52) Tsang 88
nC3H7+CH2=C3H6+CH3 1.81E+12 0.00 0. ! (52) Tsang 88
nC3H7+CH2OH=C3H6+CH3OH 4.82E+11 0.00 0. ! (52) Tsang 88
iC3H7=CH3+C2H4 1.00E+14 0.00 45000. ! (83) Dagaut 92
iC3H7+H=C3H6+H2 3.61E+12 0.00 0. ! (52) Tsang 88
iC3H7+H (+M)=C3H8 (+M) 2.40E+13 0.00 0. ! (52) Tsang 88
LOW /1.70E+58 -12.08 11263.7/
TROE /0.649 1213.1 1213.1 13369.7/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
iC3H7+H = CH3+C2H5 5.90E+23 -2.81 10009. ! (52) 88TSA RRKM 0.1 atm
iC3H7+O=CH3CHO+CH3 9.60E+13 0.00 0. ! (52) Tsang 88
iC3H7+O2=C3H6+HO2 1.26E+11 0.00 0. ! (52) Tsang 88
iC3H7+HO2=CH3CHO+OH+CH3 2.41E+13 0.00 0. ! (52) Tsang 88
iC3H7+OH=C3H6+H2O 2.41E+13 0.00 0. ! (52) Tsang 88
iC3H7+CH3=CH4+C3H6 2.19E+14 -0.68 0. ! (52) Tsang 88
iC3H7+C2H5=C3H6+C2H6 2.30E+13 -0.35 0. ! (52) Tsang 88
iC3H7+C2H5=C3H8+C2H4 1.84E+13 -0.35 0. ! (52) Tsang 88
iC3H7+C2H3=C2H4+C3H6 1.52E+14 -0.70 0. ! (52) Tsang 88
iC3H7+C2H3=C3H8+C2H2 1.52E+14 -0.70 0. ! (52) Tsang 88
iC3H7+C2H2=CH3+iiiC4H6 2.77E+10 0.00 6504. ! (52) Tsang 88
iC3H7+C2H=C3H6+C2H2 3.60E+12 0.00 0. ! (52) Tsang 88
iC3H7+iC3H7=C3H8+C3H6 2.11E+14 -0.70 0. ! (52) Tsang 88
iC3H7+HCO=CO+C3H8 1.20E+14 0.00 0. ! (52) Tsang 88
iC3H7+CH3O=C3H8+CH2O 1.21E+13 0.00 0. ! (52) Tsang 88
iC3H7+CH2SING=C3H6+CH3 1.04E+13 0.00 0. ! (52) Tsang 88
iC3H7+CH2=C3H6+CH3 3.01E+13 0.00 0. ! (52) Tsang 88
iC3H7+CH2OH=C3H6+CH3OH 2.89E+12 0.00 0. ! (52) Tsang 88
iC3H7+CH2OH=C3H8+CH2O 2.35E+12 0.00 0. ! (52) Tsang 88
!
!-----C3H6 chemistry-----
!
CH3+C2H3 (+M)=C3H6 (+M) 2.50E+13 0.00 0. ! (50) Qin/Wan 00
LOW /4.27E+58 -11.94 9770./
TROE /0.175 1341 60000 10140/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H2/3.00/ AR/0.7/
C3H6+H=H2+AC3H5 1.70E+05 2.50 2492. ! (84) Tsang 91
C3H6+H=C2H4+CH3 8.80E+16 -1.05 6461. ! (84) Tsang 91 0.1 atm
C3H6+H=SC3H5+H2 7.81E+05 2.50 12285. ! (85) Tsang 92
C3H6+H (+M)=nC3H7 (+M) 1.33E+13 0.00 3260.7 ! (84) Tsang 91
LOW /6.26E+38 -6.66 7000./
TROE /1.000 1000. 1310. 48097./
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C3H6+H (+M)=iC3H7 (+M) 1.33E+13 0.00 1559.8 ! (84) Tsang 91
LOW /8.70E+42 -7.50 4721.8/
TROE /1.000 1000. 645.4 6844.3 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/

```

C3H6+H=TC3H5+H2	3.90E+05	2.50	5821.	!	(85) Tsang 92
C3H6=H2+AC3H4	4.00E+13	0.00	80000.	!	(87) Hidaka 92
C3H6=CH4+C2H2	3.50E+12	0.00	70000.	!	(87) Hidaka 92
C3H6+O=C2H5+HCO	3.50E+07	1.65	-972.	!	(84) Tsang 91
C3H6+O=AC3H5+OH	1.75E+11	0.70	5884.	!	(84) Tsang 91
C3H6+O=SC3H5+OH	1.21E+11	0.70	8960.	!	(84) Tsang 91
C3H6+O=TC3H5+OH	6.03E+10	0.70	7633.	!	(84) Tsang 91
C3H6+O=CH3+H+CH2CO	1.20E+08	1.65	327.	!	(84) Tsang 91
C3H6+OH=AC3H5+H2O	3.12E+06	2.00	-298.	!	(84) Tsang 91
C3H6+OH=SC3H5+H2O	2.14E+06	2.00	2778.	!	(84) Tsang 91
C3H6+OH=TC3H5+H2O	1.11E+06	2.00	1451.	!	(84) Tsang 91
C3H6+HO2=AC3H5+H2O2	9.63E+03	2.60	13910.	!	(84) Tsang 91
C3H6+O2=AC3H5+HO2	6.03E+13	0.00	47590.	!	(84) Tsang 91
C3H6+CH3=AC3H5+CH4	2.20E+00	3.50	5675.	!	(84) Tsang 91
C3H6+CH3=TC3H5+CH4	8.40E-01	3.50	11660.	!	(84) Tsang 91
C3H6+C2H5=AC3H5+C2H6	2.23E+00	3.50	6637.	!	(84) Tsang 91
C3H6+C2H2=AC3H5+C2H3	4.04E+13	0.00	46818.	!	(84) Tsang 91
C3H6+C2H3=AC3H5+C2H4	2.21E+00	3.50	4682.	!	(84) Tsang 91
C3H6+C2H3=SC3H5+C2H4	1.35E+00	3.50	10842.	!	(84) Tsang 91
C3H6+C2H3=TC3H5+C2H4	8.40E-01	3.50	9670.	!	(84) Tsang 91
C3H6+C2H3=iiiC4H6+CH3	7.23E+11	0.00	5008.	!	(84) Tsang 91
C3H6+C2H4=AC3H5+C2H5	5.78E+13	0.00	51584.	!	(84) Tsang 91
C3H6+C2H4=nC3H7+C2H3	6.03E+13	0.00	75446.	!	(84) Tsang 91
C3H6+CH2OH=AC3H5+CH3OH	6.03E+01	2.95	12000.	!	(84) Tsang 91
C3H6+nC3H7=AC3H5+C3H8	2.23E+00	3.50	6637.	!	(84) Tsang 91
C3H6+nC3H7=IC4H8+C2H5	2.23E+00	3.50	-2000.	!	(84) Tsang 91
C3H6+iC3H7=C3H8+AC3H5	6.62E-02	4.00	8066.	!	(84) Tsang 91
C3H6+C3H6=AC3H5+nC3H7	2.53E+14	0.00	55179.	!	(84) Tsang 91
C3H6+C3H6=AC3H5+iC3H7	4.88E+13	0.00	52309.	!	(84) Tsang 91
!					
!-----C3H5 chemistry-----					
!					
CH3+C2H3=AC3H5+H	1.50E+24	-2.83	18618.	!	(88) Davis/Wang 99
CH3+C2H3=SC3H5+H	3.20E+35	-7.76	13300.	!	(88) Davis/Wang 99
CH3+C2H3=TC3H5+H	4.99E+22	-4.39	18850.	!	(88) Davis/Wang 99
AC3H5+H (+M)=C3H6 (+M)	2.00E14	0.00	0.	!	(84) Tsang 91
LOW	/1.33E+60	-12.00	5967.8/		
TROE /0.02 1097 10967 6860/					
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/					
AC3H5+H=AC3H4+H2	1.80E+13	0.00	0.	!	(84) Tsang 91
TC3H5+H=AC3H4+H2	3.30E+12	0.00	0.	!	(83) Dagaut 92
SC3H5+H=AC3H4+H2	3.30E+12	0.00	0.	!	(83) Dagaut 92
AC3H5+O=C2H3CHO+H	6.00E+13	0.00	0.	!	(84) Tsang 91
AC3H5+O=C2H3+CH2O	1.80E+14	0.00	0.	!	(89) Westmoreland PC
SC3H5+O=CH2CO+CH3	1.81E+14	0.00	0.	!	(83) Dagaut 92
TC3H5+O=H+HCCO+CH3	1.81E+14	0.00	0.	!	(83) Dagaut 92
AC3H5+OH = C2H3CHO+H+H	5.30E+37	-6.71	29306.	!	(84) Tsang 91 RRKM
0.1atm					
AC3H5+OH=AC3H4+H2O	6.00E+12	0.00	0.	!	(84) Tsang 91
AC3H5+O2=AC3H4+HO2	4.99E+15	-1.40	22428.	!	(90) Boz/Dean 93
AC3H5+O2=CH2O+CH3CO	1.19E+15	-1.01	20128.	!	(90) Boz/Dean 93
AC3H5+O2=OH+C2H3CHO	1.82E+13	-0.41	22859.	!	(90) Boz/Dean 93
SC3H5+O2=CH3CHO+HCO	4.34E+12	0.00	0.	!	(83) Dagaut 92
TC3H5+O2=CH3CHO+HCO	4.34E+12	0.00	0.	!	(83) Dagaut 92
AC3H5+HO2=C2H3+CH2O+OH	6.60E+12	0.00	0.	!	(10) Baulch 94
AC3H5+CH3=AC3H4+CH4	3.00E+12	-0.32	-131.	!	(84) Tsang 91
AC3H5+CH3 (+M)=IC4H8 (+M)	1.00E+14	-0.32	-262.	!	(84) Tsang 91
LOW	/3.51E+60	-12.97	6000./		
TROE /0.896 60000 1606 6118/					
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/					
SC3H5+CH3=AC3H4+CH4	1.00E+11	0.00	0.	!	(83) Dagaut 92
TC3H5+CH3=AC3H4+CH4	1.00E+11	0.00	0.	!	(83) Dagaut 92
AC3H5+C2H3=AC3H4+C2H4	1.00E+12	0.00	0.	!	(83) Dagaut 92
SC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.00	0.	!	(83) Dagaut 92
TC3H5+C2H3=AC3H4+C2H4	1.00E+11	0.00	0.	!	(83) Dagaut 92
AC3H5+CH2O=C3H6+HCO	1.26E+08	1.90	18191.	!	(83) Dagaut 92



AC3H5+HCO=C3H6+CO	6.00E+13	0.00	0.	!	(84) Tsang 91
AC3H5+AC3H5=AC3H4+C3H6	8.43E+10	0.00	-262.	!	(84) Tsang 91
AC3H5+CH2=iiC4H6+H	3.00E+13	0.00	0.	!	(84) Tsang 91
AC3H5+nC3H7=AC3H4+C3H8	7.23E+11	0.00	-131.	!	(84) Tsang 91
AC3H5+iC3H7=AC3H4+C3H8	4.58E+12	-0.35	-131.	!	(84) Tsang 91
AC3H5=TC3H5	3.90E+59	-15.42	75400.	!	(88) Davis/Wang 99
AC3H5=SC3H5	1.30E+55	-14.53	73800.	!	(88) Davis/Wang 99
TC3H5=SC3H5	1.60E+44	-12.16	52200.	!	(88) Davis/Wang 99
!					
!-----C3H4 chemistry-----					
!					
AC3H4=PC3H4	6.0256E+53	-12.18	84276.	!	(91) JAM/SJK 03
AC3H4+H=AC3H5	1.241E52	-12.02	17839.	!	(92) JAM/JPS 08
DUPLICATE					
AC3H4+H=AC3H5	6.923E36	-8.19	7462.	!	(92) JAM/JPS 08
DUPLICATE					
AC3H4+H=TC3H5	1.554E53	-13.10	14472.	!	(92) JAM/JPS 08
DUPLICATE					
AC3H4+H=TC3H5	0.988E45	-11.21	8212.	!	(92) JAM/JPS 08
DUPLICATE					
PC3H4+H=TC3H5	3.174E52	-12.69	14226.	!	(92) JAM/JPS 08
DUPLICATE					
PC3H4+H=TC3H5	2.589E45	-11.23	8046.	!	(92) JAM/JPS 08
DUPLICATE					
!PC3H4+H=AC3H5	3.379E49	-12.75	14072.	!	(92) JAM/JPS 08
! DUPLICATE					
!PC3H4+H=AC3H5	2.981E43	-11.43	8736.	!	(92) JAM/JPS 08
! DUPLICATE					
! Mistake above, should be SC3H5, fixed as below.					
PC3H4+H=SC3H5	3.379E49	-12.75	14072.	!	(92) JAM/JPS 08
DUPLICATE					
PC3H4+H=SC3H5	2.981E43	-11.43	8736.	!	(92) JAM/JPS 08
DUPLICATE					
AC3H4+H=PC3H4+H	1.476E13	0.26	4103.	!	(92) JAM/JPS 08
AC3H4+H=CH3+C2H2	2.722E9	1.20	6834.	!	(92) JAM/JPS 08
PC3H4+H=CH3+C2H2	3.891E10	0.989	4114.	!	(92) JAM/JPS 08
!C2H2+CH3=AC3H5	-0.681E+49	-12.27	16642.	!	(92) JAM/JPS 08
! DUPLICATE					
!C2H2+CH3=AC3H5	1.524E+44	-10.73	15256.	!	(92) JAM/JPS 08
! DUPLICATE					
! Mistake above, should be SC3H5, fixed as below.					
C2H2+CH3=SC3H5	-0.681E+49	-12.27	16642.	!	(92) JAM/JPS 08
DUPLICATE					
C2H2+CH3=SC3H5	1.524E+44	-10.73	15256.	!	(92) JAM/JPS 08
DUPLICATE					
!C2H2+CH3=CH3CHCH	1.4E+32	-7.14	10000.	!	!bpick jul03 actually from Wang Hai Davis/Wang 99 0.1 atm
! PLOG /0.1	1.4E+32	-7.14	10000./		
! PLOG /1.	3.2E+35	-7.76	13300./		
! PLOG /10.	2.4E+38	-8.21	17100./		
! PLOG /100.	1.4E+39	-8.06	20200./		
! PLOG /1.0E+5	1.5E+07	1.87	8200./		
C2H2+CH3=TC3H5	6.80E+20	-4.16	18000.	!	(88) Davis/Wang 99 0.1 atm
! Miller					
! C2H2+CH3=CH3CCH2	6.8E+20	-4.16	18000.	!	!bpick jul03 actually from Wang Hai Davis/Wang 99 0.1 atm
! PLOG /0.1	6.8E+20	-4.16	18000./		
! PLOG /1.	5.0E+22	-4.39	18800./		
! PLOG /10.	9.3E+27	-5.55	22900./		
! PLOG /100.	3.8E+36	-7.58	31300./		
C2H2+CH3=AC3H5	8.20E+53	-13.32	33200.	!	(88) Davis/Wang 99 0.1 atm
AC3H4+H=C3H3+H2	6.604E3	3.095	5522.	!	(92) JAM/JPS 08
AC3H4+OH=C3H3+H2O	1.00E+07	2.00	1000.	!	(46) Miller 92

```

! Miller
! C3H4+H=H2CCCH+H2      6.604E3  3.095    5522. !JAM, SJK et al (2007)
! C3H4+OH=H2CCCH+H2O    2.0E7    2.0      5000. !JAM
! C3H4+OH=CH2O+C2H3     1.0E12   0.0     -198.7 ! JAM/Liu(1988)/Butler(07)
! C3H4+OH=CH2CO+CH3     3.04E12  0.0     -198.7 !
PC3H4+H=C3H3+H2        3.57E4    2.825   4821.  ! (92) JAM/JPS 08
AC3H4+O=C2H4+CO        2.00E+07  1.80    1000.  ! (93) Davis/Wang 99
AC3H4+C2H=C3H3+C2H2    1.00E+13  0.00    0.      ! (54) Wang 97
AC3H4+CH3=C3H3+CH4     1.30E+12  0.00    7700.  ! (88) Davis/Wang 99
PC3H4+O=HCCO+CH3       7.30E+12  0.00    2250.  ! (94) Adusei 96
PC3H4+O=C2H4+CO        1.00E+13  0.00    2250.  ! (94) Adusei 96
PC3H4+O=C3H3+OH        3.44E+04  2.16    4830.  ! (94) Adusei 96
PC3H4+OH=C3H3+H2O      1.00E+07  2.00    1000.  ! (46) Miller 92
PC3H4+C2H=C3H3+C2H2    1.00E+13  0.00    0.      ! (54) Wang 97
PC3H4+CH3=C3H3+CH4     1.80E+12  0.00    7700.  ! (88) Davis/Wang 99
!
!-----C3H3 chemistry-----
!
C3H3+H=PC3H4            3.6308E+36  -7.36   6039.  ! (91) JAM/SJK 03
C3H3+H=AC3H4            3.3884E+36  -7.41   6337.  ! (91) JAM/SJK 03
!C3H3+CH3(+M)=iic4H6(+M)  1.50E+12    0.00    0.      ! (54) Wang 97
! LOW                    /2.60E+57  -11.94  9770./
! TROE /0.175 1341 60000 9770/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/

C3H3+CH3=iic4H6        3.61E13    0.0     0.0 ! [Fahr and Nayak '2000: 40%
of total] MIT PAH

C2H3+C2H3=iiiC4H6      7.00E+57   -13.82  17629. ! (54) Wang 97 RRKM 20
Torr
! C3H3+H=C3H2+H2        5.00E+13    0.00    3000.  ! (46) Miller 92
C3H3+H=C3H2+H2        2.14E+05    2.52    7453.  ! JAM&SJK 2002 30 Torr
! Miller These reactions come from JAM&SJK 2002 30 Torr
! H2CCCH+H=C3H2+H2     2.14E5     2.52    7453.  ! abstraction

C3H3+O=>C2H2+HCO       1.385E+14   0.00    0.      ! (95) Slagle 90
C3H3+O=C2H3+CO         4.615E+13   0.00    0.      ! (95) Slagle 90
C3H3+O=C2H+CH2O        4.615E+13   0.00    0.      ! (95) Slagle 90
!H2CCCH+O=CH2O+C2H     1.4E14     0.000   0.000 ! GUTMAN 23RD (PRD JAM)
C3H3+O=>C2H2+CO+H      4.615E+13   0.00    0.      ! (95) Slagle 90

! C3H3+OH=C3H2+H2O     2.00E+13    0.00    0.      ! (34) Miller 89
C3H3+OH=C3H2+H2O     2.00E+13    0.00    8000.  ! JAM 2007
! Miller H2CCCH+OH=C3H2+H2O  0.200E+14  0.000   8000.  ! JAM 2007

C3H3+HCO=AC3H4+CO     2.50E+13    0.00    0.      ! (54) Wang 97
C3H3+HCO=PC3H4+CO     2.50E+13    0.00    0.      ! (54) Wang 97
C3H3+CH=iC4H3+H       5.00E+13    0.00    0.      ! (54) Wang 97
C3H3+CH2=C4H4+H       5.00E+13    0.00    0.      ! (46) Miller 92
! C3H3+O2=CH2CO+HCO    3.00E+10    0.00    2868.  ! (99) Slagle 88
C3H3+O2=CH2CO+HCO    1.70E+05    1.70    1500.  ! JAM&SJK Faraday 119
! Miller
! H2CCCH+O2=CH2CO+HCO  1.70E5     1.7     1500.  !JAM&SJK Faraday 119

C3H3+HCCO=C4H4+CO     2.50E+13    0.00    0.      ! (54) Wang 97
C3H3+HO2=OH+CO+C2H3   8.00E+11    0.00    0.      ! (93) Davis/Wang 99
C3H3+HO2=AC3H4+O2     3.00E+11    0.00    0.      ! (93) Davis/Wang 99
C3H3+HO2=PC3H4+O2     2.50E+12    0.00    0.      ! (93) Davis/Wang 99
C3H2+O2=H+CO+HCCO     2.00E+12    0.00    1000.  ! (61) Pauwels 95
! Miller
! C3H2+O2=CO2+C2H2     11.5E5     2.245   367.6 ! JAM(based on ch2+O2)
! C3H2+O2=CO2+C2H+H    11.5E5     2.245   367.6 ! JAM
! C3H2+O2=HCCO+CO+H    2.5E5      2.245   367.6 ! JAM

```

```

C3H2+O=C2H2+CO          6.80E+13   0.00   0.   ! (100) Warnatz 83
C3H2+OH=C2H2+HCO        6.80E+13   0.00   0.   ! (100) Warnatz 83
C3H2+H=C3H3              1.1E+40  -8.0   84700. ! (101) HAR/KLI
07, WestmQRRK
!C3H2+H=C3H3              7.60E+13   0.22  -86.84 !2007HAR/KLI3789-3801
C3H2+CH=C4H2+H          5.00E+13   0.00   0.   ! (54) Wang 97
C3H2+CH2=nC4H3+H        5.00E+13   0.00   0.   ! (54) Wang 97
C3H2+CH3=C4H4+H         5.00E+12   0.00   0.   ! (54) Wang 97
C3H2+HCCO=nC4H3+CO      1.00E+13   0.00   0.   ! (54) Wang 97
!
!-----C3HxO chemistry-----
!
C2H3CO+M=>C2H3+CO+M      8.51E+15   0.00  23000. ! (76) Wilk 89
C2H3+CO+M=>C2H3CO+M      1.58E+11   0.00   6000. ! (76) Wilk 89
C2H3CHO+HO2=>C2H3CH2O+O2 1.29E+11   0.00  32000. ! (76) Wilk 89
C2H3CH2O=>C2H3CHO+H      1.00E+14   0.00  19000. ! (76) Wilk 89
C2H3CHO+H=>C2H3CH2O      1.00E+08   0.00  10000. ! (76) Wilk 89
C2H3CHO+OH=>C2H3CO+H2O   1.00E+13   0.00   0.   ! (76) Wilk 89
C2H3CO+H2O=>C2H3CHO+OH   1.91E+13   0.00  36620. ! (76) Wilk 89
C2H3CHO+H=>C2H3CO+H2     3.98E+13   0.00  4200.  ! (76) Wilk 89
C2H3CO+H2=>C2H3CHO+H     1.78E+13   0.00  23670. ! (76) Wilk 89
C2H3CHO+O=>C2H3CO+OH     5.01E+12   0.00   1790. ! (76) Wilk 89
C2H3CO+OH=>C2H3CHO+O     1.00E+12   0.00  19160. ! (76) Wilk 89
C2H3CHO+HO2=>C2H3CO+H2O2 1.70E+12   0.00  10700. ! (76) Wilk 89
C2H3CO+H2O2=>C2H3CHO+HO2 1.00E+12   0.00  14100. ! (76) Wilk 89
C2H3CHO+CH3=>C2H3CO+CH4  1.74E+12   0.00   8440. ! (76) Wilk 89
C2H3CO+CH4=>C2H3CHO+CH3  1.51E+13   0.00  28000. ! (76) Wilk 89
C2H3CH2O+O2=>C2H3CHO+HO2 1.74E+11   0.00   1750. ! (76) Wilk 89
C2H3CH2O=>CH2O+C2H3      1.00E+14   0.00  21600. ! (76) Wilk 89
CH2O+C2H3=>C2H3CH2O      1.00E+11   0.00   0.   ! (76) Wilk 89
!
! Miller C4H, only three reactions!
C4H+H2=C4H2+H            2.0E13    0.0    5000. !JAM 6/01
C4H+O2=CO+CO+C2H        1.2E12    0.0    0.0   ! JAM 1996/CJP 092899
C4H2+OH=H2O+C4H         9.15E+09  1.03   21746. ! Proc Comb Inst 31 185-193 (2007)
!
!-----C4H2 chemistry-----
!
C4H2+OH=CO+C3H3          1.69E+28  -4.59   20140. ! (103) JPS/SJK/JAM 07
C4H2+H=nC4H3             1.4375E+63 -15.66  24018  ! (102) SJK/JAM 05
DUPLICATE
C4H2+H=nC4H3             4.165E+32  -6.4928 9726.1 ! (102) SJK/JAM 05
DUPLICATE
C4H2+H (+M)=iC4H3 (+M)   4.31E10   1.158   1752.9 ! (102) SJK/JAM 05
LOW                       /2.30E45  -8.095   2506.6 /
TROE /0.0748 1.0E-50 -4215.9 1.0E50/
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
C4H2+O=C3H2+CO           2.70E+13   0.00   1720. ! (3) Warnatz 84
!
!-----C4H3 chemistry-----
!
nC4H3=iC4H3              3.70E+61  -15.81  54890. ! (54) Wang 97 20 Torr
nC4H3+H=iC4H3+H         2.40E+11   0.79   2410.  ! (54) Wang 97 20 Torr
nC4H3+H=C2H2+H2CC       1.60E+19  -1.60   2220.  ! (54) Wang 97 20 Torr
nC4H3+H=C4H4             1.10E+42  -9.65   7000.  ! (54) Wang 97 20 Torr
nC4H3+H=C4H2+H2         3.00E+13   0.00   0.   ! (54) Wang 97
nC4H3+OH=C4H2+H2O       2.00E+12   0.00   0.   ! (54) Wang 97
iC4H3+H=C2H2+H2CC       2.40E+19  -1.60   2800.  ! (54) Wang 97 20 Torr
iC4H3+H=C4H4             4.20E+44 -10.27  7890.  ! (54) Wang 97 20 Torr
iC4H3+H=C4H2+H2         5.00E+13   0.00   0.   ! (46) Miller 92
iC4H3+OH=C4H2+H2O       4.00E+12   0.00   0.   ! (54) Wang 97
iC4H3+O2=HCCO+CH2CO     7.86E+16  -1.80   0.   ! (54) Wang 97
!
!-----C4H4 chemistry-----
!
C4H4+H=n-C4H5            4.20E+50 -12.34  12500. ! (54) Wang 97 20Torr

```

```

C4H4+H=i-C4H5                9.60E+52 -12.85      14300.    ! (54) Wang 97 20Torr
!Miller These are fits from JAM&SJK 2002 30 Torr
!CH2CHCHCH=CH2CHCCH+H      1.12E47  -10.997  48397.
!CH2CHCCH2=CH2CHCCH+H      3.15E58  -13.954  64898.
C4H4+H=nC4H3+H2              6.65E+05  2.53      12240.    ! (54) Wang 97
C4H4+H=iC4H3+H2              3.33E+05  2.53      9240.     ! (54) Wang 97
! CH2CHCCH+H=HCCHCCH+H2     2.0E7    2.0    15000.    !JAM
! CH2CHCCH+H=H2CCCCH+H2     3.0E7    2.0    5000.     !JAM
C4H4+OH=nC4H3+H2O            3.10E+07  2.00      3430.    ! (54) Wang 97
C4H4+OH=iC4H3+H2O            1.55E+07  2.00      430.     ! (54) Wang 97
! CH2CHCCH+OH=HCCHCCH+H2O   7.5E6    2.0    5000.     !JAM
! CH2CHCCH+OH=H2CCCCH+H2O   1.0E7    2.0    2000.     !JAM

C4H4+O=C3H3+HCO              6.00E+08  1.45      -860.    ! (54) Wang 97
!
!-----C4H5 chemistry-----
!
n-C4H5=i-C4H5                1.30E+62 -16.38      49600.    ! (54) Wang 97 20Torr
n-C4H5+H=i-C4H5+H            1.00E+36 -6.26      17486.    ! (54) Wang 97 20Torr
n-C4H5+H=C4H4+H2             1.50E+13  0.00        0.        ! (54) Wang 97
n-C4H5+OH=C4H4+H2O           2.00E+12  0.00        0.        ! (54) Wang 97
n-C4H5+HCO=iiiC4H6+CO        5.00E+12  0.00        0.        ! (54) Wang 97
n-C4H5+HO2=C2H3+CH2CO+OH     6.60E+12  0.00        0.        ! (54) Wang 97
n-C4H5+H2O2=iiC4H6+HO2       1.21E+10  0.00      -596.     ! (54) Wang 97
n-C4H5+HO2=iiiC4H6+O2        6.00E+11  0.00        0.        ! (54) Wang 97
n-C4H5+O2=HCO+C2H3CHO        9.20E+16 -1.39      1010.    ! (54) Wang 97
i-C4H5+H=C4H4+H2             3.00E+13  0.00        0.        ! (54) Wang 97
i-C4H5+H=C3H3+CH3            1.0E14   0.00        0.        ! (66) Hansen/Miller 08
i-C4H5+OH=C4H4+H2O           4.00E+12  0.00        0.        ! (54) Wang 97
i-C4H5+HCO=iiiC4H6+CO        5.00E+12  0.00        0.        ! (54) Wang 97
i-C4H5+HO2=iiiC4H6+O2        6.00E+11  0.00        0.        ! (54) Wang 97
i-C4H5+HO2=C2H3+CH2CO+OH     6.60E+12  0.00        0.        ! (54) Wang 97
i-C4H5+H2O2=iiC4H6+HO2       1.21E+10  0.00      -596.     ! (54) Wang 97
i-C4H5+O2=CH2CO+CH2CHO       2.16E+10  0.00      2500.    ! (54) Wang 97
!
!-----C4H6 chemistry-----
!
iiiC4H6=i-C4H5+H              8.20E+51 -10.92     118409.   ! (54) Wang 97 20Torr
iiiC4H6=n-C4H5+H              3.50E+61 -13.87     129677.   ! (54) Wang 97 20Torr
! Miller CH2CHCHCH2=CH2CHCCH2+H  5.70E+36  -6.270  112353.2 ! Laskin et al.
2000
! Miller CH2CHCHCH2=CH2CHCHCH+H  5.30E+44  -8.620  123608.2 ! Laskin et al.
2000
iiiC4H6=C4H4+H2               2.50E+15  0.00      94700.    ! (106) Hidaka 96
iiiC4H6+H=n-C4H5+H2           3.0E7    2.0      13000.    ! (66) Hansen/Miller 08
JAM Est
iiiC4H6+H=i-C4H5+H2           3.0E7    2.0      6000.     ! (66) Hansen/Miller 08
JAM Est
C2H4+C2H3=iiiC4H6+H           7.40E+14 -0.66      8420.     ! (54) Wang 97 20Torr
iiiC4H6+H=PC3H4+CH3           2.00E+12  0.00      7000.     ! (86) Wang USC_II 07
iiiC4H6+H=AC3H4+CH3           2.00E+12  0.00      7000.     ! (86) Wang USC_II 07
iiiC4H6+O=n-C4H5+OH           7.50E+06  1.90      3740.     ! (86) Wang USC_II 07
iiiC4H6+O=i-C4H5+OH           7.50E+06  1.90      3740.     ! (86) Wang USC_II 07
iiiC4H6+O=HCO+AC3H5           6.02E+08  1.45     -858.     ! (66) Hansen/Miller 08
iiiC4H6+OH=CH3CHO+C2H3        6.3E12   0.00     -874.     ! (66) Hansen/Miller 08
JAM Est
iiiC4H6+OH=AC3H5+CH2O         6.3E12   0.00     -874.     ! (66) Hansen/Miller 08
! iiiC4H6+OH=n-C4H5+H2O       6.20E+06  2.00      3430.     ! (107) Liu 88
! iiiC4H6+OH=i-C4H5+H2O       3.10E+06  2.00      430.      ! (86) Wang USC_II 07
iiiC4H6+OH=n-C4H5+H2O         2.0E7    2.0      5000.     ! JAM
iiiC4H6+OH=i-C4H5+H2O         2.0E7    2.0      2000.     ! JAM
! CH2CHCHCH2+OH=CH2CHCHCH+H2O  2.0E7    2.0      5000.     ! JAM
! CH2CHCHCH2+OH=CH2CHCCH2+H2O  2.0E7    2.0      2000.     ! JAM
iiiC4H6+CH3=n-C4H5+CH4        2.00E+14  0.00      22800.    ! (106) Hidaka 96
iiiC4H6+CH3=i-C4H5+CH4        1.00E+14  0.00      19800.    ! (106) Hidaka 96
iiiC4H6+C2H3=n-C4H5+C2H4      5.00E+13  0.00      22800.    ! (106) Hidaka 96

```

```

iiiC4H6+C2H3=i-C4H5+C2H4      2.50E+13   0.00   19800.   ! (106) Hidaka 96
iiiC4H6+C3H3=n-C4H5+AC3H4      1.00E+13   0.00   22500.   ! (106) Hidaka 96
iiiC4H6+C3H3=i-C4H5+AC3H4      5.00E+12   0.00   19500.   ! (106) Hidaka 96
iiiC4H6+AC3H5=n-C4H5+C3H6      1.00E+13   0.00   22500.   ! (86) Wang USC_II 07
iiiC4H6+AC3H5=i-C4H5+C3H6      5.00E+12   0.00   19500.   ! (86) Wang USC_II 07
iiC4H6=i-C4H5+H                  4.20E+15   0.00   92600.   ! (108) Leung/Linstedt 95
iiC4H6+H=iiiC4H6+H              2.00E+13   0.00    4000.   ! (86) Wang USC_II 07
iiC4H6+H=i-C4H5+H2              1.70E+05   2.50   2490.   ! (86) Wang USC_II 07
iiC4H6+H=AC3H4+CH3              2.00E+13   0.00    2000.   ! (86) Wang USC_II 07
iiC4H6+H=PC3H4+CH3              2.00E+13   0.00    2000.   ! (86) Wang USC_II 07
iiC4H6+CH3=i-C4H5+CH4           7.00E+13   0.00   18500.   ! (86) Wang USC_II 07
iiC4H6+O=CH2CO+C2H4             1.20E+08   1.65    327.   ! (86) Wang USC_II 07
iiC4H6+O=i-C4H5+OH              1.80E+11   0.70   5880.   ! (86) Wang USC_II 07
iiC4H6+OH=i-C4H5+H2O            3.10E+06   2.00   -298.   ! (86) Wang USC_II 07
iiC4H6=iiiC4H6                  3.00E+13   0.00   65000.   ! (86) Wang USC_II 07
!
!-----1-C4H8 1-butene chemistry-----
!
IC4H8+H=C2H4+C2H5                1.60E+22   -2.39   11180.   ! (86) Wang USC_II 07
IC4H8+H=C3H6+CH3                 3.20E+22   -2.39   11180.   ! (86) Wang USC_II 07
IC4H8+H=C4H7+H2                  6.50E+05   2.54    6756.   ! (86) Wang USC_II 07
IC4H8+O=nC3H7+HCO                3.30E+08   1.45   -402.   ! (109) Ko/Adusei 91
IC4H8+O=C4H7+OH                  1.50E+13   0.00    5760.   ! (109) Ko/Adusei 91
DUPLICATE
IC4H8+O=C4H7+OH                  2.60E+13   0.00    4470.   ! (109) Ko/Adusei 91
DUPLICATE
IC4H8+OH=C4H7+H2O                7.00E+02   2.66     527.   ! (86) Wang USC_II 07
IC4H8+O2=C4H7+HO2                2.00E+13   0.00   50930.   ! (86) Wang USC_II 07
IC4H8+HO2=C4H7+H2O2              1.00E+12   0.00   14340.   ! (86) Wang USC_II 07
IC4H8+CH3=C4H7+CH4               4.50E-01   3.65    7153.   ! (86) Wang USC_II 07
C4H7=iiiC4H6+H                   1.27E24   -4.752  23777.   ! (133) Kiefer 09
C4H7+H(+M)=IC4H8(+M)             3.60E+13   0.00     0.   ! (86) Wang USC_II 07
LOW                               /3.01E+48  -9.32   5833.6/
TROE /0.498 1314 1314 50000/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C4H7+H=CH3+AC3H5                 2.00E+21   -2.00   11000.   ! (86) Wang USC_II 07
C4H7+H=iiiC4H6+H2                1.80E+12   0.00     0.   ! (86) Wang USC_II 07
C4H7+O2=iiiC4H6+HO2              1.00E+11   0.00     0.   ! (86) Wang USC_II 07
!C4H7+HO2=CH2O+OH+AC3H5          2.40E+13   0.00     0.   ! (86) Wang USC_II 07
C4H7+HCO=IC4H8+CO                6.00E+13   0.00     0.   ! (86) Wang USC_II 07
C4H7+CH3=iiiC4H6+CH4             1.10E+13   0.00     0.   ! (86) Wang USC_II 07
C2H4+C2H3=C4H7                   1.23E+35   -7.76   9930.   ! (54) Wang 97 RRKM 0.1
atm
!
!-----1-butyl nC4H9 chemistry from USC_Mech_II:
! (86) 2007 Hai Wang USC_II
IC4H8+H(+M) = nC4H9(+M)          1.33E+13   0.00   3260.7   !=(C3H6+H) TS5 600 cm-1
LOW                               /6.26E+38  -6.66   7000./
TROE /1.000 1000. 1310. 48097. /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C2H4+C2H5 = nC4H9                 1.50E+11   0.00   7300.   ! KP, P
nC4H9+H = IC4H8+H2                1.80E+12   0.00     0.   ! =(nC3H7+H) TS4
nC4H9+O = nC3H7+CH2O              9.60E+13   0.00     0.   ! =(nC3H7+O) TS3 ka+kb
nC4H9+OH = IC4H8+H2O              2.40E+13   0.00     0.   ! =(nC3H7+OH) TS3
nC4H9+O2 = IC4H8+HO2              2.70E+11   0.00     0.   ! BB75
nC4H9+HO2 = nC3H7+OH+CH2O         2.40E+13   0.00     0.   ! =(nC3H7+HO2) TS3 ?
!pC4H9+HCO = C4H10+CO             9.00E+13   0.00     0.   ! =(nC3H7+HCO) TS3
nC4H9+CH3 = IC4H8+CH4             1.10E+13   0.00     0.   ! =(nC3H7+CH3) TS3
!C4H10+H = pC4H9+H2              9.20E+05   2.54   6756.   ! =(C3H8+H scaled to BBW
at 753K)
!
!=====
! = DME and EtOH Subset =
!=====

```

C2H5OH=CH3+CH2OH 1.26E+51 -10.59 100869 !Juan's RRKM\_v0.6 for 1 atm  
 C2H5OH=C2H4+H2O 8.80E+25 -3.68 70799 !Juan's RRKM\_v0.6 for 1 atm  
 C2H5OH+OH=C2H4OH+H2O 1.81E+11 0.39 716.5 !temp  
 C2H5OH+OH=CH3CHOH+H2O 3.09E+10 0.49 -379.8 !temp  
 C2H5OH+OH=C2H5O+H2O 1.05E+10 0.79 716.9 !temp  
 C2H5OH+H=C2H4OH+H2 1.90E+7 1.8 5098.0 !temp  
 C2H5OH+H=CH3CHOH+H2 2.58E+7 1.65 2827.0 !MARINOV 1998  
 C2H5OH+H=C2H5O+H2 1.50E+7 1.60 3038.0 !MARINOV 1998  
 C2H5OH+O=C2H4OH+OH 9.41E+7 1.70 5459.0 !MARINOV 1998  
 C2H5OH+O=CH3CHOH+OH 1.88E+7 1.85 1824.0 !MARINOV 1998  
 C2H5OH+O=C2H5O+OH 1.58E+7 2.00 4448.0 !MARINOV 1998  
 C2H5OH+CH3=C2H4OH+CH4 2.19E+2 3.18 9622.0 !MARINOV 1998  
 C2H5OH+CH3=CH3CHOH+CH4 7.28E+2 2.99 7948.0 !MARINOV 1998  
 C2H5OH+CH3=C2H5O+CH4 1.45E+2 2.99 7649.0 !MARINOV 1998  
 C2H5OH+HO2=CH3CHOH+H2O2 8.20E+3 2.55 10750.0 !temp  
 C2H5OH+HO2=C2H4OH+H2O2 2.43E+4 2.55 15750.0 !temp  
 C2H5OH+HO2=C2H5O+H2O2 3.80E+12 0.0 24000.0 !temp  
 C2H5O+M=CH3CHO+H+M 0.56E+35 -5.89 25274.0 ! temp  
 C2H5O+M=CH3+CH2O+M 5.35E+37 -6.96 23800.0 !temp  
 C2H5O+CO=C2H5+CO2 4.68E+2 3.16 5380.0 !MARINOV 1998  
 C2H5O+H=CH3+CH2OH 3.00E+13 0.0 0.0 !MARINOV 1998  
 C2H5O+H=C2H4+H2O 3.00E+13 0.0 0.0 !MARINOV 1998  
 C2H5O+OH=CH3CHO+H2O 1.00E+13 0.0 0.0 !MARINOV 1998  
 CH3CHOH+O2=CH3CHO+HO2 4.82E+13 0.0 5017.0 !MARINOV 1998  
 DUP  
 CH3CHOH+O2=CH3CHO+HO2 8.43E+14 -1.2 0.0 !MARINOV 1998  
 DUP  
 CH3CHOH+O=CH3CHO+OH 1.00E+14 0.0 0.0 !MARINOV 1998  
 CH3CHOH+H=C2H4+H2O 3.00E+13 0.0 0.0 !MARINOV 1998  
 CH3CHOH+H=CH3+CH2OH 3.00E+13 0.0 0.0 !MARINOV 1998  
 CH3CHOH+HO2=CH3CHO+OH+OH 4.00E+13 0.0 0.0 !MARINOV 1998  
 CH3CHOH+OH=CH3CHO+H2O 5.00E+12 0.0 0.0 !MARINOV 1998  
 CH3CHOH+M=CH3CHO+H+M 1.00E+14 0.0 25000.0 !MARINOV 1998  
 C2H4+OH=C2H4OH 2.41E+11 0.0 -2385.0 ! Diau, 1992  
 C2H4OH+O2=HOC2H4O2 1.00E+12 0.0 -1100.0 ! MARINOV 1999  
 HOC2H4O2=CH2O+CH2O+OH 1.80E+11 0.0 24500.0 ! temp  
 CH3OCH3 = CH3+CH3O 1.87637E+49 -1.04002E+01 9.34535E+04 ! P = 0.04atm  
 CH3OCH3+OH = CH3OCH2+H2O 6.71E+06 2.0 -6.2988E+02 ! PCCP 2001, 3, 4722-4732  
 CH3OCH3+H = CH3OCH2+H2 2.97E+07 2.0 4033.61 ! PCCP 2001, 3, 4722-4732  
 CH3OCH3+O = CH3OCH2+OH 1.855E-03 5.29 -1.090E+02  
 CH3OCH3+HO2 = CH3OCH2+H2O2 1.680E+13 0.00 1.769E+04  
 CH3OCH3+CH3 = CH3OCH2+CH4 3.86E-08 6.2464 2513.9  
 CH3OCH3+O2 = CH3OCH2+HO2 4.100E+13 0.00 4.491E+04  
 CH3OCH3+CH3O = CH3OCH2+CH3OH 6.020E+11 0.00 4.074E+03  
 CH3OCH2 = CH2O+CH3 1.600E+13 0.00 2.550E+04  
 CH3OCH2+CH3O = CH3OCH3+CH2O 2.410E+13 0.00 0.000E+00  
 CH3OCH2+CH2O = CH3OCH3+HCO 5.490E+03 2.80 5.862E+03  
 CH3OCH2+O2 => CH2O + CH2O + OH 5.02345E+23 -3.80666E+00 3.10000E+03 ! p=0.04atm  
 CH3OCH2 + HO2 = CH3OCH2O + OH 9.000E+12 0.00 0.000E+00  
 CH3OCH2O = CH3OCHO+H 1.745E+16 -0.66 1.172E+04  
 CH3OCHO = CH3+OCHO 1.392E+18 -0.99 7.914E+04  
 CH3OCHO+O2 = CH3OCO+HO2 1.000E+13 0.00 4.970E+04  
 CH3OCHO+OH = CH3OCO+H2O 2.340E+07 1.61 -3.500E+01  
 CH3OCHO+HO2 = CH3OCO+H2O2 1.220E+12 0.00 1.700E+04  
 CH3OCHO+O = CH3OCO+OH 2.350E+05 2.50 2.230E+03  
 CH3OCHO+H = CH3OCO+H2 4.550E+06 2.00 5.000E+03  
 CH3OCHO+CH3 = CH3OCO+CH4 7.550E-01 3.46 5.481E+03  
 CH3OCHO+CH3O = CH3OCO+CH3OH 5.480E+11 0.00 5.000E+03  
 CH3OCO = CH3O + CO 7.451E+12 -1.76 1.715E+04  
 CH3OCO = CH3 + CO2 1.514E+12 -1.78 1.382E+04  
 OCHO + M = H + CO2 + M 2.443E+15 -0.50 2.650E+04

!=====  
 != HNO Mechanism Subset =  
 !=====

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! !!  
!! NH Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NH+M=N+H+M	2.65E+14	0.0	75500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+M=N+H+M	2.65E+14	0.0	75510.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91 keyed to Ar=1.0			
!NH+H=N+H2	3.50E+13	0.0	1728.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+H=N+H2	3.200E+13	0.000	330.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+H=N+H2	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90,rv			
!NH+H=N+H2	3.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N+H2=NH+H	2.33E+14	0.0	30830.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZT00 (JCP 113, 6152, 2000)			
NH+H=N+H2	3.20E+13	0.0	325.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+H=N+H2	3.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DAV/HAN90,rv			
!NH+H=N+H2	3.20E+13	0.00	325
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH+H=N+H2	3.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90,rv			
!NH+H=N+H2	3.0E+13	0.0	0.0
!Miller personal communication; Original comments: DAVIDSON&HANSON 1990			
NH+O=N+OH	1.70E+08	1.5	3368.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!NH+O=N+OH	3.72E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91			
!N+OH=NH+O	6.40E+12	0.10	21249.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+O=N+OH	1.70E+08	1.50	3366.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+O=N+OH	7.00E+12	0.00	0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH+OH=N+H2O	1.20E+06	2.00	-487.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+OH=N+H2O	2.000E+09	1.200	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+OH=N+H2O	5.00E+11	0.500	2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NH+OH=N+H2O	5.00E+11	0.5	2000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+OH=N+H2O	5.00E+11	0.5	2000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
NH+OH=N+H2O	1.60E+07	1.733	-576
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!NH+OH=N+H2O	2.00E+09	1.20	0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH+OH=N+H2O	5.0E+11	0.500	2000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH+OH=N+H2O	0.500E+12	0.500	2000.000
!Miller personal communication; Original comments: NH3 CST			

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! NH2 Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NH2+M=NH+H+M	3.16E+23	-2.0	91400.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+M=NH+H+M	3.16E+23	-2.0	91400
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+H=NH+H2	4.80E+08	1.50	7934.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+H=NH+H2	7.20E+05	2.320	799
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG95			
!NH2+H=NH+H2	4.00E+13	0.0	3650.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+H=NH+H2	4.000E+13	0.000	3650.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH2+H=NH+H2	4.00E+13	0.0	3650.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90			
!NH+H2=NH2+H	1.00E+14	0.0	20070.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186. [EDIT TEST]			
!NH2+H=NH+H2	7.20E+05	2.320	799
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG95			
!NH2+H=NH+H2	1.00E+06	2.32	799
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+H=NH+H2	7.2E+05	2.320	799
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG95			
NH2+H=NH+H2	4.0E+13	0.0	3650.
!Miller personal communication; Original comments: NH2-NO2 paper [EDIT TEST]			
!NH2+O=NH+OH	7.00E+12	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+O=NH+OH	3.30E+08	1.50	5074.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+O=OH+NH	3.000E+12	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
NH2+O=NH+OH	7.00E+12	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: INO/WAS99,DRA/WAG84,ADA/PHI94			
DUPLICATE			
NH2+O=NH+OH	8.60E-01	4.010	1673
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DUA/PAG95			
DUPLICATE			
!NH2+O=NH+OH	6.80E+12	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+O=NH+OH	7.00E+12	0.00	0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00			
! DUPLICATE			
!NH2+O=NH+OH	3.33E+08	1.50	5077
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00			
! DUPLICATE			
!NH2+O=NH+OH	7.00E+12	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09			
INO/WAS99,DRA/WAG84,ADA/PHI94			
! DUPLICATE			
!NH2+O=NH+OH	8.60E-01	4.010	1673
!Klippenstein et al. C&F 158 (2011) 774-789.			
! DUPLICATE			
!NH2+O=NH+OH	7.00E+12	0.00	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+O=NH+OH	7.0E+12	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:			
INO/WAS99,DRA/WAG84,ADA/PHI94			
! DUPLICATE			
!NH2+O=NH+OH	8.6E-1	4.010	1673



```

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:          DUA/PAG95
!   DUPLICATE
!NH2+O=NH+OH          0.675E+13   0.000   0.000
!Miller personal communication; Original comments:

!NH2+OH=NH+H2O          2.40E+06   2.00   50.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+OH=NH+H2O          9.000E+07   1.500  -460.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH2+OH=NH+H2O          4.00E+06   2.000  1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2+OH=NH+H2O          4.00E+06   2.0    1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+OH=NH+H2O          4.00E+06   2.0    1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
NH2+OH=NH+H2O          3.30E+06   1.949  -217
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09,adj
!NH2+OH=NH+H2O          9.00E+07   1.50   -460
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+OH=NH+H2O          4.0E+06   2.000  1000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2+OH=NH+H2O          0.400E+07   2.000  1000.000
!Miller personal communication; Original comments: JAM,9/87

NH2+O2=NH+HO2          1.00E+14   0.0    49997.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94

!NH+NH=NH2+N          5.95E+02   2.9    -2030.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
NH+NH=NH2+N          5.70E-01   3.880   342
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   NH3 Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH3(+M)=NH2+H(+M)          3.60E+16   0.0    93733.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH3+M=NH2+H+M          2.20E+16   0.000  93470
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90
NH3+M=NH2+H+M          2.20E+16   0.0    93470.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH3(+M)=NH2+H(+M)          5.50E+15   0.00   107792.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)
!   LOW/                      2.20E+16   0.00   93470. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)
!NH3+M=NH2+H+M          2.20E+16   0.0    93470.0 !Sun et al. Int.
J. Chem. Kinetics 41 (2009) 176-186.
!NH3+M=NH2+H+M          2.20E+16   0.000  93470
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DAV/HAN90
!NH3+M=NH2+H+M          2.20E+16   0.00   93500
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH3+M=NH2+H+M          2.2E+16   0.000  93470
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90
!NH3+M=NH2+H+M          2.2E+16   0.0    93470.
!Miller personal communication; Original comments: NH2-NO2 paper
!   CO/2/ H2/2/ CO2/3/ H2O/5/

NH3+M=NH+H2+M          6.30E+14   0.0    93390.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!NH3+H=NH2+H2          5.40E+05   2.40   9910.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH3+H=NH2+H2 5.400E+05 2.400 9915.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NH3+H=NH2+H2 6.40E+05 2.390 10171  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIC/SUT86  
!NH3+H=NH2+H2 6.40E+05 2.4 10171.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH3+H=NH2+H2 5.42E+05 2.40 9917.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; KMF90 (Ko, Marshall...) [EDIT TEST]  
!NH3+H=NH2+H2 5.42E+05 2.4 9920.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
!NH3+H=NH2+H2 6.40E+05 2.390 10171  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIC/SUT86  
!NH3+H=NH2+H2 5.42E+05 2.40 9920  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH3+H=NH2+H2 6.4E+05 2.390 10171  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIC/SUT86  
NH3+H=NH2+H2 0.636E+06 2.390 10171.000  
!Miller personal communication; Original comments: MICHAEL [EDIT TEST]

!NH3+O=NH2+OH 9.40E+06 1.94 6454.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH3+O=NH2+OH 9.400E+06 1.940 6460.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NH3+O=NH2+OH 9.40E+06 1.940 6460  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SUT/KLE90  
!NH3+O=NH2+OH 9.40E+06 1.9 6460.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH3+O=NH2+OH 9.40E+06 1.94 6460.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SUT/PAT/KLEMM90  
NH3+O=NH2+OH 2.80E+02 3.290 4471  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09  
!NH3+O=NH2+OH 1.10E+06 2.10 5210  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH3+O=NH2+OH 9.4E+06 1.940 6460  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SUT/KLE90  
!NH3+O=NH2+OH 9.4E+6 1.90 6460.  
!Miller personal communication; Original comments: NH2-NO2 paper

!NH3+OH=NH2+H2O 5.00E+07 1.60 953.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH3+OH=NH2+H2O 5.000E+07 1.600 955.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NH3+OH=NH2+H2O 2.00E+06 2.040 566  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SAL/HAN84  
NH3+OH=NH2+H2O 2.00E+06 2.0 566.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH3+OH=NH2+H2O 2.04E+06 2.04 566.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!NH3+OH=NH2+H2O 2.00E+06 2.040 566  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 SAL/HAN84  
!NH3+OH=NH2+H2O 3.683E+03 2.86 -197.  
!Corchado et al. J. Phys Chem 99 (1995) 687-694. ; NIST Fit.  
!NH3+OH=NH2+H2O 5.00E+07 1.60 950  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH3+OH=NH2+H2O 2.0E+06 2.040 566  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SAL/HAN84  
!NH3+OH=NH2+H2O 0.204E+07 2.040 566.000  
!Miller personal communication; Original comments: LOUGE

NH2+HO2=NH3+O2 9.20E+05 1.94 -1152.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+HO2=NH3+O2 9.20E+05 1.940 -1152  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00

!NH2+HO2=NH3+O2 9.20E+05 1.9 -1152.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2+HO2=NH3+O2 2.0E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97, 298 K  
 !NH2+HO2=NH3+O2 9.20E+05 1.940 -1152  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
 !NH2+HO2=NH3+O2 9.2E+05 1.940 -1152  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
 !NH2+HO2=NH3+O2 1.0E+13 0.0 0.0  
 !Miller personal communication; Original comments: JAM/PG

NH3+HO2=NH2+H2O2 3.00E+11 0.000 22000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
 !NH3+HO2=NH2+H2O2 3.00E+11 0.0 22000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH3+HO2=NH2+H2O2 3.00E+11 0.000 22000  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 !NH3+HO2=NH2+H2O2 3.0E+11 0.000 22000  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
 !NH3+HO2=NH2+H2O2 3.0E+11 0.0 22000.  
 !Miller personal communication; Original comments: MILLER&BOWMAN IJCK

!NH2+NH=NH3+N 9.20E+05 1.94 2443.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2+NH=NH3+N 9.20E+05 1.940 2444  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 !NH2+NH=NH3+N 9.20E+05 1.9 2444.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2+NH=NH3+N 1.00E+13 0.0 2000.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 NH2+NH=NH3+N 9.60E+03 2.460 107  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09  
 !NH2+NH=NH3+N 1.00E+13 0.00 2000  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 !NH2+NH=NH3+N 9.2E+05 1.940 2444  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2+NH2=NH3+NH 5.00E+13 0.0 9929.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2+NH2=NH3+NH 5.00E+13 0.000 10000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90  
 !NH2+NH2=NH3+NH 5.00E+13 0.0 10000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2+NH2=NH3+NH 5.00E+13 0.0 10000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90  
 !NH3+NH=NH2+NH2 3.16E+14 0.0 26770.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 NH2+NH2=NH3+NH 5.60E+00 3.530 552  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09  
 !NH3+NH=NH2+NH2 3.16E+14 0.00 26800  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 !NH2+NH2=NH3+NH 5.0E+13 0.000 10000  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! N2 Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2+M=N+N+M 3.71E+21 -1.6 225000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Baulch et al, 1973

N2+M=N+N+M	1.00E+28	-3.3	225000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+N=N2+H	1.50E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+N=N2+H	1.500E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
NH+N=N2+H	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NH+N=N2+H	3.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+N=N2+H	3.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NH+N=N2+H	9.00E+11	0.5	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+N=N2+H	3.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			
!NH+N=N2+H	9.00E+11	0.50	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH+N=N2+H	3.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH+N=N2+H	0.300E+14	0.000	0.000
!Miller personal communication; Original comments: JAM			
!NH+NH=N2+H+H	5.10E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+NH=N2+H+H	2.50E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
NH+NH=N2+H+H	2.50E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+NH=N2+H+H	5.10E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB89			
!NH+NH=N2+H+H	2.5E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH+NH=N2+H+H	0.254E+14	0.000	0.000
!Miller personal communication; Original comments: NH3 CST			
NH2+N=N2+H+H	7.10E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+N=N2+H+H	7.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 WHY/PHI83			
!NH2+N=N2+H+H	7.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+N=N2+H+H	7.20E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NH2+N=N2+H+H	6.90E+13	0.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+N=N2+H+H	7.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 WHY/PHI83			
!NH2+N=N2+H+H	6.90E+13	0.00	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+N=N2+H+H	7.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 WHY/PHI83			
!NH2+N=N2+H+H	0.720E+14	0.000	0.000
!Miller personal communication; Original comments: JAM/PG			
NH+NH=N2+H2	1.00E+08	1.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   NNH Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!NNH=N2+H 3.300E+08 0.000 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+M=N2+H+M 1.300E+14 -0.110 4980.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
! CO2/2.00/ C2H6/3.00/ AR/ .70/
!NNH=N2+H 6.50E+07 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99
!NNH=N2+H 6.50E+07 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH(+M)=N2+H(+M) 4.10E+09 1.13 5186.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D95; high P
limit [EDIT TEST]
! LOW/ 1.00E+13 0.5 3060. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D95; low P
limit
! N2O/5.0/ H2O/9.0/ N2/1.0/ O2/0.82/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; like N2O+M
! HNO3/5.0/ NH3/5.0/ NO3/5.0/
!
! DUPLICATE
!NNH=N2+H 3.00E+08 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; tunneling
term, B&D95 [EDIT TEST]
! DUPLICATE
!NNH=N2+H 3.00E+08 0.0 0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! DUPLICATE
!NNH+M=N2+H+M 1.00E+13 0.5 3060.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! DUPLICATE
NNH=N2+H 1.00E+09 0.000 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST]
!NNH=N2+H 3.00E+08 0.00 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH+M=N2+H+M 1.00E+13 0.50 3060
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH=N2+H 6.5E+07 0.000 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99
!NNH=N2+H 6.5E+7 0.0 0.0
!Miller personal communication; Original comments: JAM 6/98

!NNH+H=N2+H2 2.40E+08 1.50 -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+H=H2+N2 5.000E+13 0.000 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+H=N2+H2 1.00E+14 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NNH+H=N2+H2 1.00E+14 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+H=N2+H2 1.00E+14 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NNH+H=N2+H2 1.00E+14 0.0 0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NNH+H=N2+H2 1.00E+14 0.000 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+H=N2+H2 1.0E+14 0.000 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+H=N2+H2 0.100E+15 0.000 0.000
!Miller personal communication; Original comments: JAM,9/87

NH+NH=NNH+H 5.10E+13 0.0 0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH+NH=NNH+H 5.10E+13 0.00 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

```

!NNH+O=N2+OH	1.70E+16	-1.23	496.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+O=N2+OH	1.70E+08	1.50	-894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+O=OH+N2	2.500E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+O=N2+OH	8.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NNH+O=N2+OH	8.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O<=>OH+N2	2.500E+13	0.000	0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)			
NNH+O=N2+OH	1.20E+13	0.145	-217
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NNH+O=N2+OH	8.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NNH+O=N2+OH	8.0E+13	0.0	0.0
!Miller personal communication; Original comments:			
!NNH+OH=N2+H2O	2.40E+22	-2.88	2453.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+OH=N2+H2O	1.20E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+OH=H2O+N2	2.000E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+OH=N2+H2O	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
NNH+OH=N2+H2O	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+OH=N2+H2O	5.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NNH+OH=N2+H2O	5.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			
!NNH+OH=N2+H2O	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NNH+OH=N2+H2O	0.500E+14	0.000	0.000
!Miller personal communication; Original comments:			
!NNH+O2=N2+HO2	1.20E+12	-0.34	149.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+O2=HO2+N2	5.000E+12	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+O2=N2+HO2	2.00E+14	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+HO2	2.00E+14	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O2<=>HO2+N2	5.000E+12	0.000	0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)			
NNH+O2=N2+HO2	5.60E+14	-0.385	-13
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NNH+O2=N2+HO2	2.0E+14	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+HO2	2.0E+14	0.0	0.0
!Miller personal communication; Original comments: JAM			
!NNH+O2=N2+H+O2	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99			
NNH+O2=N2+H+O2	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O2=N2+H+O2	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+O2+H	5.0E+13	0.0	0.0
!Miller personal communication; Original comments: JAM			
NNH+HO2=N2+H2O2	1.40E+04	2.69	-1599.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NNH+N=NH+N2                3.00E+13    0.0    2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!NNH+NH=N2+NH2              5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NNH+NH=N2+NH2              5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+NH=N2+NH2              5.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NNH+NH=N2+NH2              2.00E+11    0.5    2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NNH+NH=N2+NH2              5.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+NH =N2+NH2             5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NH=N2+NH2              0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

!NNH+NH2=N2+NH3             9.20E+05    1.94    -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+NH2=N2+NH3             5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NNH+NH2=N2+NH3             5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+NH2=N2+NH3             5.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NNH+NH2=N2+NH3             1.00E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NNH+NH2=N2+NH3             5.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+NH2=N2+NH3             5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NH2=N2+NH3             0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  N2H2 Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2H2=NNH+H                  5.60E+36    -7.75    70211.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H                  1.80E+40    -8.41    73348.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H                  3.10E+41    -8.42    76000.
!10 atm                       Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H                  1.60E+37    -7.94    70717.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H                  2.60E+40    -8.53    72882.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H                  1.30E+44    -9.22    77032.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2+M=NNH+H+M              1.90E+27    -3.050    66107
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 M=N2
! H2O/7/
!N2H2+M=NNH+H+M              5.00E+16    0.0    50000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: MB89
N2H2+M=NNH+H+M              5.00E+16    0.0    50000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/
!N2H2+M=NNH+H+M              5.00E+16    0.0    50000.0

```

```

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.00/ H2/2.00/
!N2H2+M=NNH+H+M           1.90E+27   -3.050   66107
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 M=N2
!   H2O/7/
!N2H2+M=NNH+H+M           5.00E+16    0.00   50000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!   H2/2/ H2O/15/ O2/2/ N2/2/
!N2H2+M=NNH+H+M           1.9E+27   -3.050   66107
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
M=N2
!   H2O/7/
!N2H2+M=NNH+H+M           0.500E+17  0.000   50000.000
!Miller personal communication; Original comments: NH3 CST
!   H2O/15/ O2/2/ N2/2/ H2/2/

N2H2+M=NH+NH+M           3.16E+16    0.0   99400.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.00/ H2/2.00/

!NH2+NH=N2H2+H           1.50E+15   -0.50    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH=N2H2+H           5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2+NH=N2H2+H           1.50E+15   -0.5     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
!NH2+NH=N2H2+H           1.50E+15   -0.50    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90
!NH2+NH=N2H2+H           1.50E+15   -0.5     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186. [EDIT TEST]
NH2+NH=N2H2+H           4.30E+14   -0.272   -77
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09 [EDIT TEST]
!NH2+NH=N2H2+H           1.50E+15   -0.50    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+NH=N2H2+H           5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2+NH=N2H2+H           0.500E+14  0.000    0.000
!Miller personal communication; Original comments: NH3CST

!N2H2+H=NNH+H2           4.80E+08    1.50   1579.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
N2H2+H=NNH+H2           8.50E+04    2.630   230
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96
!N2H2+H=NNH+H2           4.80E+08    1.5     1580.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
!N2H2+H=NNH+H2           5.00E+13    0.0     1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!N2H2+H=NNH+H2           8.50E+04    2.6     -230.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H2+H=NNH+H2           8.50E+04    2.630   230
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96
!N2H2+H=NNH+H2           8.50E+04    2.63    -230
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!N2H2+H=NNH+H2           8.5E+04    2.630   230
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96
!N2H2+H=NNH+H2           0.500E+14  0.000   1000.000
!Miller personal communication; Original comments: NH3 CST

!2NH2=N2H2+H2           5.00E+11    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DAV90
!NH2+NH2=N2H2+H2         1.00E+13    0.0     1500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
NH2+NH2=N2H2+H2         1.70E+08    1.620   11783
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

```



!NH2+NH2=N2H2+H2	5.00E+13	0.00	1500
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NH2=N2H2+H2	8.5E+11	0.0	0.0
!Miller personal communication; Original comments: NH2-NO2 paper			
N2H2+O=NNH+OH	3.30E+08	1.50	496.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+O=NNH+OH	3.30E+08	1.500	497
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+O=NNH+OH	3.30E+08	1.5	497.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N2H2+O=NNH+OH	2.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+O=NNH+OH	3.30E+08	1.500	497
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+O=NNH+OH	2.00E+13	0.00	1000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+O=NNH+OH	3.3E+08	1.500	497
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+O=NNH+OH	0.200E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!N2H2+OH=NNH+H2O	2.40E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
N2H2+OH=NNH+H2O	5.90E+01	3.400	1360
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	2.40E+06	2.0	-600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+OH=NNH+H2O	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+OH=NNH+H2O	5.90E+01	3.400	1360
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	5.92E+01	3.40	-1360
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+OH=NNH+H2O	5.9E+01	3.400	1360
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
N2H2+N=NNH+NH	1.00E+06	2.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH=NNH+NH2	2.40E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+NH=NNH+NH2	2.40E+06	2.000	-1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	2.40E+06	2.0	-1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+NH=NNH+NH2	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
N2H2+NH=NNH+NH2	1.00E+13	0.0	6000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH=NNH+NH2	2.40E+06	2.000	-1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	2.4E+06	2.000	-1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!N2H2+NH2=NH3+NNH	1.80E+06	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+NH2=NNH+NH3	8.80E-02	4.050	1610
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96			
N2H2+NH2=NH3+NNH	1.80E+06	1.9	-1152.0

!Catoire et al. C&F (2012) doi:10.1016/j.combust.ame.2011.12.007 ; Original comments: DEA/BOZ 2000

!N2H2+NH2=NH3+NNH	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+NH2=NH3+NNH	8.80E-02	4.0	-1610.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH2=NNH+NH3	8.80E-02	4.050	1610
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+NH2=NH3+NNH	8.80E-02	4.05	-1610
!Duynslaeger et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+NH2=NNH+NH3	8.8E-2	4.050	1610
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+NH2=NH3+NNH	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
NNH+NNH=N2H2+N2	1.00E+13	0.0	4000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!                           !!  
!! H2NN Chemistry       !!  
!!                           !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!H2NN=NNH+H	5.90E+32	-6.99	51762.
!0.1 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!H2NN=NNH+H	9.60E+35	-7.57	54810.
!1.0 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!H2NN=NNH+H	5.00E+36	-7.43	57263.
!10 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!H2NN=NNH+H	7.20E+28	-7.77	50729.
!0.1 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!H2NN=NNH+H	3.20E+31	-6.22	52288.
!1.0 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!H2NN=NNH+H	5.10E+33	-6.52	54185.
!10 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
H2NN=NNH+H	3.40E+26	-4.830	46228
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM			
!H2NN=NNH+H	3.40E+26	-4.830	46228
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM			
!H2NN=NNH+H	3.4E+26	-4.830	46228
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM			

!N2H2=H2NN	9.20E+38	-9.01	67689.
!0.1 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
N2H2=H2NN	2.00E+41	-9.38	68413.
!1.0 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!N2H2=H2NN	1.30E+45	-10.13	70717.
!10 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		

!H2NN+H=N2H2+H	1.80E+10	0.97	4468.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
H2NN+H=N2H2+H	7.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!H2NN+H=N2H2+H	7.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!H2NN+H=N2H2+H	7.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			

H2NN+H=NNH+H2	4.80E+08	1.50	-894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!H2NN+H=NNH+H2	4.80E+08	1.500	-894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			

```

!H2NN+H=NNH+H2                4.80E+08    1.500    -894
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+H=NNH+H2                4.8E+08    1.500    -894
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2+NH2=H2NN+H2                2.40E+20    -2.91    2135.
!0.1 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                1.20E+21    -3.08    3366.
!1.0 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                2.30E+19    -2.54    4180.
!10 atm                         Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                1.20E+21    -3.080   3368
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2
NH2+NH2=H2NN+H2                7.20E+04    1.880    8802
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!NH2+NH2=H2NN+H2                1.2E+21    -3.080   3368
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1
ATM N2

H2NN+O=OH+NNH                  3.30E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+O=NNH+OH                  3.30E+08    1.500    -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NNH+OH                  3.30E+08    1.500    -894
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NNH+OH                  3.3E+08    1.500    -894
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

H2NN+OH=NNH+H2O                2.40E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+OH=NNH+H2O                2.40E+06    2.000    -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=NNH+H2O                2.40E+06    2.000    -1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=NNH+H2O                2.4E+06    2.000    -1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

H2NN+HO2=NNH+H2O2              2.90E+04    2.69    -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+HO2=NNH+H2O2              2.90E+04    2.690    -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=NNH+H2O2              2.90E+04    2.690    -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=NNH+H2O2              2.9E+04    2.690    -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

H2NN+NH2=NH3+NNH               1.80E+06    1.94    -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+NH2=NNH+NH3               1.80E+06    1.940    -1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+NH2=NNH+NH3               1.80E+06    1.940    -1152
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+NH2=NNH+NH3               1.8E+06    1.940    -1152
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                                !!
!! N2H3 Chemistry                !!
!!                                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2H3=N2H2+H                    2.30E+43    -9.55    64432.
!0.1 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
N2H3=N2H2+H                    3.60E+47    -10.38   68970.
!1.0 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!N2H3=N2H2+H	1.80E+45	-9.39	70101.
!10 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!N2H3=N2H2+H	3.60E+47	-10.380	69009
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2 600-2500K			
!N2H3+M=N2H2+H+M	1.00E+16	0.0	37000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H3=N2H2+H	3.60E+47	-10.380	69009
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2 600-2500K			
!N2H3=N2H2+H	3.6E+47	-10.380	69009
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2 600-2500K			
N2H3+M=NH2+NH+M	5.00E+16	0.0	60000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+NH2=N2H3+H	9.20E+11	-0.01	10009.
!0.1 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
NH2+NH2=N2H3+H	1.20E+12	-0.03	10078.
!1.0 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!NH2+NH2=N2H3+H	4.70E+12	-0.20	10615.
!10 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!NH2+NH2=N2H3+H	1.20E+12	-0.030	10084
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !			
!NH2+NH2=N2H3+H	1.79E+13	-0.35	11320.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D93, AMD, priv. comm.			
!N2H3+H=NH2+NH2	5.00E+13	0.0	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+NH2=N2H3+H	1.20E+12	-0.030	10084
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !			
!NH2+NH2=N2H3+H	1.2E+12	-0.030	10084
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !			
N2H3+H=N2H2+H2	2.40E+08	1.50	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+H=N2H2+H2	2.40E+08	1.500	-10
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+H=N2H2+H2	2.40E+08	1.50	-10
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION 1/15/96 (DB00)			
!N2H3+H=N2H2+H2	1.00E+13	0.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H3+H=N2H2+H2	2.40E+08	1.500	-10
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+H=N2H2+H2	2.4E+08	1.500	-10
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
N2H3+H=NH+NH3	1.00E+11	0.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
NH3+NH2=N2H3+H2	1.00E+11	0.5	21600.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
N2H3+O=N2H2+OH	1.70E+08	1.50	-645.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+O=N2H2+OH	1.70E+08	1.500	-646
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+O=N2H2+OH	1.70E+08	1.50	-646
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION 1/15/96 (DB00)			
!N2H3+O=N2H2+OH	1.70E+08	1.500	-646
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			

$\text{N}_2\text{H}_3+\text{O}=\text{N}_2\text{H}_2+\text{OH}$  1.7E+08 1.500 -646  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

$\text{N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$  1.20E+06 2.00 -1192.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 $\text{N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$  1.20E+06 2.000 -1192  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$  1.20E+06 2.00 -1192  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
 1/15/96 (DB00)  
 $\text{N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$  1.20E+06 2.000 -1192  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$  1.2E+06 2.000 -1192  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

$\text{N}_2\text{H}_3+\text{OH}=\text{H}_2\text{NN}+\text{H}_2\text{O}$  3.00E+13 0.0 0.0  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 $\text{N}_2\text{H}_3+\text{OH}=\text{H}_2\text{NN}+\text{H}_2\text{O}$  3.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{OH}=\text{H}_2\text{NN}+\text{H}_2\text{O}$  3.00E+13 0.000 0  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{OH}=\text{H}_2\text{NN}+\text{H}_2\text{O}$  3.0E+13 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

$\text{N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$  2.90E+04 2.69 -1599.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 $\text{N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$  1.40E+04 2.690 -1600  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$  2.90E+04 2.69 -1600  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; UPDATE  
 10/18/97 (DB00)  
 $\text{N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$  1.40E+04 2.690 -1600  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$  1.4E+04 2.690 -1600  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

$\text{N}_2\text{H}_3+\text{N}=\text{N}_2\text{H}_2+\text{NH}$  1.00E+06 2.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

$\text{N}_2\text{H}_3+\text{NH}=\text{N}_2\text{H}_2+\text{NH}_2$  2.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
 $\text{N}_2\text{H}_3+\text{NH}=\text{N}_2\text{H}_2+\text{NH}_2$  2.00E+13 0.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 $\text{N}_2\text{H}_3+\text{NH}=\text{N}_2\text{H}_2+\text{NH}_2$  2.00E+13 0.000 0  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 $\text{N}_2\text{H}_3+\text{NH}=\text{N}_2\text{H}_2+\text{NH}_2$  2.0E+13 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

$\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$  9.20E+05 1.94 -1152.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$  9.20E+05 1.940 -1152  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$  9.20E+05 1.94 -1152  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
 1/15/96 (DB00)  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{NH}_3+\text{N}_2\text{H}_2$  1.00E+11 0.5 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$  9.20E+05 1.940 -1152  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$  9.2E+05 1.940 -1152  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

$\text{N}_2\text{H}_3+\text{NH}_2=\text{H}_2\text{NN}+\text{NH}_3$  3.00E+13 0.0 0.0  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 $\text{N}_2\text{H}_3+\text{NH}_2=\text{H}_2\text{NN}+\text{NH}_3$  3.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00

```

!N2H3+NH2=H2NN+NH3          3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+NH2=H2NN+NH3          3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

N2H3+NNH=N2H2+N2H2          1.00E+13    0.0      4000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

N2H3+N2H3=NH3+NH3+N2        3.00E+12    0.0      0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  N2H4 Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2+NH2=N2H4                2.00E+46   -10.93   9989.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                5.60E+48   -11.30   11876.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                3.20E+49   -11.18   13981.
!10 atm                       Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                5.60E+48   -11.300  11882
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2(600-2500K)!
!NH2+NH2+M=N2H4+M            2.98E+47   -9.44    9680.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D93, AMD,
priv. comm.
!N2H4 (+M)=NH2+NH2 (+M)       5.00E+14    0.0      60000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   LOW/                       1.50E+15    0.0      39000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.40/ NH3/3.00/ N2H4/4.00/
NH2+NH2 (+M)=N2H4 (+M)       5.60E+14   -0.414   66
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!   LOW/                       1.60E+34   -5.49    1987 /
!Klippenstein et al. C&F 158 (2011) 774-789.
!   TROE/ 0.31 1E-30 1E30 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: (Fc=0.31) ??
!NH2+NH2=N2H4                5.6E+48   -11.300  11882
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
1ATM N2(600-2500K)!

N2H4+M=N2H3+H+M              1.00E+15    0.0      63600.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.40/ NH3/3.00/ N2H4/4.00/

!N2H4=H2NN+H2                4.00E+44   -9.85    71313.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
N2H4=H2NN+H2                 5.30E+39   -8.35    69267.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4=H2NN+H2                2.50E+39   -8.19    69625.
!10 atm                       Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!N2H4+H=N2H3+H2              9.60E+08    1.50     4836.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
N2H4+H=N2H3+H2               7.00E+12    0.000    2500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 VAG95
!N2H4+H=N2H3+H2              4.90E+12    0.00     2130.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; fit to data
from 6 sources in NIST (WRA)
!N2H4+H=N2H3+H2              7.00E+12    0.0      2500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

```

!N2H4+H=N2H3+H2	7.00E+12	0.000	2500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 VAG95			
!N2H4+H=N2H3+H2	7.0E+12	0.000	2500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 VAG95			
N2H4+H=NH2+NH3	2.40E+09	0.0	3100.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
N2H4+O=N2H3+OH	6.70E+08	1.50	2850.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H4+O=N2H3+OH	1.50E+11	0.000	-1270
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG96,VAG01			
!N2H4+O=N2H3+OH	6.70E+08	1.50	2851
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST. 12/22/95 (DB00)			
!N2H4+O=N2H3+OH	6.70E+08	1.500	2851
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H4+O=N2H3+OH	1.5E+11	0.000	-1270
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG96,VAG01			
N2H4+O=N2H2+H2O	4.40E+11	0.000	-1270
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 VAG96			
!N2H4+OH=N2H3+H2O	4.80E+06	2.00	-645.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H4+OH=N2H3+H2O	1.30E+13	0.000	-318
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG01			
!N2H4+OH=N2H3+H2O	4.80E+06	2.00	-646
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST. 12/22/95 (DB00)			
N2H4+OH=N2H3+H2O	4.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HAR/ATK79			
!N2H4+OH=N2H3+H2O	1.3E+13	0.000	-318
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG01			
N2H3+HO2=N2H4+O2	9.20E+05	1.94	2125.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+HO2=N2H4+O2	9.20E+05	1.940	2126
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+HO2=N2H4+O2	9.20E+05	1.94	2126
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; NH2 WITH ADJUSTED THERMO (DB00)			
!N2H3+HO2=N2H4+O2	9.20E+05	1.940	2126
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+HO2=N2H4+O2	9.2E+05	1.940	2126
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
N2H4+N=N2H3+NH	1.00E+10	1.0	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
N2H4+NH=NH2+N2H3	1.00E+09	1.5	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H4+NH2=N2H3+NH3	3.70E+06	1.94	1628.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
N2H4+NH2=N2H3+NH3	3.90E+12	0.000	1500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 GEH/WAG71,JAM est			
!N2H4+NH2=N2H3+NH3	1.80E+06	1.7	-1380.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H4+NH2=N2H3+NH3	3.90E+12	0.000	1500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 GEH/WAG71,JAM est			
!N2H4+NH2=N2H3+NH3	3.9E+12	0.000	1500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 GEH/WAG71,JAM est			
N2H3+N2H2=N2H4+NNH	1.00E+13	0.0	6000.0

```

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

N2H3+N2H3=N2H4+N2H2                1.20E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                                !!
!!  NO Chemistry                 !!
!!                                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NO(+M)=N+O(+M)                      1.45E+15    0.0    148345.
!1.4      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO(+M)=N+O(+M)                      1.40E+15    0.0    148345.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO+M=N+O+M                          1.40E+15    0.0    148429.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
NO+M=N+O+M                          1.40E+15    0.0    148430.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
N2/1.0/ H2/2.2/ H2O/6.7/ CO2/3.0/
N2O/2.2/

!NO+H=N+OH                          1.69E+14    0.0    48773.
!1.5      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO+H=N+OH                          1.70E+14    0.0    48800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HS85
!N+OH=NO+H                          1.10E+14    0.0    1122.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N+OH=NO+H                          3.360E+13   0.000   385.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
N+OH=NO+H                          3.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 FLO/HAN77,HOW/SMI80
!N+OH=NO+H                          3.80E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N+OH=NO+H                          3.80E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04
FLO/HAN77,HOW/SMI80
!N+OH=NO+H                          2.80E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!N+OH=NO+H                          3.8E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04
FLO/HAN77,HOW/SMI80
!N+OH=NO+H                          0.380E+14   0.000    0.000
!Miller personal communication; Original comments: SMITH,FLOWER

!NH+O=NO+H                          6.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O=NO+H                          4.000E+13   0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+O=NO+H                          9.20E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 CEC94
NH+O=NO+H                          9.20E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+O=NO+H                          5.50E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91
!NH+O=NO+H                          9.20E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 CEC94
!NH+O=NO+H                          7.00E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH+O=NO+H                          9.2E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 CEC94
!NH+O=NO+H                          9.2E+13     0.0    0.0
!Miller personal communication; Original comments: MERTENS

```



NH2+O=NO+H2	5.00E+12	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: COH91			
!NH2+O=H2+NO	5.00E+12	0.00	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
NH+OH=NO+H2	2.00E+13	0.00	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
NO+O=O2+N	1.81E+09	1.0	38725.
!1.5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!O+NO=N+O2	3.80E+09	1.0	41375.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91			
!N+O2=NO+O	9.00E+09	1.00	6494.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N+O2=NO+O	9.000E+09	1.000	6500.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N+O2=NO+O	6.40E+09	1.000	6280
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	6.40E+09	1.0	6280.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N+O2=NO+O	6.40E+09	1.000	6280
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	9.00E+09	1.00	6500
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N+O2=NO+O	6.4E+09	1.000	6280
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	0.640E+10	1.000	6280.000
!Miller personal communication; Original comments:			
!NH+O2=NO+OH	7.60E+10	0.0	1529.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+O2=NO+OH	1.280E+06	1.500	100.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+O2=NO+OH	1.30E+06	1.500	100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
NH+O2=NO+OH	1.30E+06	1.5	100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+O2=NO+OH	1.28E+06	1.5	100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC, 92			
!NH+O2=NO+OH	1.30E+06	1.500	100
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=NO+OH	4.50E+08	0.790	1190
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH+O2=NO+OH	1.3E+06	1.500	100
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=NO+OH	1.28E+6	1.5	100.
!Miller personal communication; Original comments: MILL&MEL 24TH			
!O+N2=N+NO	2.00E+14	0.0	76774.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N+NO=N2+O	2.700E+13	0.000	355.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N+NO=N2+O	2.10E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05			
N+NO=N2+O	3.30E+12	0.3	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N+NO=N2+O	3.27E+12	0.3	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N+NO=N2+O	2.10E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09 CEC05			
!N2+O=NO+N	1.80E+14	0.00	76100
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N+NO=N2+O	2.1E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: CEC05			

!N+NO=N2+O	0.327E+13	0.300	0.000
!Miller personal communication; Original comments: LEEDS,MONAT			
!NH+NO=N2+OH	1.40E+17	-1.49	1311.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+NO=N2+OH	2.160E+13	-0.230	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+NO=N2+OH	2.20E+13	-0.230	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
NH+NO=N2+OH	2.20E+13	-0.2	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+NO=N2+OH	2.16E+13	-0.23	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC, 92			
!NH+NO=N2+OH	2.70E+12	-0.0721	-512
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NH+NO=N2+OH	6.10E+13	-0.50	120
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH+NO=N2+OH	2.2E+13	-0.230	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+NO=N2+OH	2.16E+13	-0.23	0.0
!Miller personal communication; Original comments: MILL&MEL 24TH			
!NH+NO=NNH+O	1.70E+14	-0.20	12193.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+O=NH+NO	7.000E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+O=NH+NO	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
!NNH+O=NH+NO	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O=NO+NH	3.30E+14	-0.23	-1013.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ditto			
NNH+O=NH+NO	5.20E+11	0.381	-409
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NNH+O=NH+NO	2.00E+14	0.00	4000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NNH+O=NH+NO	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92			
!NNH+O=NH+NO	5.0E+13	0.0	0.0
!Miller personal communication; Original comments: JAM&CFM 24TH			
!NH2+NO=N2+H2O	4.70E+12	-0.25	-1201.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+NO=N2+H2O	2.80E+20	-2.654	1258
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99			
NH2+NO=N2+H2O	2.80E+20	-2.7	1258.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+NO=N2+H2O	2.77E+20	-2.65	1258.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99			
!NH2+NO=N2+H2O	1.30E+16	-1.25	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: MILKLI00,fit			
!	DUPLICATE		
!NH2+NO=N2+H2O	-3.1E+13	-0.48	1180
!Klippenstein et al. C&F 158 (2011) 774-789.			
!	DUPLICATE		
!NH2+NO=N2+H2O	2.77E+20	-2.65	1260
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NO=N2+H2O	2.8E+20	-2.654	1258
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99			
!NH2+NO=N2+H2O	2.77E+20	-2.654	1258.3
!Miller personal communication; Original comments: JAM 3/98			
!NH2+NO=NNH+OH	3.50E+10	0.34	-765.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+NO=NNH+OH	2.30E+10	0.425	-814

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99
!NH2+NO=NNH+OH                2.30E+10    0.4    -814.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+NO=NNH+OH                2.29E+10    0.425   -815.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99 [EDIT
TEST]
!NH2+NO=NNH+OH                3.10E+13    -0.48    1180
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: MILKLI00,fit [EDIT TEST]
[EDIT TEST]
NH2+NO=NNH+OH                2.29E+10    0.425   -814
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+NO=NNH+OH                2.3E+10    0.425   -814
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99
!NH2+NO=NNH+OH                2.294E+10  0.425   -813.56
!Miller personal communication; Original comments: JAM 6/98

!N2H2+O=NH2+NO                1.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
N2H2+O=NH2+NO                1.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94
!N2H2+O=NH2+NO                1.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!N2H2+O=NH2+NO                1.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!N2H2+O=NH2+NO                1.00E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!N2H2+O=NH2+NO                1.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!N2H2+O=NH2+NO                0.100E+14  0.000    0.000
!Miller personal communication; Original comments: NH3 CST

H2NN+O=NH2+NO                7.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NH2+NO                3.20E+09    1.03    2701.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+O=NH2+NO                7.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NH2+NO                7.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

H2NN+OH=>NH2+NO+H            2.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=>NH2+NO+H            2.00E+12    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=>NH2+NO+H            2.0E+12    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

N2H3+O=>NH2+NO+H            3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=>NH2+NO+H            3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=>NH2+NO+H            3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

H2NN+HO2=>NH2+NO+OH          9.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=>NH2+NO+OH          9.00E+12    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=>NH2+NO+OH          9.0E+12    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!          !!
!!   HNO Chemistry   !!

```

```

!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NO+H(+M)=HNO(+M)                1.52E+15   -0.41   0.
!4      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!      LOW/                        8.96E+19   -1.32   735. /
!1.5-3  Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!      TROE/ 0.167 12.94 100000 /
!      DUPLICATE
!HNO(+M)=H+NO(+M)                1.20E+16   -0.43   49492.
!4      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!      LOW/                        6.02E+21   -1.61   50808. /
!1.5-3  Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!      TROE/ 0.157 12.94 100000 /
!      DUPLICATE
!HNO(+M)=H+NO(+M)                2.60E+16    0.0    48654.
!1.0 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H+NO+M=HNO+M                4.480E+19   -1.320   740.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)
!      H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!      CO2/2.00/ C2H6/3.00/ AR/ .70/
!NO+H(+M)=HNO(+M)                1.50E+15   -0.410   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 NBS91
!      LOW/                        2.40E+14    0.206   -1550 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 RIL/FON03
!      TROE/ 0.82 1E-30 1E30 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.82 (NBS91)
!      N2/1.6/
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 RIL/FON03
!H+NO(+M)=HNO(+M)                1.50E+15   -0.4    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!      LOW/                        0.23E+15    0.206   -1550.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!      N2/1.0/ H2O/10.0/ O2/1.5/ H2/2.0/
!      CO2/3.0/
!H+NO(+M)=HNO(+M)                1.52E+15   -0.41   0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Fall-off, TH91
!      LOW/                        4.00E+20   -1.75   0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Glarborg et
al, ISC 1998
!      N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.3/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 from
TH91
!NO+H(+M)=HNO(+M)                1.50E+15   -0.410   0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 NBS91 [EDIT
TEST]
!      LOW/                        2.40E+14    0.206   -1550 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 RIL/FON03 [EDIT
TEST]
!      TROE/ 0.82 1E-30 1E30 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.82 (NBS91)
[EDIT TEST]
!      N2/1.6/
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 RIL/FON03 [EDIT
TEST]
!H+NO(+M)=HNO(+M)                1.52E+15   -0.41   0.0
!Duynslaeher et al. Proceedings of the European Combustion Meeting 2011
!      LOW/                        4.00E+20   -1.75   0.0 /
!Duynslaeher et al. Proceedings of the European Combustion Meeting 2011
!      H2/2/ H2O/10/ O2/1.5/ AR/0.75/
!NO+H(+M)=HNO(+M)                1.5E+15   -0.410   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 NBS91
!      LOW/                        2.4E+14    0.206   -1550 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 RIL/FON03
!      TROE/ 0.82 1E-30 1E+30 1E+30/

```

```

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.82
(NBS91)
!      N2/1.6/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 RIL/FON03
!H+NO+M=HNO+M      4.0E+20      -1.75      0.0
!Miller personal communication; Original comments: Glarborg,et al 27th
!      H2O/10/ O2/1.5/ H2/2/ CO2/3/ N2/0.0/

!NO+H2=HNO+H      1.39E+13      0.0      56498.
!3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!H+HNO=H2+NO      1.81E+13      0.0      993.
!4      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
HNO+H=H2+NO      4.50E+11      0.72      655.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+H=H2+NO      9.000E+11      0.720      660.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNO+H=NO+H2      4.40E+11      0.720      650
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=NO+H2      4.40E+11      0.7      650.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!H+HNO=H2+NO      4.46E+11      0.72      655.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SP92
!HNO+H=NO+H2      4.40E+11      0.720      650
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=NO+H2      4.46E+11      0.72      655
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!HNO+H=NO+H2      4.4E+11      0.720      650
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=H2+NO      4.46E+11      0.720      655.
!Miller personal communication; Original comments: SOTO&PAGE JCP 1992

!NH+OH=HNO+H      2.00E+13      0.0      0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+OH=HNO+H      2.000E+13      0.000      0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+OH=HNO+H      2.00E+13      0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH+OH=HNO+H      2.00E+13      0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
NH+OH=HNO+H      3.20E+14      -0.376      -46
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!H+HNO=NH+OH      3.00E+14      0.0      18000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, 1993
jannaf est
!NH+OH=HNO+H      2.00E+13      0.00      0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH+OH=HNO+H      2.0E+13      0.000      0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH+OH=HNO+H      0.200E+14      0.000      0.000
!Miller personal communication; Original comments: NH3 CST

!HNO+H=O+NH2      3.50E+15      -0.30      29252.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+H=O+NH2      3.50E+15      -0.30      29252.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+O=HNO+H      4.60E+13      0.0      0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+O=H+HNO      3.900E+13      0.000      0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH2+O=HNO+H      6.60E+13      0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: INO/WAS99,DRA/WAG84,ADA/PHI94
!NH2+O=HNO+H      6.60E+14      -0.5      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+O=HNO+H      4.60E+13      0.00      0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00 [EDIT
TEST]

```

```

!NH2+O=HNO+H                6.60E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09
DRA/WAG84,ADA/PHI94
!NH2+O=HNO+H                4.50E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+O=HNO+H                6.6E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
INO/WAS99,DRA/WAG84,ADA/PHI94
NH2+O=HNO+H                0.663E+15  -0.500    0.000
!Miller personal communication; Original comments: [EDIT TEST]

NH+H2O=HNO+H2              2.000E+13    0.000    13850.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+H2O=HNO+H2              2.00E+13    0.00    13900
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

HNO+O=OH+NO                1.81E+13    0.0    0.
!3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!HNO+O=OH+NO                4.50E+11    0.72    655.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+O=NO+OH                2.500E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNO+O=NO+OH                2.30E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 INO/WAS99
!HNO+O=NO+OH                2.30E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNO+O=OH+NO                3.61E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
!HNO+O=NO+OH                2.30E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 INO/WAS99
!HNO+O=OH+NO                5.00E+11    0.50    2000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!HNO+O=NO+OH                2.3E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 INO/WAS99
!HNO+O=OH+NO                1.0E+13    0.0    0.0
!Miller personal communication; Original comments: NH2-NO2 paper

NH+O2=HNO+O                4.60E+05    2.00    6494.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O2=HNO+O                4.610E+05    2.000    6500.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+O2=HNO+O                4.60E+05    2.000    6500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92
!NH+O2=HNO+O                4.60E+05    2.0    6500.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+O2=HNO+O                4.61E+05    2.0    6500.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC,
92
!NH+O2=HNO+O                4.60E+05    2.000    6500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIL/MEL92
!NH+O2=HNO+O                4.00E+13    0.00    17900
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH+O2=HNO+O                4.6E+05    2.000    6500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92
!NH+O2=HNO+O                4.61E+5    2.0    6500.
!Miller personal communication; Original comments: MILL&MEL 24TH

!OH+HNO=H2O+NO            4.82E+13    0.0    993.
!3-<10      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!HNO+OH=NO+H2O            1.30E+07    1.88    -953.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+OH=NO+H2O            1.300E+07    1.900    -950.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNO+OH=NO+H2O            3.60E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 BAU73
HNO+OH=NO+H2O            3.60E+13    0.0    0.0

```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+OH=NO+H2O 1.295E+07 1.884 -958.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SPM91  
!HNO+OH=NO+H2O 3.60E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 BAU73  
!HNO+OH=NO+H2O 1.30E+07 1.88 -956  
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011  
!HNO+OH=NO+H2O 3.6E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 BAU73  
!HNO+OH=NO+H2O 0.360E+14 0.000 0.000  
!Miller personal communication; Original comments: NH3 CST

!NH2+O2=HNO+OH 6.20E+07 1.23 35081.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+O2=HNO+OH 6.20E+07 1.230 35100  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!NH2+O2=HNO+OH 6.20E+07 1.2 35100.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+O2=HNO+OH 4.50E+12 0.0 25000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
NH2+O2=HNO+OH 2.90E-02 3.764 18185  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw  
!NH2+O2=HNO+OH 1.00E+13 0.00 26300  
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011  
!NH2+O2=HNO+OH 6.2E+07 1.230 35100  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

NH2+HO2=HNO+H2O 5.68E+15 -1.12 707  
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

HNO+O2=NO+HO2 2.00E+13 0.0 15887.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO+O2=HO2+NO 1.000E+13 0.000 13000.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HNO+O2=HO2+NO 2.00E+13 0.000 16000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNO+O2=HO2+NO 2.00E+13 0.0 16000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+O2=HO2+NO 1.00E+13 0.0 25000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB91  
!HNO+O2=HO2+NO 2.00E+13 0.000 16000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNO+O2=HO2+NO 2.0E+13 0.000 16000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNO+O2=HO2+NO 2.0E+12 0.0 25000.  
!Miller personal communication; Original comments: JAM 3/98

!HNO+NH2=NH3+NO 9.20E+05 1.94 -1152.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
NH2+HNO=NH3+NO 3.60E+06 1.630 -1250  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
!NH2+HNO=NH3+NO 3.60E+06 1.6 -1250.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+NH2=NH3+NO 2.00E+13 0.0 1000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!NH2+HNO=NH3+NO 3.60E+06 1.630 -1250  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN96  
!HNO+NH2=NH3+NO 2.00E+13 0.00 1000  
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011  
!NH2+HNO=NH3+NO 3.6E+06 1.630 -1250  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
!HNO+NH2=NH3+NO 3.63E+6 1.63 -1252  
!Miller personal communication; Original comments: Lin,Morokuma JPC 1996

N2H3+O=NH2+HNO 3.00E+13 0.0 0.0  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!N2H3+O=NH2+HNO          3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=NH2+HNO          3.00E+13    0.00    0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; (DB00)
!N2H3+O=NH2+HNO          3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=NH2+HNO          3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

N2H3+OH=NH3+HNO          1.00E+12    0.000    15000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!N2H3+OH=NH3+HNO          1.00E+12    0.000    15000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!N2H3+OH=NH3+HNO          1.0E+12    0.000    15000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

!NNH+NO=N2+HNO           1.20E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+NO=N2+HNO           5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NNH+NO=N2+HNO           5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+NO=N2+HNO           2.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, est,
040596
!NNH+NO=N2+HNO           5.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+NO=N2+HNO           5.00E+13    0.00    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NNH+NO=N2+HNO           5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NO=N2+HNO           0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

H+NO+N2=HNO+N2           4.0E+20    -1.75    0.0
!Miller personal communication; Original comments: Glarborg,et al 27th

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!          !!
!!  HON Chemistry  !!
!!          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!HON (+M)=NO+H(+M)        5.10E+19    -1.73    16036.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HON+M=NO+H+M             5.10E+19    -1.7    16045.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
AR/0.7/ H2O/7.0/ CO2/2.0/

HON+H=HNO+H              2.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+H=HNO+H             2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

HON+H=OH+NH              2.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+H=OH+NH             2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

HON+O=OH+NO              7.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+O=OH+NO             7.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```



```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!   !!! change NHOH to HNOH
!!  HNOH Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

HNOH+M=H+HNO+M                    2.00E+24   -2.84   58901.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+M=HNO+H+M                    2.00E+24   -2.840   58934
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/
!HNOH+M=HNO+H+M                    2.00E+24   -2.8     58934.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   H2O/10.0/
!HNOH+M=HNO+H+M                    2.00E+24   -2.840   58934
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/
!HNOH+M=HNO+H+M                    2.0E+24   -2.840   58934
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/

HNOH+H=NH2+OH                      4.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+H=NH2+OH                      4.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=NH2+OH                      4.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+H=NH2+OH                      4.00E+13    0.00     0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION
!HNOH+H=NH2+OH                      4.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=NH2+OH                      4.0E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

HNOH+H=HNO+H2                      4.80E+08    1.50    377.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+H=HNO+H2                      4.80E+08    1.500    378
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=HNO+H2                      4.80E+08    1.5     378.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+H=HNO+H2                      4.80E+08    1.50     378
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!HNOH+H=HNO+H2                      4.80E+08    1.500    378
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=HNO+H2                      4.8E+08     1.500    378
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

HNOH+O=HNO+OH                      7.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
DUPLICATE
HNOH+O=HNO+OH                      3.30E+08    1.50    -357.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
DUPLICATE
!HNOH+O=HNO+OH                      7.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                      3.30E+08    1.500    -358
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                      7.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+O=HNO+OH                      3.30E+08    1.5     -358.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+O=HNO+OH                      7.00E+13    0.00     0

```

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION
!   DUPLICATE
!HNOH+O=HNO+OH           3.30E+08    1.50    -358
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!   DUPLICATE
!HNOH+O=HNO+OH           7.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH           3.30E+08    1.500    -358
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH           7.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH           3.3E+08    1.500    -358
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE

HNOH+OH=HNO+H2O           2.40E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+OH=HNO+H2O           2.40E+06    2.000    -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+OH=HNO+H2O           2.40E+06    2.0    -1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+OH=HNO+H2O           2.40E+06    2.00    -1192
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!HNOH+OH=HNO+H2O           2.40E+06    2.000    -1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+OH=HNO+H2O           2.4E+06    2.000    -1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNOH+O2=HNO+HO2           3.00E+12    0.000    25000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
HNOH+O2=HNO+HO2           3.00E+12    0.0    25000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+O2=HNO+HO2           3.00E+12    0.000    25000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!HNOH+O2=HNO+HO2           3.0E+12    0.000    25000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

HNOH+HO2=HNO+H2O2         2.90E+04    2.69    -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+HO2=HNO+H2O2         2.90E+04    2.690    -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+HO2=HNO+H2O2         2.90E+04    2.7    -1600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+HO2=HNO+H2O2         2.90E+04    2.690    -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+HO2=HNO+H2O2         2.9E+04    2.690    -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNOH+NH2=N2H3+OH         6.70E+06    1.82    715.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNOH+NH2=N2H3+OH         1.00E+01    3.460    -467
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+NH2=N2H3+OH         1.00E+01    3.460    -467
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+NH2=N2H3+OH         1.0E+01    3.460    -467
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNOH+NH2=H2NN+H2O         4.60E+19    -1.94    1926.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNOH+NH2=H2NN+H2O         8.80E+16    -1.080    1113
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+NH2=H2NN+H2O         8.80E+16    -1.080    1113
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00

```

```

!HNOH+NH2=H2NN+H2O                                8.8E+16   -1.080   1113
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

HNOH+NH2=HNO+NH3                                    1.80E+06   1.94    -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+NH2=NH3+HNO                                    1.80E+06   1.940   -1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+NH2=NH3+HNO                                    1.80E+06   1.9      -1152.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+NH2=NH3+HNO                                    1.80E+06   1.940   -1152
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+NH2=NH3+HNO                                    1.8E+06    1.940   -1152
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!** change H2NO to NH2O
!!                !!
!!  NH2O Chemistry !!
!!                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2O(+M)=HNO+H(+M)                                  2.80E+24   -2.83   64879.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+M=HNO+H+M                                       2.80E+24   -2.830   64915
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
NH2O+M=HNO+H+M                                       2.80E+24   -2.8     64915.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
  H2O/10.0/
!NH2O+M=HNO+H+M                                       2.80E+24   -2.830   64915
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNO+H+M                                       2.8E+24    -2.830   64915
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNO+H+M                                       7.5E+15    0.0     50000.0
!Miller personal communication; Original comments: JAM 12/96
!  H2O/5/  N2/2/

!NH2O=HNOH                                           8.20E+25   -4.94   43769.
!0.1 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O=HNOH                                         1.30E+27   -4.99   43957.
!1.0 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O=HNOH                                         2.60E+28   -5.06   44742.
!10 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O(+M)=HNOH(+M)                                1.10E+29   -3.99   43957.
!T>1000K     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+M=HNOH+M                                       1.10E+29   -4.000   44000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
NH2O+M=HNOH+M                                       1.10E+29   -4.0     44000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
  H2O/10.0/
!NH2O+M=HNOH+M                                       1.10E+29   -4.000   44000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNOH+M                                       1.1E+29    -4.000   44000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/

!NH2O+H=NH2+OH                                       4.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+H=NH2+OH                                       5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NH2O+H=NH2+OH                                       5.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

!NH2O+H=NH2+OH 4.00E+13 0.00 0  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION  
 !NH2O+H=NH2+OH 5.00E+13 0.000 0  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 !NH2O+H=NH2+OH 5.0E+13 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
 !NH2O+H=NH2+OH 5.0E+13 0.0 0.0  
 !Miller personal communication; Original comments:  
  
 !NH2O+H=HNO+H2 4.80E+08 1.50 1559.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2O+H=HNO+H2 3.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
 NH2O+H=HNO+H2 3.00E+07 2.0 2000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2O+H=HNO+H2 4.80E+08 1.50 1560  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
 !NH2O+H=HNO+H2 3.00E+07 2.000 2000  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 !NH2O+H=HNO+H2 3.0E+07 2.000 2000  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
 !NH2O+H=HNO+H2 3.0E+7 2.0 2000.  
 !Miller personal communication; Original comments: JAM,PG EST  
  
 !NH2O+O=HNO+OH 3.30E+08 1.50 487.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2O+O=HNO+OH 3.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
 NH2O+O=HNO+OH 3.00E+07 2.0 2000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2O+O=HNO+OH 3.30E+08 1.50 487  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
 !NH2O+O=HNO+OH 3.00E+07 2.000 2000  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 !NH2O+O=HNO+OH 3.0E+07 2.000 2000  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
 !NH2O+O=HNO+OH 3.0E+7 2.0 2000.  
 !Miller personal communication; Original comments:  
  
 NH2+O2=NH2O+O 2.50E+11 0.48 29570.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2+O2=NH2O+O 2.50E+11 0.480 29586  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
 !NH2+O2=NH2O+O 2.50E+11 0.5 29586.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2+O2=NH2O+O 2.60E+11 0.4872 29050  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw  
 !NH2+O2=NH2O+O 2.5E+11 0.480 29586  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
  
 !NH2O+OH=HNO+H2O 2.40E+06 2.00 -1192.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NH2O+OH=HNO+H2O 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SUN/CUR01  
 !NH2O+OH=HNO+H2O 2.00E+07 2.0 1000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NH2O+OH=HNO+H2O 2.40E+06 2.00 -1192  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
 NH2O+OH=HNO+H2O 2.00E+07 2.000 1000  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
 !NH2O+OH=HNO+H2O 1.0E+14 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SUN/CUR01  
 !NH2O+OH=HNO+H2O 2.0E+7 2.0 1000.  
 !Miller personal communication; Original comments:  
  
 !NH2+HO2=NH2O+OH 2.50E+13 0.0 0.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+HO2=NH2O+OH          5.00E+13  0.000  0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NH2+HO2=NH2O+OH          5.00E+13  0.0  0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+HO2=NH2O+OH          5.00E+13  0.000  0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2+HO2=NH2O+OH          5.0E+13  0.000  0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2+HO2=NH2O+OH          5.0E+13  0.0  0.0
!Miller personal communication; Original comments: JAM/PG

!NH2O+O2=HNO+HO2          3.00E+12  0.000  25000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NH2O+O2=HNO+HO2          3.00E+12  0.0  25000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+O2=HNO+HO2          3.00E+12  0.000  25000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+O2=HNO+HO2          3.0E+12  0.000  25000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+O2=HNO+HO2          3.0E+12  0.0  25000.
!Miller personal communication; Original comments: JAM

NH2O+HO2=HNO+H2O2          2.90E+04  2.69  -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+HO2=HNO+H2O2          2.90E+04  2.690  -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!NH2O+HO2=HNO+H2O2          2.90E+04  2.7  1600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+HO2=HNO+H2O2          2.90E+04  2.690  -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!NH2O+HO2=HNO+H2O2          2.9E+04  2.690  -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2O+NH2=HNO+NH3          1.80E+06  1.94  -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+NH2=HNO+NH3          3.00E+12  0.000  1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NH2O+NH2=HNO+NH3          3.00E+12  0.0  1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+NH2=HNO+NH3          1.80E+06  1.94  -1152
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!NH2O+NH2=HNO+NH3          3.00E+12  0.000  1000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+NH2=HNO+NH3          3.0E+12  0.000  1000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+NH2=NH3+HNO          3.0E+12  0.0  1000.
!Miller personal communication; Original comments:

!NH2O+NO=HNO+HNO          2.00E+04  2.000  13000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NH2O+NO=HNO+HNO          2.00E+04  2.0  13000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+NO=HNO+HNO          2.00E+04  2.000  13000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+NO=HNO+HNO          2.0E+04  2.000  13000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+NO=HNO+HNO          2.0E+7  2.0  13000.
!Miller personal communication; Original comments:

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  NH2OH Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

!NH2+OH=NH2OH	1.80E+32	-6.91	4111.
!0.1 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!NH2+OH=NH2OH	3.90E+33	-7.00	4438.
!1.0 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
!NH2+OH=NH2OH	5.60E+34	-7.02	5362.
!10 atm	Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)		
NH2OH(+M)=NH2+OH(+M)	1.40E+20	-1.310	64080
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
LOW/	5.40E+37	-5.96	66783 /
!Klippenstein et al. C&F 158 (2011) 774-789.			
TROE/ 0.31 1E-30 1E30 1E30 /			
NH2OH+H=HNOH+H2	4.80E+08	1.50	6246.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+H=HNOH+H2	4.80E+08	1.50	6249
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
NH2OH+H=NH2O+H2	2.40E+08	1.50	5064.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+H=NH2O+H2	2.40E+08	1.50	5067
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
NH2OH+O=HNOH+OH	3.30E+08	1.50	3863.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+O=HNOH+OH	3.30E+08	1.50	3865
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
NH2OH+O=NH2O+OH	1.70E+08	1.50	3009.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+O=NH2O+OH	1.70E+08	1.50	3010
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
!NH2OH+OH=HNOH+H2O	2.40E+06	2.00	-328.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
NH2OH+OH=HNOH+H2O	1.50E+04	2.61	-3537
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!NH2OH+OH=NH2O+H2O	1.20E+06	2.00	-596.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
NH2OH+OH=NH2O+H2O	1.50E+05	2.28	-1296
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
NH2O+HO2=O2+NH2OH	2.90E+04	2.69	-1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
HNOH+HO2=NH2OH+O2	2.90E+04	2.69	-1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
NH2OH+HO2=HNOH+H2O2	2.90E+04	2.69	9552.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+HO2=HNOH+H2O2	2.90E+04	2.69	9557
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
NH2OH+HO2=NH2O+H2O2	1.40E+04	2.69	6414.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2OH+HO2=NH2O+H2O2	1.40E+04	2.69	6418
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS			
N2H4+O=NH2OH+NH	2.90E+11	0.000	-1270
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG96,VAG01			
!N2H4+O=NH2OH+NH	2.9E+11	0.000	-1270
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG96,VAG01			
NH2OH+NH=HNOH+NH2	2.90E-03	4.40	1564
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			

NH2OH+NH=NH2O+NH2 1.50E-03 4.60 2424  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+NH2=HNOH+NH3 1.80E+06 1.94 3227.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 NH2OH+NH2=HNOH+NH3 1.10E-01 4.00 -97  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+NH2=NH2O+NH3 9.20E+05 1.94 1887.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 NH2OH+NH2=NH2O+NH3 9.50E+00 3.42 -1013  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! HNNNH2 Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!

H2NN+NH2=HNNNH2+H 7.90E+06 1.90 -1331.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! N2O Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2O(+M)=N2+O(+M) 1.30E+11 0.0 59576.  
 !2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! LOW/ 7.23E+17 -0.73 62754. /  
 !Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! TROE/ 0.0175 12.94 100000 /  
 !N2O(+M)=N2+O(+M) 5.70E+14 0.0 56061.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !N2O(+M)=N2+O(+M) 7.910E+10 0.000 56020.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 ! LOW/ 6.370E+14 0.000 56640.00 /  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 ! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/  
 ! CO2/2.00/ C2H6/3.00/ AR/ .625/  
 !N2O(+M)=N2+O(+M) 1.30E+12 0.000 62570  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JOH/GLA92,ROH/HAN96  
 ! LOW/ 4.00E+14 0.0 56600 /  
 ! N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/  
 !N2O(+M)=N2+O(+M) 1.30E+12 0.0 62570.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! LOW/ 0.40E+15 0.0 56600.0 /  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! N2/1.70/ O2/1.40/ CO2/3.00/ H2O/12.00/  
 !N2O(+M)=N2+O(+M) 1.26E+12 0.0 62620.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Rohrig et al,  
 1996 preprint [EDIT TEST]  
 ! LOW/ 5.97E+14 0.0 56640. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; to appear in  
 IJCK; rekeyed to N2  
 ! N2O/5.0/ H2O/9.0/ N2/1.0/ CO2/3.2/  
 ! O2/0.82/  
 N2O(+M)=N2+O(+M) 1.30E+12 0.000 62570  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04  
 JOH/GLA92,ROH/HAN96 [EDIT TEST]

LOW/	4.00E+14	0	56600	/
N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/				
!N2O(+M)=N2+O(+M)	1.26E+12	0.00	62600	
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011				
! LOW/	4.00E+14	0.00	56600	/
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011				
! NO/3/ N2O/3.5/ O2/1.4/ N2/1.7/				
! H2O/12/				
!N2O(+M)=N2+O(+M)	1.3E+12	0.000	62570	
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JOH/GLA92,ROH/HAN96				
! LOW/	4.0E+14	0	56600	/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:				
! N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/				
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:				
!N2O+M=N2+O+M	4.0E+14	0.0	56100.	
!Miller personal communication; Original comments: PG,ET AL 24TH [EDIT TEST]				
! N2/1.7/ O2/1.4/ H2O/12/ CO/1.5/ CO2/3/				
!Miller personal communication; Original comments: PG,et al 25th except CO [EDIT TEST]				
!N2O+H=N2+OH	9.64E+13	0.0	15093.	
!1.7 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663				
!N2O+H=N2+OH	2.20E+14	0.0	16741.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!N2O+H=N2+OH	3.870E+14	0.000	18880.00	
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )				
N2O+H=N2+OH	3.30E+10	0.000	4729	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MAR/FON87				
DUPLICATE				
N2O+H=N2+OH	4.40E+14	0.000	19254	
!Tian et al. C&F 156 (2009) 1413-1426				
DUPLICATE				
!N2O+H=N2+OH	3.30E+10	0.0	4729.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007				
!N2O+H=N2+OH	4.40E+14	0.0	19254.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007				
!N2O+H=N2+OH	1.30E+11	0.938	15210.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA01 (Fit#8, WRA, 3/16/01)				
!N2O+H=N2+OH	6.40E+07	1.835	13492	
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw				
!N2O+H=N2+OH	5.00E+13	0.00	15200	
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011				
!N2O+H=N2+OH	3.3E+10	0.000	4729	
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MAR/FON87				
! DUPLICATE				
!N2O+H=N2+OH	4.4E+14	0.000	19254	
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:				
! DUPLICATE				
!N2O+H=N2+OH	3.31E+10	0.0	4729.	
!Miller personal communication; Original comments: FONTIJN 1987				
! DUPLICATE				
!N2O+H=N2+OH	4.40E+14	0.0	19254	
!Miller personal communication; Original comments: FONTIJN 1987				
! DUPLICATE				
!H+N2O=NH+NO	8.50E+20	-1.62	35349.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
! DUPLICATE				
!NH+NO=N2O+H	3.00E+18	-1.65	1430.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
! DUPLICATE				
!NH+NO=N2O+H	3.650E+14	-0.450	0.00	
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )				
!NH+NO=N2O+H	2.90E+14	-0.400	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92 [EDIT TEST]				



```

!      DUPLICATE
!NH+NO=N2O+H                -2.20E+13  -0.230  0
!Tian et al. C&F 156 (2009) 1413-1426 [EDIT TEST]
!      DUPLICATE
!NH+NO=N2O+H                2.90E+14   -0.4    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+NO=N2O+H                -2.2E+13  -0.2    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+NO=N2O+H                3.50E+14   -0.46   16.1
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B.Williams fit
of MM calc
!NH+NO=N2O+H                1.80E+14   -0.351  -244
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST] [EDIT TEST
2]
!NH+NO=N2O+H                5.00E+14   -0.40   0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
NH+NO=N2O+H                2.9E+14   -0.400  0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92
[EDIT TEST]
      DUPLICATE
NH+NO=N2O+H                -2.2E+13  -0.230  0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: [EDIT TEST]
      DUPLICATE
!NH+NO=N2O+H                2.94E+14   -0.4    0.0
!Miller personal communication; Original comments: MILL&MEL 24TH
!      DUPLICATE
!NH+NO=N2O+H                -2.16E+13 -0.23   0.0
!Miller personal communication; Original comments: MILL&MEL 24TH
!      DUPLICATE

!H+N2O=NNH+O                2.40E+19   -1.26  47065.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+O=N2O+H                1.00E+14   0.000  0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NNH+O=N2O+H                1.00E+14   0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 [EDIT TEST]
!NNH+O=N2O+H                1.40E+14   -0.40  477.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
B&D95,QRRK,preprint on O+NNH
!NNH+O=N2O+H                1.90E+14   -0.274  -22
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST]
NNH+O=N2O+H                1.0E+14   0.000  0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est [EDIT
TEST]
!NNH+O=N2O+H                0.100E+15  0.000  0.000
!Miller personal communication; Original comments:

!NH2+NO=N2O+H2              5.00E+13   0.0    24481.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94
!NH2+NO=N2O+H2              7.00E+13   0.0    2780.
!Roose et al. Int. Symp. on Combust. 18 (1981) 853-862.
NH2+NO=H2+N2O              1.00E+13   0.00  33700
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

NO+NO=N2O+O                3.61E+12   0.0    65335.
!2      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      DUPLICATE
N2O+O=NO+NO                6.62E+13   0.0    26611.
!Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      DUPLICATE
!N2O+O=NO+NO                2.90E+13   0.0    23135.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2O+O=2NO                  2.900E+13  0.000  23150.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!N2O+O=NO+NO                9.20E+13   0.000  27679
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEA/AND00

```

!N2O+O=NO+NO	9.20E+13	0.0	27679.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N2O+O=NO+NO	9.155E+13	0.0	27680.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&A00			
!N2O+O=NO+NO	9.20E+13	0.000	27679
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEA/AND00			
!N2O+O=NO+NO	6.92E+13	0.00	26600
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!N2O+O=NO+NO	9.2E+13	0.000	27679
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEA/AND00			
!N2O+O=NO+NO	9.16E+13	0.0	27679.
!Miller personal communication; Original comments: Meagher&Anderson JPC A 2000			
N2O+O=O2+N2	1.02E+14	0.0	28001.
!2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!N2O+O=N2+O2	1.40E+12	0.0	10803.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2O+O=N2+O2	1.400E+12	0.000	10810.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N2O+O=N2+O2	3.70E+12	0.000	15936
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEA/AND00			
!N2O+O=N2+O2	3.70E+12	0.0	15936.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N2O+O=N2+O2	3.692E+12	0.0	15940.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&A00			
!N2O+O=N2+O2	3.70E+12	0.000	15936
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEA/AND00			
!N2O+O=N2+O2	1.00E+14	0.00	28200
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!N2O+O=N2+O2	3.7E+12	0.000	15936
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEA/AND00			
!N2O+O=N2+O2	3.69E+12	0.0	15936.
!Miller personal communication; Original comments:			
!HNO+NO=N2O+OH	8.50E+12	0.0	29570.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2O+OH=HNO+NO	1.20E-04	4.330	25080
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96			
N2O+OH=HNO+NO	1.20E-04	4.3	25080.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNO+NO=N2O+OH	1.70E+13	0.0	29590.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; comment follows			
!N2O+OH=HNO+NO	1.20E-04	4.330	25080
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96			
!N2O+OH=HNO+NO	1.2E-4	4.330	25080
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96			
!N2O+OH=HNO+NO	1.18E-4	4.33	25081
!Miller personal communication; Original comments:			
!N2O+OH=N2+HO2	1.30E-02	4.72	36540.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2O+OH=N2+HO2	2.000E+12	0.000	21060.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N2O+OH=N2+HO2	1.30E-02	4.720	36560
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96			
!N2O+OH=N2+HO2	1.30E-02	4.7	36560.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N2O+OH=N2+HO2	1.29E-02	4.72	36561
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Mebel et al 96, per DB00			
!N2O+OH=N2+HO2	1.30E-02	4.720	36560
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96			
N2O+OH=N2+HO2	1.00E+14	0.00	30000
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!N2O+OH=N2+HO2	1.3E-2	4.720	36560

```

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96
!N2O+OH=N2+HO2                1.29E-2    4.72    36561
!Miller personal communication; Original comments: Mebel,Lin IJCK 1996

NNH+O2=N2O+OH                  2.90E+11   -0.34   149.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+O2=N2O+OH                  2.90E+11   -0.34   150
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

!HNO+HNO=H2O+N2O              8.43E+08    0.0    3100.
!2-10 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!HNO+HNO=N2O+H2O              8.50E+08    0.0    3078.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+HNO=N2O+H2O              9.00E+08    0.000   3100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91
HNO+HNO=N2O+H2O              9.00E+08    0.0    3100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNO+HNO=N2O+H2O              3.63E-03    3.98    1190.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; LHM92
!HNO+HNO=N2O+H2O              9.00E+08    0.000   3100
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 NBS91
!HNO+HNO=N2O+H2O              9.0E+08     0.000   3100
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 NBS91
!HNO+HNO=N2O+H2O              9.0E+8      0.0     3100
!Miller personal communication; Original comments: NH2-NO2 paper

NH+N2O=N2+HNO                  2.00E+12    0.00    6000
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

!N2H2+NO=N2O+NH2              4.00E+12    0.000   11922
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H2+NO=NH2+N2O              4.00E+12    0.0     11922.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
!N2H2+NO=N2O+NH2              4.00E+12    0.0     11915.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000) [EDIT TEST[
!N2H2+NO=N2O+NH2              4.00E+12    0.000   11922
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
N2H2+NO=N2O+NH2              3.00E+10    0.00    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011 [EDIT TEST]
!N2H2+NO=N2O+NH2              4.0E+12     0.000   11922
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H2+NO=N2O+NH2              0.300E+13   0.000   0.000
!Miller personal communication; Original comments: NH3 CST

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  HNNO Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

HNNO+M=H+N2O+M                 2.20E+15    0.0     21600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+M=H+N2O+M                 2.2E+15     0.0     21600.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,
IJCK 27,867(1995)
!N2O+H=HNNO                     1.20E+24   -4.46   10694.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2O+H=HNNO                     1.30E+25   -4.48   10763.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2O+H=HNNO                     3.20E+26   -4.58   11220.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2O+H(+M)=HNNO(+M)             1.10E+27   -3.48   10763.
!10 atm & T>1000K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!N2O+H(+M)=HNNO(+M)                1.10E+27   -3.48   10763.
!1 atm & T>300K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HNNO+M=N2+OH+M                        1.00E+15    0.0    25600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+M=N2+OH+M                        1.0E+15    0.0    25600.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,
IJCK 27,867(1995)

HNNO+H=H2+N2O                          2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+H=H2+N2O                          2.0E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra est

NH2+NO=HNNO+H                          8.000E+13   0.00    28000
!Miller, Smooke, Green, Kee Combust. Sci. Technol., Vol. 34 (1983), pp 149-176

!HNNO+OH=H2O+N2O                       2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+OH=H2O+N2O                       2.0E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra est
NNH+HO2=HNNO+OH                        2.40E+13    0.0    1698.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HNNO+NO=N2O+HNO                         1.00E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                                     !!
!!  NH2NO Chemistry                   !!
!!                                     !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2+NO=NH2NO                           1.90E+30   -6.67   3495.
!0.1 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
NH2+NO=NH2NO                           3.50E+31   -6.75   3724.
!1.0 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NO=NH2NO                           1.70E+33   -6.92   4607.
!10 atm       Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO=N2+H2O                            4.10E+33   -7.18   35150.
!0.1 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
NH2NO=N2+H2O                            3.10E+34   -7.11   36262.
!1.0 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2NO=N2+H2O                            2.90E+31   -5.91   36153.
!10 atm       Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NO+H=HNNO+H2                         4.80E+08    1.50    7407.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

N2H3+O=NH2NO+H                          3.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

H2NN+OH=NH2NO+H                          2.00E+12    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NO+O=HNNO+OH                          3.30E+08    1.50    4697.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NO+OH=HNNO+H2O                       2.40E+06    2.00    -70.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

H2NN+HO2=NH2NO+OH                       6.60E+05    1.94    7050.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

NH2NO+HO2=HNNO+H2O2 2.90E+04 2.69 12620.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NO+NH2=HNNO+NH3 1.80E+06 1.94 4538.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! \*\*\*\*\* MUST INCLUDE HNNHO  
!! NH2NHO Chemistry !! \*\*\*\* rename to H2NNHO  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2NHO=NH2+HNO 2.70E+39 -8.74 41594.  
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
NH2NHO=NH2+HNO 2.40E+40 -8.73 41584.  
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2NHO=NH2+HNO 1.20E+41 -8.64 41554.  
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NHO+H=NHNHO+H2 4.80E+08 1.50 -894.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NHO+O=NHNHO+OH 3.30E+08 1.50 -894.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NHO+OH=NHNHO+H2O 2.40E+06 2.00 -1192.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

N2H3+HO2=NH2NHO+OH 3.00E+13 0.0 0.0  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NHO+HO2=NHNHO+H2O2 2.90E+04 2.69 -1599.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NH2NHO+NH2=NHNHO+NH3 1.80E+06 1.94 -1152.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! NO2 Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NO2(+M)=NO+O(+M) 7.60E+18 -1.27 73245.  
!3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
LOW/ 2.47E+28 -3.37 74756. /  
!2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
TROE/ 0.100 295.1 972.7 4981.6 /

!NO2(+M)=NO+O(+M) 5.70E+15 0.0 59954.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NO2(+M)=NO+O(+M) 7.60E+18 -1.27 73290.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Original  
comments: Tsang & Herron

! LOW/ 2.47E+28 -3.37 74800. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; keyed to  
N2=1.0  
! T&H/ 0.95 -1.0E-04 /  
N2O/1.5/ H2O/4.4/ N2/1.0/ CO2/2.3/  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; EFFICIENCIES  
FROM Baulch et al,  
DUPLICATE

```

NO+O(+M)=NO2(+M) 1.30E+15 -0.75 0.
!3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
LOW/ 4.71E+24 -2.87 1551. /
!1.3-3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
TROE/ 0.100 295.1 972.7 4681.6 /
DUPLICATE
!NO+O+M=NO2+M 1.060E+20 -1.410 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
! CO2/2.00/ C2H6/3.00/ AR/ .70/
!NO+O(+M)=NO2(+M) 1.30E+15 -0.750 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 ALL/DRY97,NBS91
! LOW/ 4.72E+24 -2.87 1550 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 ALL/DRY97 (Fc=0.95-1E-
04*T)
! TROE/ 0.880 1E03 1E04 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a ( 1bar)
! AR/0/
!NO+O(+M)=NO2(+M) 1.30E+15 -0.8 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
! LOW/ 0.75E+20 -1.41 0.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
! N2/1.7/ O2/1.5/ H2O/10.0/
!NO+O(+M)=NO2(+M) 1.30E+15 -0.750 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 ALL/DRY97,NBS91
! LOW/ 4.72E+24 -2.87 1550 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 ALL/DRY97
(Fc=0.95-1E-04*T)
! TROE/ 0.880 1E03 1E04 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
! AR/0/
!NO+O(+AR)=NO2(+AR) 1.30E+15 -0.750 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08aLL/DRY97,NBS91
! LOW/ 7.56E+19 -1.41 0 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 YAR/SUT91 (Fc=0.95-1E-
04*T)
! TROE/ 0.750 1E03 1E05 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a ( 1bar)
!NO+O(+AR)=NO2(+AR) 1.30E+15 -0.750 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08aLL/DRY97,NBS91
! LOW/ 7.56E+19 -1.41 0 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 YAR/SUT91
(Fc=0.95-1E-04*T)
! TROE/ 0.750 1E03 1E05 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!NO+O(+M)=NO2(+M) 1.30E+15 -0.75 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
! LOW/ 4.72E+24 -2.87 1550 /
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
! TROE/ 9.62E-01 1.00E+01 7.96E+03 /
! O2/0.8/ N2O/4.4/ H2O/10/ AR/0.6/
! NO2/6.2/ NO/1.8/
!NO+O=NO2 1.30E+15 -0.75 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NO+O(+M)=NO2(+M) 1.3E+15 -0.750 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08
ALL/DRY97,NBS91
! LOW/ 4.72E+24 -2.87 1550 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 ALL/DRY97
(Fc=0.95-1E-04*T)
! TROE/ 0.880 1E+03 1E+04 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a ( 1bar) Ć
AR/0/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
!NO+O(+AR)=NO2(+AR) 1.3E+15 -0.750 0

```

```

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
RAS/GLA08aLL/DRY97,NBS91
!      LOW/                                7.56E+19  -1.41      0 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 YAR/SUT91
(Fc=0.95-1E-04*T)
!      TROE/ 0.750  1E+03  1E+05  1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a ( 1bar)
C!NO+O+M=NO2+M                                7.5E+19  -1.41      0.0
!Miller personal communication; Original comments: PG
!      N2/1.7/  O2/1.5/  H2O/10/

!NO2+H=NO+OH                                8.43E+13  0.0      0.
!1.3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
NO2+H=NO+OH                                1.30E+14  0.0      357.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO2+H=NO+OH                                1.320E+14  0.000    360.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NO2+H=NO+OH                                1.30E+14  0.000    362
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 KO/FON91
!NO2+H=NO+OH                                1.30E+14  0.0      362.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO2+H=NO+OH                                1.30E+14  0.0      361.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; KF91
!NO2+H=NO+OH                                1.30E+14  0.000    362
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 KO/FON91
!NO2+H=NO+OH                                1.32E+14  0.00    362
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NO2+H=NO+OH                                1.3E+14  0.000    362
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 KO/FON91
!NO2+H=NO+OH                                8.4E+13  0.0      0.0
!Miller personal communication; Original comments: TSANG&HERRON (PG)

NH+O2=H+NO2                                2.30E+10  0.0      2482.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NO2+O=O2+NO                                3.91E+12  0.0      -238.
!1.2      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO2+O=NO+O2                                3.90E+12  0.0      -238.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO2+O=NO+O2                                3.900E+12  0.000    -240.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NO2+O=NO+O2                                1.10E+14  -0.520    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BEM/CLY74
!NO2+O=NO+O2                                3.90E+12  0.0      -238.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO2+O=NO+O2                                3.90E+12  0.0      -238.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 89
!NO2+O=NO+O2                                1.10E+14  -0.520    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BEM/CLY74
!NO2+O=NO+O2                                3.91E+12  0.00    -238
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NO2+O=NO+O2                                1.1E+14  -0.520    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BEM/CLY74
!NO2+O=NO+O2                                3.9E+12  0.0      -238.
!Miller personal communication; Original comments: TSANG&HERRON (PG)

NO2+OH=HO2+NO                                1.81E+13  0.0      6673.
!1.2      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO+HO2=NO2+OH                                2.10E+12  0.000    -497
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 CEC05
!NO+HO2=NO2+OH                                2.10E+12  0.0      -480.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO+HO2=NO2+OH                                2.11E+12  0.0      -479.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HS84 (from CJ
Howard)
!HO2+NO=NO2+OH                                2.20E+12  0.0      -476

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HO2+NO=NO2+OH 2.110E+12 0.000 -480.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NO+HO2=NO2+OH 2.10E+12 0.000 -497  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 CEC05  
!NO2+OH=HO2+NO 1.81E+13 0.00 6680  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NO+HO2=NO2+OH 2.1E+12 0.000 -497  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 CEC05  
!HO2+NO=NO2+OH 0.211E+13 0.000 -479.000  
!Miller personal communication; Original comments: HOWARD

HON+O2=NO2+OH 1.00E+12 0.0 4968.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

NO2+N=N2O+O 3.49E+12 0.0 -437.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!NO2+N=N2O+O 3.49E+12 0.0 -437.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97

!NH+NO2=N2O+OH 1.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HAR/PHI86  
!NH+NO2=N2O+OH 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH+NO2=N2O+OH 4.00E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; branching per QH95  
NH+NO2=N2O+OH 4.10E+12 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: HAR/PHI86  
!NH+NO2=N2O+OH 1.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HAR/PHI86  
!NO2+NH=N2O+OH 1.0E+13 0.0 0.0  
!Miller personal communication; Original comments: PHILLIPS

!NH+NO2=NO+HNO 5.70E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; branching per QH95  
NH+NO2=HNO+NO 5.90E+12 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: HAR/PHI86

!NO2+NH2=N2O+H2O 1.50E+16 -1.44 268.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+NO2=N2O+H2O 1.60E+16 -1.440 268  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 PAR/LIN97  
NH2+NO2=N2O+H2O 3.00E+14 -0.770 242  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SONG  
!NH2+NO2=N2O+H2O 1.60E+16 -1.4 268.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+NO2=N2O+H2O 1.62E+16 -1.44 270  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH2+NO2=N2O+H2O 1.6E+16 -1.440 268  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 PAR/LIN97  
!NO2+NH2=N2O+H2O 1.62E+16 -1.44 268  
!Miller personal communication; Original comments: Park&Lin JPC 1997

!NO2+NH2=NH2O+NO 6.60E+16 -1.44 268.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
NH2+NO2=NH2O+NO 1.30E+15 -0.770 242  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SONG  
!NH2+NO2=NH2O+NO 6.50E+16 -1.440 268  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 PAR/LIN97  
!NH2+NO2=NH2O+NO 6.50E+16 -1.4 268.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+NO2=NH2O+NO 6.5E+16 -1.440 268  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 PAR/LIN97  
!NH2+NO2=NH2O+NO 6.48E+16 -1.44 268



```

!Miller personal communication; Original comments:

!H2NN+O2=NH2+NO2                1.50E+12    0.000    5961
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
H2NN+O2=NH2+NO2                1.50E+12    0.0      5958.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+O2=NH2+NO2                1.50E+12    0.000    5961
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O2=NH2+NO2                1.5E+12     0.000    5961
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

HNNO+NO=NNH+NO2                3.20E+12    0.0      270.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+NO=NNH+NO2                3.2E+12     0.00     270.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,
IJCK 27,867(1995)

N2O+NO=NO2+N2                  5.30E+05    2.230    46280
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96
!N2O+NO=NO2+N2                  5.30E+05    2.2      46280.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N2O+NO=NO2+N2                  5.30E+05    2.230    46280
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96!
!N2O+NO=N2+NO2                  4.29E+13    0.00     47130.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, 11/95;
fit to reanalyzed
!N2O+NO=N2+NO2                  2.75E+14    0.00     50000
!Duynslaeher et al. Proceedings of the European Combustion Meeting 2011
!N2O+NO=NO2+N2                  5.3E+05     2.230    46280
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96
!N2O+NO=NO2+N2                  5.26E+5     2.23     46281
!Miller personal communication; Original comments:

NO+NO+NO=N2O+NO2              1.07E+10    0.0      26800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GVO 79

HNO+NO+NO=HNNO+NO2            1.70E+11    0.0      2100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNO+NO+NO=HNNO+NO2            1.70E+11    0.00     2100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,
IJCK 27,867(1995)

NO2+NO2=NO+NO+O2              1.63E+12    0.0      26108.
!1.5-2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO2+NO2=NO+NO+O2              4.50E+12    0.000    27599
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98
!NO2+NO2=NO+NO+O2              1.60E+12    0.0      26123.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO2+NO2=NO+NO+O2              4.51E+12    0.0      27600.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; PGML00
!NO2+NO2=NO+NO+O2              4.50E+12    0.000    27599
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98
!NO2+NO2=NO+NO+O2              4.5E+12     0.000    27599
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98
!NO2+NO2=NO+NO+O2              1.63E+12    0.0      26123.
!Miller personal communication; Original comments: TSANG&HERRON

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                                !!
!! HONO Chemistry                !!
!!                                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

HONO(+M)=OH+NO(+M)             1.20E+19    -1.23    49667.
!1.4-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663

```

LOW/ 3.01E+30 -3.8 50322. /  
 !Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 TROE/ 0.370 11.98 100000 /  
 DUPLICATE  
 !HONO(+M)=OH+NO(+M) 2.00E+31 -4.56 51146.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 NO+OH(+M)=HONO(+M) 1.99E+12 -0.05 -721.  
 !1.4-3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 LOW/ 5.08E+23 -2.51 -68. /  
 !1.5-4 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 TROE/ 0.370 11.98 100000 /  
 DUPLICATE  
 !NO+OH(+M)=HONO(+M) 1.10E+14 -0.300 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 FUL/TRO98  
 ! LOW/ 3.392E+23 -2.5 0 /  
 ! TROE/ 0.75 1E-30 1E30 1E30 /  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 FUL/TRO98 [M=He,T=400K]  
 !NO+OH(+M)=HONO(+M) 2.00E+12 -0.1 -721.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! LOW/ 0.50E+24 -2.51 -68.0 /  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! N2/1.0/ O2/1.0/ H2O/6.7/ AR/0.67/  
 !NO+OH(+M)=HONO(+M) 1.988E+12 -0.05 -721.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang & Herron  
 ! LOW/ 5.08E+23 -2.51 -67.6 /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; keyed to  
 N2=1.0.  
 ! T&H/ 0.62 /  
 ! N2O/5.0/ H2O/8.3/ N2/1.0/ CO2/1.5/  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 from  
 TH91;  
 !NO+OH(+M)=HONO(+M) 1.10E+14 -0.300 0  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 FUL/TRO98  
 ! LOW/ 3.392E+23 -2.5 0 /!  
 ! TROE/ 0.75 1E-30 1E30 1E30 /  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 FUL/TRO98  
 [M=He,T=400K]  
 !NO+OH(+M)=HONO(+M) 1.1E+14 -0.300 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 FUL/TRO98  
 ! LOW/ 3.392E+23 -2.5 0 /  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
 ! TROE/ 0.75 1E-30 1E+30 1E+30 /  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 FUL/TRO98  
 [M=He,T=400K]  
 !OH+NO+M=HONO+M 5.08E+23 -2.51 -67.6  
 !Miller personal communication; Original comments: TSANG&HERRON  
 ! CO2/0.0/ H2O/5/  
  
 !HONO+H=H2+NO2 1.20E+13 0.0 7348.  
 !20 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 !HONO+H=H2+NO2 2.00E+08 1.55 6613.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NO2+H2=HONO+H 2.41E+13 0.0 28795.  
 !5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 NO2+H2=HONO+H 1.30E+04 2.760 29770  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98  
 !NO2+H2=HONO+H 4.50E+12 0.0 27600.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !H2+NO2=HONO+H 1.30E+04 2.76 29770.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; PGML98; see  
 also MGYD00  
 !NO2+H2=HONO+H 1.30E+04 2.760 29770  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98  
 !NO2+H2=HONO+H 1.3E+04 2.760 29770  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98  
 !HONO+H=H2+NO2 1.2E+13 0.0 7352

!Miller personal communication; Original comments: TSANG&HERRON

HONO+H=H2O+NO	8.10E+06	1.89	3843.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HONO+H=NO+H2O	8.10E+06	1.890	3850
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HSU/MEL97			
!HONO+H=NO+H2O	8.10E+06	1.9	3850.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HONO+H=H2O+NO	8.13E+06	1.89	3847.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLMM97			
!HONO+H=NO+H2O	8.10E+06	1.890	3850
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HSU/MEL97			
!HONO+H=NO+H2O	8.1E+06	1.890	3850
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HSU/MEL97			
HONO+H=OH+HNO	5.60E+10	0.86	4965.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HONO+H=HNO+OH	5.60E+10	0.860	5000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HSU/MEL97			
!HONO+H=HNO+OH	5.60E+10	0.9	5000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HONO+H=HNO+OH	5.63E+10	0.86	4969.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLMM97			
!HONO+H=HNO+OH	5.60E+10	0.860	5000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HSU/MEL97			
!HONO+H=HNO+OH	5.6E+10	0.860	5000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HSU/MEL97			
HON+OH=HONO+H	4.00E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HON+OH=HONO+H	4.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
HONO+O=OH+NO2	1.20E+13	0.0	5958.
!10 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!HONO+O=OH+NO2	1.70E+08	1.50	3028.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HONO+O=NO2+OH	1.20E+13	0.000	5960
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91			
!HONO+O=NO2+OH	1.20E+13	0.0	6000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HONO+O=OH+NO2	1.2E+13	0.0	5961.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91			
!HONO+O=NO2+OH	1.20E+13	0.000	5960
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 NBS91			
!HONO+O=NO2+OH	1.2E+13	0.000	5960
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 NBS91			
!HONO+O=OH+NO2	1.2E+13	0.0	5961.
!Miller personal communication; Original comments: TSANG&HERRON			
HON+O2=HONO+O	1.00E+12	0.0	4965.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
HONO+OH=H2O+NO2	1.26E+10	1.0	135.
!2-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!HONO+OH=H2O+NO2	1.20E+06	2.00	-596.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HONO+OH=NO2+H2O	4.00E+12	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HONO+OH=NO2+H2O	1.70E+12	0.000	-520
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BUR/RAV92			
!HONO+OH=H2O+NO2	1.27E+10	1.0	135.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91			
!HONO+OH=NO2+H2O	1.70E+12	0.000	-520
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BUR/RAV92			
!HONO+OH=NO2+H2O	1.7E+12	0.000	-520

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BUR/RAV92  
!HONO+OH=H2O+NO2 4.0E+12 0.0 0.0  
!Miller personal communication; Original comments: RAVI IJCK 1992

!NO2+HO2=HONO+O2 1.90E+00 3.320 3044  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a  
NO2+HO2=HONO+O2 6.30E+08 1.2 5000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO2+HO2=HONO+O2 1.00E+12 0.0 5000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler  
!NO2+HO2=HONO+O2 1.90E+00 3.320 3044  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a  
!NO2+HO2=HONO+O2 1.9E+00 3.320 3044  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

!NH+HONO=NH2+NO2 1.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
NH+HONO=NH2+NO2 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH+HONO=NH2+NO2 1.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH+HONO=NH2+NO2 1.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

!HONO+NH2=NO2+NH3 9.20E+05 1.94 1916.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+HONO=NH3+NO2 7.10E+01 3.020 -4940  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
NH2+HONO=NH3+NO2 7.10E+01 3.0 -4940.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HONO+NH2=NO2+NH3 1.0E+10 1.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra, est, better analysis than B&T72  
!NH2+HONO=NH3+NO2 7.10E+01 3.020 -4940  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN96  
!NH2+HONO=NH3+NO2 7.1E+01 3.020 -4940  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
!HONO+NH2=NO2+NH3 71.1 3.02 -4941  
!Miller personal communication; Original comments: Lin,Morokuma JPC 1996

HNNO+NO=N2+HONO 2.60E+11 0.0 810.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+NO=N2+HONO 2.6E+11 0.0 810.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al, IJCK 27,867(1995)

HNO+NO2=HONO+NO 4.40E+04 2.640 4040  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 MEB/MOR98  
!HNO+NO2=HONO+NO 6.00E+11 0.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+NO2=HONO+NO 4.42E+04 2.64 4042.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MLM98  
!HNO+NO2=HONO+NO 4.40E+04 2.640 4040  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 MEB/LIN98  
!HNO+NO2=HONO+NO 4.4E+04 2.640 4040  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 MEB/MOR98  
!NO2+HNO=HONO+NO 6.0E+11 0.0 2000.  
!Miller personal communication; Original comments: TSANG&HERRON

!NH2O+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
NH2O+NO2=HONO+HNO 6.00E+11 0.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2O+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est

```

!NH2O+NO2=HONO+HNO                6.0E+11    0.000    2000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+NO2=HNO+HONO                6.0E+11    0.0      2000.
!Miller personal communication; Original comments: HNO+NO2

!HNOH+NO2=HONO+HNO                6.00E+11    0.000    2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
HNOH+NO2=HONO+HNO                6.00E+11    0.0      2000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+NO2=HONO+HNO                6.00E+11    0.0      2000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99, est.
!HNOH+NO2=HONO+HNO                6.00E+11    0.000    2000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!HNOH+NO2=HONO+HNO                6.0E+11    0.000    2000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

HNNO+NO2=N2O+HONO                1.00E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

HONO+HONO=NO+NO2+H2O              3.50E-01    3.640    12140
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 MEB/MEL98
!HONO+HONO=NO+NO2+H2O              3.50E-01    3.6      12100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!2HONO=NO+NO2+H2O                  0.349      3.64     12140.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MLM98
!HONO+HONO=NO+NO2+H2O              3.50E-01    3.640    12140
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 MEB/MEL98
!HONO+HONO=NO+NO2+H2O              3.5E-01    3.640    12140
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 MEB/MEL98

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  HNO2 Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!HNO2=HONO                          7.10E+27    -5.40    52507.
!0.1 atm                            Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2=HONO                          1.30E+29    -5.47    52785.
!1.0 atm                            Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2=HONO                          2.00E+30    -5.50    53658.
!10 atm                             Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNO2 (+M)=HONO (+M)                 2.50E+14    0.000    32300
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a
  LOW/                               3.10E+18    0.0      31500   /
  TROE/ 1.149 1E-30 3125 1E30 /
!HNO2 (+M)=HONO (+M)                 2.50E+14    0.000    32300
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!  LOW/                               3.10E+18    0.0      31500   /!
!  TROE/ 1.149 1E-30 3125 1E30 /
!HNO2 (+M)=HONO (+M)                 2.5E+14    0.000    32300
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a
!  LOW/                               3.1E+18    0.0      31500   /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
!  TROE/ 1.149 1E-30 3125 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:

!HNO2+H=H2+NO2                      2.40E+08    1.50     4160.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+H=H2+NO2                      2.40E+08    1.50     4163
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95
NO2+H2=HNO2+H                      2.40E+00    3.730    32400
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a

```

```

!NO2+H2=HNO2+H                2.40E+00    3.730    32400
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!NO2+H2=HNO2+H                2.4E+00    3.730    32400
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

HNO2+O=OH+NO2                  1.70E+08    1.50    2363.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+O=NO2+OH                 1.70E+08    1.500    2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 DEA/BOZ00
!HNO2+O=OH+NO2                 1.70E+08    1.50    2365
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95
!HNO2+O=NO2+OH                 1.70E+08    1.500    2000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 DEA/BOZ00
!HNO2+O=NO2+OH                 1.7E+08    1.500    2000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 DEA/BOZ00

HNO2+OH=H2O+NO2                1.20E+06    2.00    -794.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+OH=NO2+H2O               4.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a
!HNO2+OH=H2O+NO2              1.20E+06    2.00    -795
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95
!HNO2+OH=NO2+H2O               4.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!HNO2+OH=NO2+H2O               4.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

NO2+HO2=HNO2+O2                1.90E+01    3.260    4983
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a
!NO2+HO2=HNO2+O2              1.90E+01    3.260    4983
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!NO2+HO2=HNO2+O2              1.9E+01    3.260    4983
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

HNO2+NH2=NO2+NH3                9.20E+05    1.94    874.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+NH2=NO2+NH3              9.20E+05    1.94    874
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95

HNO+NO2=HNO2+NO                 6.02E+11    0.0    1986.
!5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!! HNOO Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH+O2=HNOO                      3.50E+23    -5.00    2274.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
NH+O2=HNOO                        3.70E+24    -5.00    2294.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O2=HNOO                        5.40E+25    -5.05    2453.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
NH+O2+M=HNOO+M                    3.00E+26    -4.00    2274.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HNOO+M=OH+NO+M                   1.50E+36    -6.18    31119.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! HONHO Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

HNOH+HO2=HONHO+OH 4.00E+13 0.0 0.0  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! NH2NO2 Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NH2+NO2=NH2NO2 3.50E+31 -6.8 3726.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ  
2000

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! NO3 Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NO2+O(+M)=NO3(+M) 1.32E+13 0.0 0.  
!2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
LOW/ 1.49E+28 -4.08 2466. /  
!1.3-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
TROE/ 0.326 500.0 6204.9 2606.0 /  
!NO2+O(+M)=NO3(+M) 3.50E+12 0.240 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 HAH/TRO00  
! LOW/ 2.50E+20 -1.50 0 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 (M=N2)  
! TROE/ 0.71 1E-30 1700 1E30 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.71\*exp(-T/1700)  
!NO2+O(+M)=NO3(+M) 1.30E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! LOW/ 0.10E+29 -4.08 2470.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! N2/1.50/ O2/1.50/ H2O/10.0/  
!NO2+O=NO3 1.32E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
TSA/HER86  
!O+NO2(+M)=NO3(+M) 1.33E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 keyed to  
N2  
! LOW/ 1.49E+28 -4.08 2470. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
! T&H/ 0.79 -1.8E-04 /  
N2O/5.0/ H2O/9./ N2/1.0/ HNO3/5.0/  
NH3/5.0/ NO3/5.0/  
!NO2+O(+M)=NO3(+M) 3.50E+12 0.240 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 HAH/TRO00  
! LOW/ 2.50E+20 -1.50 0 /  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 (M=N2)  
! TROE/ 0.71 1E-30 1700 1E30 /  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.71\*exp(-  
T/1700)  
!NO2+O(+M)=NO3(+M) 3.5E+12 0.240 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 HAH/TRO00

```

!      LOW/                                2.5E+20   -1.50      0      /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 (M=N2)
!      TROE/ 0.71 1E-30 1700 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.71*exp(-
T/1700)
!NO2+O(+M)=NO3(+M)                        1.3E+13    0.0        0.0
!Miller personal communication; Original comments: TSANG&HERRON
!      LOW/                                1.0E+28    -4.08      2470.    /
!      N2/1.5/ O2/1.5/ H2O/18.6/

!NO3+H=NO2+OH                             6.00E+13   0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/SCH92
NO3+H=NO2+OH                             6.00E+13   0.0        0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO3+H=NO2+OH                             6.00E+13   0.0        0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; from refs in
NIST database
!NO3+H=NO2+OH                             6.00E+13   0.000      0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 BEC/SCH92
!NO3+H=NO2+OH                             6.0E+13    0.000      0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 BEC/SCH92
!NO3+H=NO2+OH                             6.0E+13    0.0        0.0
!Miller personal communication; Original comments: BECKER ET AL 92/N (PG)

!NO3+O=NO2+O2                             1.00E+13   0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 ATK/TRO92
NO3+O=NO2+O2                             1.00E+13   0.0        0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO3+O=NO2+O2                             1.00E+13   0.0        0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 92/99
!NO3+O=NO2+O2                             1.00E+13   0.000      0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 ATK/TRO92
!NO3+O=NO2+O2                             1.0E+13    0.000      0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 ATK/TRO92
!NO3+O=NO2+O2                             1.0E+13    0.0        0.0
!Miller personal communication; Original comments: ATKINSON ET AL 92 (PG)

!NO3+OH=NO2+HO2                          1.40E+13   0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 ATK/TRO92
NO3+OH=NO2+HO2                          1.40E+13   0.0        0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO3+OH=HO2+NO2                          1.20E+13   0.0        0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 99
!NO3+OH=NO2+HO2                          1.40E+13   0.000      0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 ATK/TRO92
!NO3+OH=NO2+HO2                          1.4E+13    0.000      0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 ATK/TRO92
!NO3+OH=NO2+HO2                          1.4E+13    0.0        0.0
!Miller personal communication; Original comments: ATKINSON ET AL 92 (PG)

!NO3+HO2=NO2+O2+OH                       1.50E+12   0.000      0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/SCH92
NO3+HO2=NO2+O2+OH                       1.50E+12   0.0        0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NO3+HO2=NO2+O2+OH                       2.50E+12   0.0        0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; controversial
reaction
!NO3+HO2=NO2+O2+OH                       1.50E+12   0.000      0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 BEC/SCH92
!NO3+HO2=NO2+O2+OH                       1.5E+12    0.000      0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 BEC/SCH92
!NO3+HO2=NO2+O2+OH                       1.5E+12    0.0        0.0
!Miller personal communication; Original comments: BECKER ET AL 92 (PG)

NO3+NH=HNO+NO2                           1.50E+13   0.0        0.

```



!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler

NO3+NH2=NH2O+NO2 9.00E+05 0.0 100.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP DB00

HNNO+NO2=NNH+NO3 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

!NO2+NO2=NO3+NO 9.64E+09 -0.73 20911.  
!2-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
!NO2+NO2=NO3+NO 9.60E+09 0.730 20900  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 NBS91  
NO2+NO2=NO3+NO 9.60E+09 0.7 20900.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO2+NO2=NO+NO3 9.64E+09 0.73 20920.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; T&H91  
!NO2+NO2=NO3+NO 9.60E+09 0.730 20900  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 NBS91  
!NO2+NO2=NO3+NO 9.6E+09 0.730 20900  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 NBS91  
!NO2+NO2=NO3+NO 9.6E+9 0.73 20900.  
!Miller personal communication; Original comments: TSANG&HERRON

!NO3+NO2=NO+NO2+O2 5.00E+10 0.000 2940  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DEM/RAV90  
NO3+NO2=NO+NO2+O2 5.00E+10 0.0 2940.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO2+NO3=NO+NO2+O2 2.71E+10 0.0 2500.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97  
!NO3+NO2=NO+NO2+O2 5.00E+10 0.000 2940  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 DEM/RAV90  
!NO3+NO2=NO+NO2+O2 5.0E+10 0.000 2940  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 DEM/RAV90  
!NO3+NO2=NO+NO2+O2 5.0E+10 0.0 2940.  
!Miller personal communication; Original comments: DEMORE ET AL 90 (PG)

NO3+NO3=NO2+NO2+O2 5.12E+11 0.0 4870.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DeMore97  
!NO3+NO3=2NO2+O2 5.12E+11 0.0 4870.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! \*\*\* change HONO2 to HNO3  
!! HNO3 Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NO2+OH(+M)=HNO3(+M) 2.41E+13 0.0 0.  
!1.2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
LOW/ 6.42E+32 -5.49 2349. /  
!2.5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
TROE/ 0.400 450.7 1584.0 /  
!NO2+OH(+M)=HNO3(+M) 3.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 TRO01  
! LOW/ 2.938E+25 -3.0 0 /  
! TROE/ 0.4 1E-30 1E30 1E30 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.4  
!NO2+OH(+M)=HNO3(+M) 2.40E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! LOW/ 0.64E+33 -5.49 2351.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

! N2/1.00/ AR/0.70/ H2O/6.00/  
 !OH+NO2(+M)=HNO3(+M) 2.41E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 keyed to N2  
 ! LOW/ 6.42E+32 -5.49 2350. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
 ! T&H/ 0.725 -2.5E-04 /  
 N2O/5.0/ H2O/9./ N2/1.0/ HNO3/5.0/  
 NH3/5.0/ NO3/5.0/  
 !NO2+OH(+M)=HNO3(+M) 3.00E+13 0.000 0  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 TRO01  
 ! LOW/ 2.938E+25 -3.0 0 /  
 !Klippenstein et al. C&F 158 (2011) 774-789.  
 ! TROE/ 0.4 1E-30 1E30 1E30 /  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.4  
 !NO2+OH(+M)=HNO3(+M) 3.0E+13 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 TRO01  
 ! LOW/ 2.938E+25 -3.0 0 /  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
 ! TROE/ 0.4 1E-30 1E+30 1E+30 /  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.4  
  
 !HNO3+H=H2+NO3 5.60E+08 1.500 16400  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
 HNO3+H=NO3+H2 5.60E+08 1.5 16400.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
 BOUGHT97  
 !HNO3+H=NO3+H2 2.40E+08 1.5 11600.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
 following DB00 EP  
 !HNO3+H=H2+NO3 5.60E+08 1.500 16400  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
 !HNO3+H=H2+NO3 5.6E+08 1.500 16400  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97  
  
 HNO3+H=H2O+NO2 6.10E+01 3.300 6285  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
 !HNO3+H=NO2+H2O 6.00E+13 0.0 9800.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
 !HNO3+H=NO2+H2O 6.00E+13 0.0 9800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
 following Laidler EP  
 !HNO3+H=H2O+NO2 6.10E+01 3.300 6285  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
 !HNO3+H=H2O+NO2 6.1E+01 3.300 6285  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97  
  
 HNO3+H=OH+HONO 3.80E+05 2.300 6976  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
 !HNO3+H=HONO+OH 2.00E+13 0.0 8000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
 !HNO3+H=HONO+OH 2.00E+13 0.0 8000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; JWB est  
 !HNO3+H=OH+HONO 3.80E+05 2.300 6976  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
 !HNO3+H=OH+HONO 3.8E+05 2.300 6976  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97  
  
 HNO3+H=HNO2+OH 6.00E+13 0.0 7000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
 following Laidler EP  
  
 HNO3+O=OH+NO3 1.80E+07 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
 DeMore97  
 !HNO3+O=NO3+OH 2.00E+13 0.0 12000.

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est following Laidler EP

!HNO3+OH=H2O+NO3	1.00E+10	0.000	-1240
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 LAM/BEN84			
HNO3+OH=H2O+NO3	9.00E+10	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: ATK2004			
HNO3+OH(+M)=H2O+NO3(+M)	2.47E+08	0.0	-2860.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
LOW/	6.89E+14	0.0	-1440.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
N2O/5.00/ H2O/9.00/ HNO3/5.00/ NO3/5.00/ NH3/5.00/			
!HNO3+OH=H2O+NO3	4.34E+09	0.0	-1560.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97			
!HNO3+OH(+M)=H2O+NO3(+M)	2.47E+08	0.0	-2860.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97			
! LOW/	6.89E+14	0.00	-1440. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
! N2O/5.00/ H2O/9.00/ N2/1.00/ HNO3/5.00/ ! NH3/5.00/ NO3/5.00/			
!HNO3+OH=H2O+NO3	1.00E+10	0.000	-1240
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 LAM/BEN84			
!HNO3+OH=H2O+NO3	1.0E+10	0.000	-1240
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 LAM/BEN84			
NO3+H2O2=HNO3+HO2	1.00E+12	0.0	8500.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid			
!NO3+H2O2=HNO3+HO2	1.00E+12	0.0	8500.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est following Laidler EP			
NO3+NH=HNO3+N	1.00E+12	0.0	5000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler			
NO3+NH2=HNO3+NH	1.00E+12	0.0	10000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler			
HNO3+NH=HNOH+NO2	1.50E+13	0.0	6000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler			
HNO3+NH2=NO3+NH3	9.00E+05	2.0	7300.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est following DB00 EP			
HNO3+NH2=NH2O+HNO2	3.00E+12	0.0	9000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler			
HNO3+NH3=NH2O+H2O+NO	23.2	3.5	44930.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML98 + Liau et al 1999 JANNAF			
NH3+HNO3=H2O+NH2NO2	8.00E-01	3.5	43100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: MUSIN98			
!HNO3+NO=HONO+NO2	8.00E+06	2.0	11000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; est Ea from Laidler EP, set			
HONO+NO2=HNO3+NO	2.00E+11	0.000	32700
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98			
!NO2+HONO=NO+HNO3	6.03E+01	0.0	0.0

```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:
STREIT79
!HONO+NO2=HNO3+NO                2.00E+11    0.000    32700
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98
!HONO+NO2=HNO3+NO                2.0E+11    0.000    32700
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98

HONO+NO3=HNO3+NO2                1.00E+12    0.0      6000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HONO+NO3=HNO3+NO2                1.00E+12    0.0      6000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP
Laidler

HNO2+NO3=HNO3+NO2                1.00E+12    0.0      5000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP
Laidler

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  N2O4 Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

N2O4 (+M)=NO2+NO2 (+M)            4.05E+18   -1.1     12840.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:
BORRELL88
  LOW/                             1.96E+28   -3.80    12840.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N2O4 (+M)=NO2+NO2 (+M)            4.05E+18   -1.1     12840.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)
!  LOW/                             1.96E+28   -3.8     12800. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)

N2O4+H2O=HONO+HNO3                2.52E+14    0.0     11586.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: FIT
NIST

!-----
!=====
!=  H/C/N/O Reactions Subset  =
!=====

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  No CN Chemistry           !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NH+CH3=CH4+N                      8.20E+05    1.87     5848.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH=N+CH4                      8.20E+05    1.870    5852
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!NH+CH3=N+CH4                      8.20E+05    1.9      5852.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH=N+CH4                      8.2E05     1.870    5852
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

C2H5+N=C2H4+NH                    4.30E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: STI95
!C2H5+N=C2H4+NH                    4.3E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: STI95

```

CH3+NH2=CH4+NH 2.80E+06 1.94 9205.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH4+NH 2.80E+06 1.940 9210  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+NH2=CH4+NH 2.80E+06 1.9 9210.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3+NH2=CH4+NH 2.8E06 1.940 9210  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
 !CH4+NH=CH3+NH2 9.0E13 0.000 20000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ROH/WAG94 Ć  
 CH3+NH2=CH2+NH3 1.60E+06 1.87 7566.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2+NH3 1.6E06 1.870 7570  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
 !CH3+NH2=CH2+NH3 1.60E+06 1.870 7570  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+NH2=CH2+NH3 1.60E+06 1.9 7570.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
  
 CH2SING+NH3=CH3+NH2 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: v9 (change products) \*  
  
 CH4+NH2=CH3+NH3 1.50E+03 3.010 9940  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SON/FRI03  
 !CH4+NH2=CH3+NH3 1.5E03 3.010 9940  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SON/FRI03  
  
 C2H+NH3=C2H2+NH2 7.20E+12 0.000 -735  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: CAR/PEE04 (i  
 !C2H+NH3=C2H2+NH2 7.2E12 0.000 -735  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/PEE04 (i  
  
 C2H4+NH2=C2H3+NH3 5.30E+12 0.000 10274  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: HEN/WAG95(p)  
 !C2H4+NH2=C2H3+NH3 5.3E12 0.000 10274  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HEN/WAG95(p)  
  
 C2H6+NH2=C2H5+NH3 4.50E+01 3.460 5600  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: MEB/LIN99  
 !C2H6+NH2=C2H5+NH3 4.5E01 3.460 5600  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: MEB/LIN99  
  
 NNH+CH3<=>CH4+N2 2.50E+13 0.000 0.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
  
 N2H2+CH3=NNH+CH4 1.60E+06 1.87 2969.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H2=NNH+CH4 1.60E+06 1.870 2971  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H2=NNH+CH4 1.6E06 1.870 2971  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 H2NN+CH3=CH4+NNH 1.60E+06 1.87 129.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NN=CH4+NNH 1.60E+06 1.870 129  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NN=CH4+NNH 1.6E06 1.870 129  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 N2H3+CH3=N2H2+CH4 8.20E+05 1.87 1817.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H3=N2H2+CH4 8.20E+05 1.870 1818  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H3=N2H2+CH4 8.2E05 1.870 1818  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

```

N2H3+CH3=H2NN+CH4          3.00E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+N2H3=H2NN+CH4          3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3+N2H3=H2NN+CH4          3.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

N2H4+CH3=N2H3+CH4          3.30E+06    1.87    5322.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+N2H4=N2H3+CH4          3.30E+06    1.870    5325
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3+N2H4=N2H3+CH4          3.3E06    1.870    5325
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2SING+NO=CH2+NO          1.00E+14    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94
!CH2SING+NO=CH2+NO          1.0E14    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

!NO+C=CO+N                  1.70E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
C+NO<=>CO+N                  2.90E+13    0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!NO+C=CO+N                  1.70E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!C+NO=CO+N                  2.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94
!C+NO<=>CO+N                  2.90E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!C+NO=CO+N                  2.8E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

!CH+NO=N+HCO                2.90E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO<=>N+HCO                2.46E+13    0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
CH+NO=HCO+N                  6.80E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO<=>N+HCO                2.46E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH+NO=HCO+N                  6.8E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

!CH+NO=NH+CO                5.50E+12    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CH+NO=CO+NH                  9.10E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO=CO+NH                  9.1E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

CH2+NO=NH2+CO                2.30E+16    -1.43    1331.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

C2+NO=C2O+N                  2.30E+13    0.000    8640
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: KRU/ROT99
!C2+NO=C2O+N                  2.3E13    0.000    8640
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KRU/ROT99

N+CO2<=>NO+CO                3.00E+12    0.000    11300.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

NH+CO2<=>HNO+CO              1.00E+13    0.000    14350.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

HNO+CH3=NO+CH4              8.20E+05    1.87    480.

```

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+CH3=NO+CH4          8.20E+05    1.9      953.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH3+HNO=NO+CH4          2.30E+14    0.000    8400
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d (Ea from [XIA/ZHA06],A
scaled to match room-T data)
!CH3+HNO=NO+CH4          2.3E14     0.000    8400
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d (Ea from [XIA/ZHA06],A
scaled to match room-T data)

C2H3+NO=C2H2+HNO          1.00E+12    0.000    1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: JAM est
!C2H3+NO=C2H2+HNO          1.0E12     0.000    1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est

HCO+NO=HNO+CO             7.23E+12    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91; test
!HCO+NO=HNO+CO             7.00E+13    -0.4     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCO+NO=HNO+CO             6.9E12     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07
!HCO+NO=HNO+CO             6.90E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07

HCO+HNO=CH2O+NO           6.00E+11    0.0      2000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 -
estimated
!HCO+HNO=NO+CH2O           6.00E+11    0.0      2000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCO+HNO=NO+CH2O           5.80E-01    3.840    115
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN04
!HCO+HNO=NO+CH2O           5.8E-01    3.840    115
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN04

!CH3O+NO=CH2O+HNO          8.40E+12    0.0      2050.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; HE88
!CH3O+NO=CH2O+HNO          1.30E+14    -0.70    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99
CH3O+NO=HNO+CH2O           7.50E+12    0.000    2017
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d CAR/DEV98
DUPLICATE
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
CH3O+NO=HNO+CH2O           2.50E+18    -2.560    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
DUPLICATE
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!CH3O+NO=HNO+CH2O           7.5E12     0.000    2017
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d CAR/DEV98
!
DUPLICATE
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!CH3O+NO=HNO+CH2O           2.5E18    -2.560    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!
DUPLICATE
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

CH2OH+NO=CH2O+HNO          1.30E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NES/STI89/p
!CH2OH+NO=CH2O+HNO          1.3E12     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NES/STI89/p

CH3O+HNO=NO+CH3OH          3.20E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d HE/LIN88
!CH3O+HNO=NO+CH3OH          3.2E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d HE/LIN88

CH2OH+HNO=NO+CH3OH          3.00E+13    0.000    0

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
 !CH2OH+HNO=NO+CH3OH 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
  
 CH2CHO+NO=HNO+CH2CO 1.00E+12 0.0 8600.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est. E/P  
  
 NH2O+CH3=CH3O+NH2 2.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NO=CH3O+NH2 2.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NO=CH3O+NH2 2.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 NH2O+CH3=CH4+HNO 1.60E+06 1.87 2959.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NO=CH4+HNO 1.60E+06 1.870 2961  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NO=CH4+HNO 1.6E06 1.870 2961  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 HNOH+CH3=CH4+HNO 1.60E+06 1.87 2095.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 NH2OH+CH3=HNOH+CH4 1.60E+06 1.87 6345.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 NH2OH+CH3=NH2O+CH4 8.20E+05 1.87 5491.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 CH+NO2=HCO+NO 1.01E+14 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WCF8S2  
 !CH+NO2=HCO+NO 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 WAG/SAD82,RIM/HER98  
 !CH+NO2=HCO+NO 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 WAG/SAD82,RIM/HER98  
  
 CH2+NO2=CH2O+NO 5.00E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ave STWW89 & DM95  
 !CH2+NO2=CH2O+NO 5.90E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SEI/WAG89  
 !CH2+NO2=CH2O+NO 5.9E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SEI/WAG89  
  
 NO2+CH3=NO+CH3O 1.40E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NO2=CH3O+NO 1.40E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ave GT74, YSG81,  
 !CH3+NO2=CH3O+NO 1.30E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; GLA74  
 !CH3+NO2=CH3O+NO 1.10E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/BEN98,WOL/CRO00  
 !CH3+NO2=CH3O+NO 1.1E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/BEN98,WOL/CRO00  
  
 C2H3+NO2=NO+CH2CHO 7.70E+14 -0.600 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GEP/HAL04 (i  
 !C2H3+NO2=NO+CH2CHO 7.7E14 -0.600 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GEP/HAL04 (i  
  
 C2H5+NO2=NO+C2H5O 4.00E+13 -0.200 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NO2+CH3=NO+CH3O  
 !C2H5+NO2=NO+C2H5O 4.0E13 -0.200 0



!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NO2+CH3=NO+CH3O

CO+NO2=NO+CO2 9.04E+13 0.0 33780.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91  
!CO+NO2=CO2+NO 9.00E+13 0.0 33800.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CO+NO2=NO+CO2 9.00E+13 0.000 33800  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 NBS91  
!CO+NO2=NO+CO2 9.0E13 0.000 33800  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 NBS91

HCO+NO2=CO+NO+OH 1.20E+23 -3.3 2355.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCO+NO2=NO+CO+OH 5.00E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (15%)  
!HCO+NO2=NO+CO+OH 5.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (15%)

HCO+NO2=H+CO2+NO 8.39E+15 -0.75 1930.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al;  
TH91  
!HCO+NO2=H+CO2+NO 8.40E+15 -0.8 1930.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCO+NO2=NO+CO2+H 2.30E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (70%)  
!HCO+NO2=NO+CO2+H 2.3E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (70%)

!CH2CHO+NO2=CHOCH2O+NO 8.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DOU/HAY96 (i

CH3CO+NO2=>CH3+CO2+NO 1.50E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: (CH3CO2+NO) (i  
!CH3CO+NO2=>CH3+CO2+NO 1.5E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: (CH3CO2+NO) (i

!HONO+CH3=NO2+CH4 8.10E+05 1.87 5501.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH4+NO2=CH3+HONO 1.20E+13 0.0 30000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SG81  
CH4+NO2=HONO+CH3 6.50E+14 0.000 45800  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d YAM/SUZ99  
!CH4+NO2=HONO+CH3 6.5E14 0.000 45800  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d YAM/SUZ99

C2H4+NO2=HONO+C2H3 6.50E+14 0.000 41400  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
!C2H4+NO2=HONO+C2H3 6.5E14 0.000 41400  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol

C2H6+NO2=HONO+C2H5 6.50E+14 0.000 41400  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
!C2H6+NO2=HONO+C2H5 6.5E14 0.000 41400  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol

HOCO+NO=CO+HONO 1.50E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: PET/MOO93,OLK/SMI01  
!HOCO+NO=CO+HONO 1.5E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: PET/MOO93,OLK/SMI01

HCO+NO2=CO+HONO 1.24E+23 -3.29 2355.

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al;  
TH91  
!HCO+NO2=HONO+CO 5.00E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (15%)  
!HCO+NO2=HONO+CO 5.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (15%)

CH2O+NO2=HCO+HONO 8.02E+02 2.77 13730.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al;  
TH91  
!CH2O+NO2=HONO+HCO 1.40E-07 5.640 9220  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN03  
!CH2O+NO2=HONO+HCO 1.4E-07 5.640 9220  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN03

CH3O+NO2=CH2O+HONO 6.00E+12 0.00 2285.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH2OH+NO2=HONO+CH2O 5.00E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NES/STI89  
!CH2OH+NO2=HONO+CH2O 5.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NES/STI89

CH3OH+NO2=HONO+CH2OH 1.50E+02 3.320 20035  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XIA/ZHA06  
!CH3OH+NO2=HONO+CH2OH 1.5E02 3.320 20035  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XIA/ZHA06

!CH2CHO+NO2=HONO+CH2CO 8.90E+12 0.0 -160.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
CH2CHO+NO2=CH2CO+HONO 8.90E+12 0.000 -159  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: BAR/WEI91 (i  
!CH2CHO+NO2=CH2CO+HONO 8.9E12 0.000 -159  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: BAR/WEI91 (i  
!CH2CHO+NO2=CH2CO+HONO 2.0E15 -0.680 1430  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DOU/HAY96 (i

CH3CHO+NO2=HONO+CH2CHO 1.30E+12 0.0 3700.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

!HNO2+CH3=NO2+CH4 8.10E+05 1.87 4836.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
CH4+NO2=HNO2+CH3 6.00E+14 0.000 37600  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d YAM/SUZ99  
!CH4+NO2=HNO2+CH3 6.0E14 0.000 37600  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d YAM/SUZ99

C2H4+NO2=HNO2+C2H3 6.00E+14 0.000 33200  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
!C2H4+NO2=HNO2+C2H3 6.0E14 0.000 33200  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol

C2H6+NO2=HNO2+C2H5 6.00E+14 0.000 33200  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
!C2H6+NO2=HNO2+C2H5 6.0E14 0.000 33200  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol

CH2O+NO2=HNO2+HCO 1.10E-01 4.220 19850  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN03  
!CH2O+NO2=HNO2+HCO 1.1E-01 4.220 19850  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN03

CH3OH+NO2=HNO2+CH2OH 2.40E+03 2.900 27470  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XIA/ZHA06  
 !CH3OH+NO2=HNO2+CH2OH 2.4E03 2.900 27470  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XIA/ZHA06  
  
 ! OCHCHO+NO2=>p 7.9E11 0.000 1980  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: (i  
  
 CH2SING+N2O=CH2O+N2 3.80E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: KOC/WAG90(p)  
 !CH2SING+N2O=CH2O+N2 3.8E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KOC/WAG90(p)  
  
 CO+N2O=N2+CO2 2.70E+11 0.0 20237.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CO+N2O=N2+CO2 2.70E+11 0.000 20237  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91  
 !CO+N2O=N2+CO2 2.7E11 0.000 20237  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SKR/GLA04 NBS91  
  
 NH2NO+CH3=HNNO+CH4 1.60E+06 1.87 7179.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 NH2NHO+CH3=NHNHO+CH4 1.60E+06 1.87 377.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! CN Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 CN+M=C+N+M 2.50E+14 0.0 141100.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92,  
 keyed to Ar=1.0  
 N2/1.5/ CO2/2.4/  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92  
  
 CH+N=CN+H 1.70E+14 -0.09 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH+N=CN+H 1.30E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
 !CH+N=CN+H 1.70E+14 -0.1 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH+N=CN+H 1.30E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MES/CAR81  
 !CH+N=CN+H 1.30E+13 0.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH+N=CN+H 1.3E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MES/CAR81  
  
 !CN+O=CO+N 7.70E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CN+O=CO+N 2.05E+13 0.0 417.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992.  
 !CN+O=CO+N 1.90E+12 0.5 723.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CN+O=CO+N 1.90E+12 0.460 723  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 COB96  
 !CN+O<=>CO+N 7.70E+13 0.000 0.00  
 !GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)  
 !CN+O=CO+N 1.9E12 0.460 723  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 COB96  
  
 NO+C=CN+O 1.10E+13 0.0 0.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!C+NO=CN+O 6.60E+13 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NO+C=CN+O 1.10E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!C+NO=CN+O 2.00E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94
!C+NO<=>CN+O 1.90E+13 0.000 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!C+NO=CN+O 2.0E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

CH+NO=OH+CN 3.30E+12 0.0 0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO=CN+OH 1.10E+12 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO=CN+OH 1.1E12 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

CN+O2=NO+CO 2.80E+17 -2.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+O2=NO+CO 2.80E+17 -2.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05, RIM/HER99
!CN+O2=NO+CO 2.8E17 -2.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05, RIM/HER99

!CN+N=C+N2 2.40E+13 0.0 -556.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+N=C+N2 1.04E+15 -0.5 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!CN+N=C+N2 2.40E+13 0.0 -556.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CN+N=C+N2 5.90E+14 -0.400 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!C+N2<=>CN+N 6.30E+13 0.000 46020.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+N=C+N2 1.80E+14 0.0 0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!C+N2=CN+N 6.3E13 0.000 46000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98
!CN+N=C+N2 5.9E14 -0.400 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

CN+NO=N2+CO 3.90E+11 0.0 27820.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95, tst
calc

C+N2O=CN+NO 4.80E+12 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DOR/MAR91
!C+N2O=CN+NO 4.8E12 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 DOR/MAR91

!CN+NO2=CO+N2O 4.90E+14 -0.8 344.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
CN+NO2=CO+N2O 4.90E+14 -0.752 344
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05
!CN+NO2=CO+N2O 4.9E14 -0.752 344
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

!CN+NO2=N2+CO2 3.70E+14 -0.8 344.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
CN+NO2=N2+CO2 3.70E+14 -0.752 344
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05
!CN+NO2=N2+CO2 3.7E14 -0.752 344
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

```

```

C2+N2=CN+CN                1.50E+13    0.000    41730
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: Sommer+97
!C2+N2=CN+CN                1.5E13    0.000    41730
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: Sommer+97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                          !!
!!   HCN Chemistry        !!
!!                          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
HCN(+M)=H+CN(+M)           8.30E+17   -0.93    123800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; T&H91 [13,0]
  LOW/                      3.57E+26   -2.6     124900. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!   TSA/ 0.95  -1.0E-04 /
  TROE/0.7342 1120.08 1.0E5/
  N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed
per Tsang;
!HCN+M=H+CN+M              3.40E+35   -5.1     133000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   N2/0.0/ O2/1.5/ H2O/10.0/
!HCN+M=H+CN+M              3.40E+35   -5.130   133000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS91
!   N2/0.0/ O2/1.5/ H2O/10/
!HCN+M<=>H+CN+M            1.04E+29   -3.300   126600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
  H2/2.00/ CH4/2.00/ CO/1.50/ !H2O/6.00/
  C2H6/3.00/ AR/0.70/ !CO2/2.00/
!HCN+M = H+CN+M            3.4E35   -5.130   133000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS91
!   N2/0.0/ O2/1.5/ H2O/10/

CH2+N=HCN+H                5.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+N=HCN+H                5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!CH2+N=HCN+H                5.00E+13    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89
!CH2+N=HCN+H                5.00E+13    0.0      0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2+N=HCN+H                5.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

CN+H2=HCN+H                3.60E+08    1.55     2999.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+H2=HCN+H                3.61E+08    1.55     3000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992.;
whb95 is similar
!CN+H2=HCN+H                1.10E+05    2.6      1908.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+H2=HCN+H                1.10E+05    2.600    1908
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!CN+H2<=>HCN+H              2.95E+05    2.450    2240.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+H2=HCN+H                3.60E+08    1.6      3000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CN+H2 = HCN+H              1.1E05    2.600    1908
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

CH+NH=HCN+H                3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est
!CH+NH=HCN+H                3.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est

```

CH3+N=HCN+H2 3.70E+12 0.15 -89.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N<=>HCN+H2 3.70E+12 0.150 -90.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH3+N<=>HCN+H2 3.70E+12 0.150 -90.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH3+N<=>HCN+H2 3.70E+12 0.1 -90.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

C2H3+N=HCN+CH2 2.00E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89  
 !C2H3+N=HCN+CH2 2.00E+13 0.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CN+CH4=HCN+CH3 1.20E+05 2.64 -159.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 CH4+CN=CH3+HCN 8.60E+05 2.300 -32  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 HER/SPE92  
 !CH4+CN=CH3+HCN 8.6E05 2.300 -32  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 HER/SPE92

C3H3+N=HCN+C2H2 1.00E+13 0.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!H2CCCH+N=HCN+C2H2 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est

C2H6+CN=C2H5+HCN 1.20E+08 1.800 -994  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 HER/SPE92  
 !C2H6+CN=C2H5+HCN 1.2E08 1.800 -994  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 HER/SPE92

CH+N2=HCN+N 4.40E+12 0.0 21964.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH+N2=HCN+N 4.40E+12 0.0 21976.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH+N2<=>HCN+N 3.12E+09 0.880 20130.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH+N2=HCN+N 4.40E+12 0.0 21976.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH2+N2=HCN+NH 1.00E+13 0.0 73954.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2+N2<=>HCN+NH 1.00E+13 0.000 74000.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2+N2=HCN+NH 1.00E+13 0.0 74000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89  
 !CH2+N2=HCN+NH 1.00E+13 0.000 74000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !CH2+N2<=>HCN+NH 1.00E+13 0.000 74000.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH2+N2=HCN+NH 1.00E+13 0.0 74000.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2+N2=HCN+NH 1.0E13 0.000 74000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

CH2SING+N2<=>NH+HCN 1.00E+11 0.000 65000.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2SING+N2<=>NH+HCN 1.00E+11 0.000 65000.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

CN+NH3=HCN+NH2 9.20E+12 0.0 -357.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HCN+N2=H+CN+N2 3.60E+26 -2.6 124890.0

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+N2=H+CN+N2 3.60E+26 -2.600 124890  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS91  
!HCN+N2 = H+CN+N2 3.6E26 -2.600 124890  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS91

!HCN+O=NH+CO 5.40E+08 1.21 7487.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HCN+O=NH+CO 3.45E+03 2.64 4980.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89; Perry&Melius 85 similar  
HCN+O=NH+CO 3.50E+03 2.6 4980.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+O=NH+CO 3.50E+03 2.640 4980  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89  
!HCN+O<=>NH+CO 5.07E+03 2.640 4980.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HCN+O=NH+CO 3.5E03 2.640 4980  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

HCN+O=CN+OH 4.20E+10 0.40 20663.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HCN+O=CN+OH 2.70E+09 1.58 26600.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89; from Perry&Melius 85  
!HCN+O=CN+OH 4.20E+10 0.4 20665.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+O=CN+OH 4.20E+10 0.400 20665  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!HCN+O<=>CN+OH 3.91E+09 1.580 26600.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HCN+O=CN+OH 4.2E10 0.400 20665  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HCN+OH=CN+H2O 3.90E+06 1.83 10287.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CN+H2O=HCN+OH 7.80E+12 0.0 7447.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HCN+OH=CN+H2O 3.90E+06 1.83 10290.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WHB95  
!HCN+OH=CN+H2O 3.90E+06 1.8 10300.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+OH=CN+H2O 3.90E+06 1.830 10300  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO/BOW95  
!CN+H2O<=>HCN+OH 8.00E+12 0.000 7460.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HCN+OH=CN+H2O 3.9E06 1.830 10300  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO/BOW95

!OH+HCN=NH2+CO 1.60E+02 2.56 8996.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
OH+HCN=NH2+CO 7.83E-04 4.0 4000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!HCN+OH=NH2+CO 7.80E-04 4.0 4000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+OH=NH2+CO 7.80E-04 4.000 4000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89  
!HCN+OH<=>NH2+CO 1.60E+02 2.560 9000.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HCN+OH=NH2+CO 7.8E-04 4.000 4000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

HCN+O2=CN+HO2 3.00E+13 0.0 75100.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+O2=CN+HO2 3.00E+13 0.000 75100  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 est

!HCN+O2 = CN+HO2 3.0E13 0.000 75100  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 est

HCCO+N=HCN+CO 5.00E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
 !HCCO+N=HCN+CO 5.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !HCCO+N=HCN+CO 5.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

!CN+CH2O=HCN+HCO 4.20E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust.ame.2011.12.007  
 CH2O+CN=HCO+HCN 1.70E+03 2.720 -1427  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: FEN/PAN97  
 !CH2O+CN=HCO+HCN 1.7E03 2.720 -1427  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: FEN/PAN97

CH+NO=HCN+O 5.30E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH+NO=HCN+O 1.10E+14 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
 !CH+NO=HCN+O 7.90E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05  
 !CH+NO<=>HCN+O 4.10E+13 0.000 0.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH+NO=HCN+O 7.9E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

CH2+NO=HCN+OH 2.90E+14 -0.69 755.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2+NO<=>OH+HCN 2.90E+14 -0.690 760.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2+NO=HCN+OH 3.90E+11 0.000 -378  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: ATA/WOL92,FIC/TEM01  
 !CH2+NO<=>OH+HCN 2.90E+14 -0.690 760.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH2+NO=HCN+OH 3.9E11 0.000 -378  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ATA/WOL92,FIC/TEM01

CH2SING+NO<=>OH+HCN 2.90E+14 -0.690 760.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2SING+NO=HCN+OH 2.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !CH2SING+NO<=>OH+HCN 2.90E+14 -0.690 760.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH2SING+NO=HCN+OH 2.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

CH3+NO=HCN+H2O 4.90E+08 0.46 12392.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NO<=>HCN+H2O 9.60E+13 0.000 28800.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH3+NO=HCN+H2O 1.50E-01 3.520 3950  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MIL98  
 !CH3+NO<=>HCN+H2O 9.60E+13 0.000 28800.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH3+NO=HCN+H2O 1.5E-1 3.520 3950  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MIL98

C2H+NO=HCN+CO 6.00E+13 0.000 570  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: PEE/CEU96  
 !C2H+NO=HCN+CO 6.0E13 0.000 570  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: PEE/CEU96

C2H3+NO=HCN+CH2O 7.00E+21 -3.382 1025  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: STR/TAA04 (i



```

!C2H3+NO=HCN+CH2O          7.0E21  -3.382   1025
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          STR/TAA04 (i

!NO+HCCO=HCN+CO2          1.40E+13   0.0    695.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HCCO+NO=HCN+CO2          3.70E+14  -0.750  -90
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/GLA03
!HCCO+NO=HCN+CO2          3.7E14  -0.750  -90
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          MIL/GLA03

CN+HNO=HCN+NO          1.80E+13   0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+HNO=HCN+NO          1.80E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!CN+HNO=HCN+NO          1.8E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

CN+HONO=HCN+NO2        1.20E+13   0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+HONO=HCN+NO2        1.20E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!CN+HONO=HCN+NO2        1.2E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

CH+N2O=HCN+NO          1.90E+13   0.000  -511
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/WIE93
!CH+N2O=HCN+NO          1.9E13   0.000  -511
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 BEC/WIE93

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
!!   HNC Chemistry   !!
!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
HCN=HNC          1.50E+23   -4.20   49428.
!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN=HNC          1.90E+24   -4.23   49548.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN=HNC          5.30E+25   -4.34   50163.
!10 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN (+M)=HNC (+M) 1.60E+26   -3.23   49548.
!T>1000K          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HCN+M=HNC+M      1.60E+26   -3.2    54600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
AR/0.7/ H2O/7.0/ CO2/2.0/
!HCN+M=HNC+M      4.36E+26   -3.34   50194.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; 2nd order
form, easiest to use
!HCN+M=HNC+M      1.60E+26   -3.230   54600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00, mod Ea
AR/0.7/ H2O/7.0/ CO2/2.0/
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!HCN+M = HNC+M      1.6E26  -3.230   54600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00, mod Ea
AR/0.7/ H2O/7.0/ CO2/2.0/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

HNC+H=HCN+H          7.80E+13   0.0    3600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+H=HCN+H          7.80E+13   0.000   3600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 SUM/NGU98
!HNC+H = HCN+H      7.8E13   0.000   3600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 SUM/NGU98

O+HNC=NH+CO          4.60E+12   0.0    2184.

```

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNC+O=NH+CO 5.44E+12 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TDLLM (Lin),
1994, preprint
!HNC+O=NH+CO 4.60E+12 0.0 2200.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+O=NH+CO 4.60E+12 0.000 2200
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HNC+O = NH+CO 4.6E12 0.000 2200
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HNC+OH=CN+H2O 1.50E+12 0.00 7680.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TST result
from TDLLM, 1994

HNC+O2=NH+CO2 1.60E+19 -2.25 1777.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! !!
!! CH2N Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!NCH2=HCN+H 1.30E+29 -6.03 29878.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2=HCN+H 6.00E+31 -6.46 32092.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2=HCN+H 3.50E+29 -5.46 32529.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000) ratioed
per Tsang;
!NCH2=HCN+H 4.00E+28 -6.0 29897.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+M=HCN+H+M 3.00E+14 0.0 22000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89
!NCH2=HCN+H 1.30E+29 -6.030 29894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 atm
H+HCN(+M)<=>NCH2(+M) 3.30E+13 0.000 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
LOW/ 1.40E+26 -3.400 1900.00 /
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
CO2/2.00/ C2H6/3.00/ AR/0.70/
!HCN+H(+M)=NCH2(+M) 3.31E+13 0.0 4844.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
! LOW/ 1.60E+24 -2.73 7660. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
! TSA/ 0.95 -1.0E-04 /
N2O/5.0/ N2/1.0/ !H2O/5.0/ CO2/2.0/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2
!H+HCN(+M)<=>NCH2(+M) 3.30E+13 0.0 0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! LOW/ 1.40E+26 -3.40 1900. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NCH2=HCN+H 1.3E29 -6.030 29894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 atm

CH+NH3=NCH2+H+H 4.40E+13 0.000 -630
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 BEC/WIE93

NCH2+H=HCN+H2 2.40E+08 1.50 -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+H=HCN+H2 4.00E+13 0.00 0.0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; lower limit
!NCH2+H=HCN+H2 2.40E+08 1.5 -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

!NCH2+H=HCN+H2	2.40E+08	1.500	-894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!NCH2+H=HCN+H2	2.40E+08	1.5	-894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NCH2+H=HCN+H2	2.4E08	1.500	-894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
CH3+N=NCH2+H	6.10E+14	-0.31	288.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!CH3+N<=>NCH2+H	6.10E+14	-0.310	290.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!CH3+N=NCH2+H	6.10E+14	-0.3	288.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000			
!CH3+N=NCH2+H	7.10E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DAV/HAN91B			
!CH3+N<=>NCH2+H	6.10E+14	-0.310	290.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!CH3+N<=>NCH2+H	6.10E+14	-0.3	290.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!CH3+N=NCH2+H	7.1E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 DAV/HAN91B			
CH+NH2=NCH2+H	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est			
!CH+NH2=NCH2+H	3.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est			
CH3+NH=NCH2+H2	3.50E+13	0.0	290.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WF97			
NCH2+CH3=HCN+CH4	8.10E+05	1.87	-1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+CH3=HCN+CH4	8.10E+05	1.9	-1113.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
C2H5+N=CH3+NCH2	2.30E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: STI95			
!C2H5+N=CH3+NCH2	2.3E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: STI95			
NCH2+N=HCN+NH	7.20E+13	0.00	400.0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
NCH2+N=N2+CH2	6.00E+13	0.0	397.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+N<=>N2+CH2	6.00E+13	0.000	400.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!NCH2+N=N2+CH2	2.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89			
!NCH2+N=CH2+N2	2.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est			
!NCH2+N<=>N2+CH2	6.00E+13	0.000	400.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NCH2+N=N2+CH2	6.00E+13	0.0	397.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NCH2+N=CH2+N2	2.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est			
NCH2+NH=HCN+NH2	1.70E+08	1.500	-894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est NCH2+O			
!NCH2+NH=HCN+NH2	1.7E08	1.500	-894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est NCH2+O			
NCH2+NH2=HCN+NH3	9.20E+05	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0

```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+NH2=HCN+NH3          9.20E+05  1.940  -1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCH2+NH2=HCN+NH3          9.20E+05  1.9  -1152.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NCH2+NH2=HCN+NH3          9.2E05  1.940  -1152
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

CH2+NO=NCH2+O              8.10E+07  1.42  4111.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NCH2+O=HCN+OH              1.70E+08  1.50  -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+O=HCN+OH              1.00E+07  2.0  6100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!NCH2+O=HCN+OH              1.70E+08  1.5  -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+O=HCN+OH              1.70E+08  1.500  -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCH2+O=HCN+OH              1.7E08  1.500  -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!CH3+NO=NCH2+OH            2.20E+09  0.75  11717.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NO<=>NCH2+OH            1.00E+12  0.000  21750.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
CH3+NO=NCH2+OH              1.50E-01  3.520  3950
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MIL98
!CH3+NO<=>NCH2+OH            1.00E+12  0.000  21750.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)
!CH3+NO=NCH2+OH              1.5E-1  3.520  3950
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MIL98

!NCH2+OH=HCN+H2O           2.10E+17  -1.68  318.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+OH=HCN+H2O           1.50E+19  -2.18  2165.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+OH=HCN+H2O           9.50E+21  -2.91  5630.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+OH=HCN+H2O           1.20E+06  2.00  -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+OH=HCN+H2O           1.00E+07  2.0  3700.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
NCH2+OH=HCN+H2O            1.50E+19  -2.2  2166.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
DUPLICATE
NCH2+OH=HCN+H2O            1.20E+06  2.0  -1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
DUPLICATE
!NCH2+OH=HCN+H2O           2.10E+17  -1.680  318
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2
!
DUPLICATE
!NCH2+OH=HCN+H2O           1.20E+06  2.000  -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!
DUPLICATE
!NCH2+OH=HCN+H2O           2.1E17  -1.680  318
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2
!
DUPLICATE
!NCH2+OH=HCN+H2O           1.2E06  2.000  -1192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!
DUPLICATE

NCH2+O2=CH2O+NO            3.00E+12  0.0  5958.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!NCH2+O2=CH2O+NO          3.00E+12    0.0    5961.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+O2=CH2O+NO          3.00E+12    0.000    5961
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCH2+O2=CH2O+NO          3.0E12    0.000    5961
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

NCH2+O2=HCN+HO2           2.70E+04    2.0    17300.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!NCH2+O2=HCN+HO2           2.70E+04    2.0    17300.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

NCH2+HO2=HCN+H2O2         1.40E+04    2.69    -1609.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NCH2+NO=HCN+HNO           1.00E+07    2.0    4400.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!NCH2+NO=HCN+HNO           1.00E+07    2.0    4400.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  CHNH Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CHNH=HCN+H                 7.70E+25    -5.20    21974.
!0.1 atm                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CHNH=HCN+H                 6.10E+28    -5.69    24257.
!1.0 atm                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH=HCN+H                 6.20E+26    -4.77    24804.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH=HCN+H                 6.10E+28    -5.7     24271.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH=HCN+H                 7.70E+25    -5.200    21986
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
!CHNH=HCN+H                 6.10E+28    -5.7     24271.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH=HCN+H                 7.7E25     -5.200    21986
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

CH3+N=CHNH+H               1.20E+11    0.52    -367.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CHNH+H=NCH2+H              2.00E+13    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+H=NCH2+H              2.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+H=NCH2+H              2.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+H=NCH2+H              2.00E+13    0.0     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+H=NCH2+H              2.0E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CHNH+H=HCN+H2              2.40E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+H=HCN+H2              2.40E+08    1.5     -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+H=HCN+H2              2.40E+08    1.500    -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+H=HCN+H2              2.40E+08    1.5     -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+H=HCN+H2              2.4E08     1.500    -894

```

```

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CHNH+O=HCN+OH                1.70E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+O=HCN+OH                1.70E+08    1.5    -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+O=HCN+OH                1.70E+08    1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+O=HCN+OH                1.7E08    1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CHNH+OH=HCN+H2O              1.20E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+OH=HCN+H2O              1.20E+06    2.0    -1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+OH=HCN+H2O              1.20E+06    2.000   -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+OH=HCN+H2O              1.2E06    2.000   -1192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CHNH+CH3=HCN+CH4             8.20E+05    1.87    -1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+CH3=HCN+CH4             8.20E+05    1.870   -1113
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+CH3=HCN+CH4             8.20E+05    1.9    -1113.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+CH3=HCN+CH4             8.2E05    1.870   -1113
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  CH2NH Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CH2NH+M=HCN+H2+M              1.00E+14    0.0    10000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH2NH+M=HCN+H2+M              1.00E+14    0.0    10000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; CAT96
!CH2NH=HCN+H2                  1.00E+14    0.0    9060.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+M=HCN+H2+M              1.00E+14    0.0    10000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

NH+CH3=CH2NH+H                4.00E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH=CH2NH+H                4.00E+13    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!NH+CH3=CH2NH+H                4.00E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH=CH2NH+H                4.0E13    0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH+H=NCH2+H2              2.40E+08    1.50    7318.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+H=NCH2+H2              2.40E+08    1.500   7322
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+H=NCH2+H2              2.40E+08    1.5    7322.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+H=NCH2+H2              2.4E08    1.500   7322
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH+H=CHNH+H2              3.00E+08    1.50    6126.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+H=CHNH+H2              3.00E+08    1.500   6130

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+H=CHNH+H2 3.00E+08 1.5 6130.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH+H=CHNH+H2 3.0E08 1.500 6130  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH+NH3=CH2NH+H 4.4E13 0.000 -630  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 BEC/WIE93, prod est (v12)  
  
 CH2SING+NH2=CH2NH+H 3.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est  
 !CH2SING+NH2=CH2NH+H 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est  
  
 CH2SING+NH3=CH2NH+H+H 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est  
  
 !CH3+NH2=CH2NH+H2 2.10E+11 -0.10 19084.  
 !0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2NH+H2 4.80E+11 -0.20 19392.  
 !1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2NH+H2 2.90E+12 -0.40 20494.  
 !10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2NH+H2 2.10E+11 -0.100 19095  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2  
 CH3+NH2<=>CH2NH+H2 2.40E+06 1.2 17369.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3+NH2=CH2NH+H2 2.1E11 -0.100 19095  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2  
  
 CH2NH+O=NCH2+OH 1.70E+08 1.50 4627.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=NCH2+OH 3.16E+08 2.0 6100.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+O=NCH2+OH 1.70E+08 1.5 4630.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+O=NCH2+OH 1.70E+08 1.500 4630  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=NCH2+OH 1.7E08 1.500 4630  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+O=CHNH+OH 2.20E+08 1.50 5402.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=CHNH+OH 2.20E+08 1.500 5404  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=CHNH+OH 2.2E08 1.500 5404  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+O=CH2O+NH 1.70E+06 2.08 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=CH2O+NH 1.00E+07 2.0 2800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+O=CH2O+NH 1.70E+06 2.1 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+O=CH2O+NH 1.70E+06 2.080 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=CH2O+NH 1.7E06 2.080 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+OH=NCH2+H2O 1.20E+06 2.00 -89.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+OH=NCH2+H2O 1.00E+07 2.0 4000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH2NH+OH=NCH2+H2O 1.20E+06 2.0 -89.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+OH=NCH2+H2O 1.20E+06 2.000 -89  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+OH=NCH2+H2O 1.2E06 2.000 -89  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+OH=CHNH+H2O 2.40E+06 2.00 457.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+OH=CHNH+H2O 2.40E+06 2.000 457  
 !Tian et al. C&F (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+OH=CHNH+H2O 2.4E06 2.000 457  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+OH=CH2O+NH2 1.80E+05 2.0 14800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+OH=CH2O+NH2 1.80E+05 2.0 14800.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97  
  
 NCH2+HO2=CH2NH+O2 1.40E+04 2.69 -1609.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCH2+HO2=CH2NH+O2 7.87E+04 2.0 21700.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !NCH2+HO2=CH2NH+O2 1.40E+04 2.7 -1609.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
  
 CH2NH+CH3=NCH2+CH4 8.20E+05 1.87 7119.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+CH3=NCH2+CH4 8.20E+05 1.870 7123  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+CH3=NCH2+CH4 8.20E+05 1.9 7123.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH+CH3=NCH2+CH4 8.2E05 1.870 7123  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+CH3=CHNH+CH4 5.30E+05 1.87 9681  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000).  
 !CH2NH+CH3=CHNH+CH4 5.30E+05 1.870 9687  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+CH3=CHNH+CH4 5.30E+05 1.9 9687.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH+CH3=CHNH+CH4 5.3E05 1.870 9687  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+NH2=NCH2+NH3 9.20E+05 1.94 4438.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+NH2=NCH2+NH3 9.20E+05 1.940 4441  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+NH2=NCH2+NH3 9.20E+05 1.9 4441.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH+NH2=NCH2+NH3 9.2E05 1.940 4441  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH2NH+NH2=CHNH+NH3 1.80E+06 1.94 6087.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+NH2=CHNH+NH3 1.80E+06 1.940 6090  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+NH2=CHNH+NH3 1.80E+06 1.9 6090.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH+NH2=CHNH+NH3 1.8E06 1.940 6090  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!



```

!!          !!
!!  CH3N Chemistry  !!
!!          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CH3N(+AR)<=>CH2NH(+AR)          1.83E+13    0.2      43980.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
  LOW/          2.23E+28    -4.45    46000. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
  TROE/ 1.0 911000 10.0 0.260E+09 /
CH3N(+AR)<=>NCH2+H(+AR)        7.40E+11    0.9      35470.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
  LOW/          1.87E+30    -4.52    37950. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
  TROE/ 0.749 218 10.0 0.260E+09 /

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!          !!
!!  CH3NH Chemistry  !!
!!          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH3NH=CH2NH+H          1.60E+36    -7.92    36322.
!0.1 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CH3NH=CH2NH+H          1.30E+42    -9.24    41316.
!1.0 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH=CH2NH+H          2.30E+44    -9.51    45218.
!10 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+M=CH2NH+H+M      1.00E+16    0.0      23800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NH=CH2NH+H          1.60E+36    -7.920   36342
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
(600-2500K)
DUPLICATE
CH3NH(+AR)<=>CH2NH+H(+AR)        7.91E+11    0.3      36260.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
  LOW/          1.64E+39    -7.02    40100. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
DUPLICATE
!CH3NH=CH2NH+H          1.6E36    -7.920   36342
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2
(600-2500K)

CH3NH+M=CH3+NH+M          1.00E+14    0.0      18000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96

!CH3+NH2=CH3NH+H          1.20E+13    -0.15    16135.
!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH+H          4.40E+13    -0.31    16632.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH+H          1.40E+14    -0.42    17853.
!10 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+H=CH3+NH2          6.00E+13    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3+NH2=CH3NH+H          1.20E+13    -0.150   16144
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
CH3+NH2<=>CH3NH+H          9.08E+13    -0.4     15714.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH2=CH3NH+H          1.2E13    -0.150   16144
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

CH3NH+H=CH2NH+H2          7.20E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!CH3NH+H=CH2NH+H2 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96  
 !CH3NH+H=CH2NH+H2 7.20E+08 1.500 -894  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH+H=CH2NH+H2 7.20E+08 1.5 -894.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3NH+H=CH2NH+H2 7.2E08 1.500 -894  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH3NH+O=CH2NH+OH 5.00E+08 1.50 -894.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH+O=CH2NH+OH 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+O=CH2NH+OH 5.00E+08 1.5 -894.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH3NH+O=CH2NH+OH 5.00E+08 1.500 -894  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH+O=CH2NH+OH 5.0E08 1.500 -894  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH3NH+O=CH3O+NH 6.00E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+O=CH3O+NH 6.00E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97  
  
 CH3NH+OH=CH2NH+H2O 3.60E+06 2.00 -1192.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH+OH=CH2NH+H2O 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+OH=CH2NH+H2O 3.60E+06 2.0 -1192.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH3NH+OH=CH2NH+H2O 3.60E+06 2.000 -1192  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH+OH=CH2NH+H2O 3.6E06 2.000 -1192  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 CH3NH+OH=CH4+HNO 6.00E+12 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+OH=CH4+HNO 6.00E+12 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97  
  
 HNOH+CH3=CH3NH+OH 2.00E+13 0.0 0  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 CH3NH+O2=CH2NH+HO2 1.00E+07 2.0 6300.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+O2=CH2NH+HO2 1.00E+07 2.0 6300.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97  
  
 CH3NH+O2=CH3O+HNO 6.00E+12 0.0 4000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98  
 !CH3NH+O2=CH3O+HNO 6.00E+12 0.0 4000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97  
  
 CH3NH+CH3=CH2NH+CH4 2.40E+06 1.87 -1112.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH+CH3=CH2NH+CH4 2.40E+06 1.870 -1113  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH+CH3=CH2NH+CH4 2.40E+06 1.9 -1113.0

```

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH+CH3=CH2NH+CH4          2.4E06  1.870  -1113
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!! CH2NH2 Chemistry           !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH2NH2=CH2NH+H                1.10E+45  -10.24  47790.
!0.1 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CH2NH2=CH2NH+H                2.40E+48  -10.82  52010.
!1.0 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2=CH2NH+H                3.20E+46  -9.95   53500.
!10 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2=CH2NH+H                1.10E+45  -10.240 47817
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
(600-2500K)
DUPLICATE
CH2NH2(+AR)<=>CH2NH+H(+AR)      7.91E+11  0.3     36260.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
LOW/                             1.64E+39  -7.02   40100. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
TROE/ 1.0 911000 10.0 0.260E+09 /
DUPLICATE
!CH2NH2=CH2NH+H                1.1E45 -10.240 47817
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2
(600-2500K)

!CH3+NH2=CH2NH2+H              1.10E+13  -0.13   9900.
!0.1 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H              1.40E+14  -0.43   11101.
!1.0 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H              7.40E+12  0.0     12064.
!10 atm                        Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H              1.10E+13  -0.130  9905
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
CH3+NH2<=>CH2NH2+H              5.15E+14  -0.6    10155.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH2=CH2NH2+H              1.1E13  -0.130  9905
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

!CH2NH2+H=CH2NH+H2              4.00E+08  1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+H=CH2NH+H2              4.80E+08  1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
CH2NH2+H=CH2NH+H2              4.80E+08  1.5     -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH2+H=CH2NH+H2              4.8E08  1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+O=CH2O+NH2              7.00E+13  0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+O=CH2O+NH2              7.00E+13  0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+O=CH2O+NH2              7.0E13  0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+O=CH2NH+OH              3.30E+08  1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+O=CH2NH+OH              3.30E+08  1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+O=CH2NH+OH              3.3E08  1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

```

CH2NH2+OH=CH2OH+NH2 4.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH2+OH=CH2OH+NH2 4.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH2+OH=CH2OH+NH2 4.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+OH=CH2NH+H2O 2.40E+06 2.00 -1192.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH2+OH=CH2NH+H2O 2.40E+06 2.000 -1192  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH2+OH=CH2NH+H2O 2.4E06 2.000 -1192  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+O2=CH2NH+HO2 1.00E+22 -3.09 6752.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH2+O2=CH2NH+HO2 1.00E+22 -3.090 6756  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH2+O2=CH2NH+HO2 1.0E22 -3.090 6756  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+O2=NH2+CH2O+O 6.00E+18 -1.59 30175.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NH2+CH3=C2H5+NH2 2.00E+13 0.0 2701.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH2+CH3=C2H5+NH2 2.00E+13 0.000 2702  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH2+CH3=C2H5+NH2 2.00E+13 0.0 2702.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH2+CH3=C2H5+NH2 2.0E13 0.000 2702  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH2NH2+CH3=CH2NH+CH4 1.60E+06 1.87 -626.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH2+CH3=CH2NH+CH4 1.60E+06 1.870 -626  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH2+CH3=CH2NH+CH4 1.60E+06 1.9 -626.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2NH2+CH3=CH2NH+CH4 1.6E06 1.870 -626  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

! CH2NH2+O2=PROD 4.7E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JANSIL99  
 addition?

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! CH3NH2 Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !CH3+NH2=CH3NH2 1.30E+54 -12.72 15599.  
 !0.1 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH3NH2 5.10E+52 -11.99 16781.  
 !1.0 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH3NH2 1.60E+47 -10.15 15679.  
 !10 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH3NH2 1.30E+54 -12.720 15608  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2  
 (600-2500K)  
 CH3+NH2<=>CH3NH2 1.03E+33 -6.3 5750.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 CH3+NH2 (+M)=CH3NH2 (+M) 7.2E12 0.420 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JODGRO95  
 LOW /2.2E30 -3.85 0/

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
!CH3+NH2=CH3NH2 1.3E54 -12.720 15608  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2  
(600-2500K)

!CH3NH2+M=CH2NH+H2+M 2.40E+13 0.000 107260  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 ZHA/LEE00  
CH3NH2(+AR)<=>CH2NH+H2(+AR) 9.99E+08 1.2 102880.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 2.46E+30 -4.75 107000. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.82 154.59 1.0 401000 /  
CH3NH2+M=CH2NH+H2+M 2.4E13 0.000 107260  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00

CH3NH2(+AR)<=>CH2NH2+H(+AR) 3.93E+15 -0.1 93820.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 6.82E+40 -7.01 98400 /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 231.01 1.0 401000 /

CH3NH2(+AR)<=>CH3NH+H(+AR) 1.44E+16 -0.3 100940.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 1.14E+38 -6.35 105000. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.67 169.67 1.0 401000 /

!CH3NH2+M=CHNH2+H2+M 1.3E14 0.000 82560  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00

!CH3NH2+M=CH3N+H2+M 9.8E14 0.000 117550  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00

CH3NH2+H=CH2NH2+H2 5.60E+08 1.50 5461.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3NH2+H=CH2NH2+H2 5.60E+08 1.500 5464  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3NH2+H=CH2NH2+H2 5.60E+08 1.5 5464.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
!CH3NH2+H=CH2NH2+H2 5.6E08 1.500 5464  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+H=CH3NH+H2 4.80E+08 1.50 9701.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3NH2+H=CH3NH+H2 4.80E+08 1.500 9706  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3NH2+H=CH3NH+H2 4.80E+08 1.5 9706.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
!CH3NH2+H=CH3NH+H2 4.8E08 1.500 9706  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+O=CH2NH2+OH 4.00E+08 1.50 5193.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3NH2+O=CH2NH2+OH 4.00E+08 1.500 5196  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3NH2+O=CH2NH2+OH 4.0E08 1.500 5196  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+O=CH3NH+OH 3.30E+08 1.50 6345.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3NH2+O=CH3NH+OH 3.30E+08 1.500 6348  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3NH2+O=CH3NH+OH 3.3E08 1.500 6348  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+OH=CH2NH2+H2O 3.60E+06 2.00 238.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+OH=CH2NH2+H2O 1.00E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 CAR/CRO98
!CH3NH2+OH=CH2NH2+H2O 8.0E12 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/CRO98,GALALV08

CH3NH2+OH=CH3NH+H2O 2.40E+06 2.00 447.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+OH=CH3NH+H2O 2.40E+06 2.000 447
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH2+OH=CH3NH+H2O 2.0E12 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/CRO98,GALALV08

CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.87 9163.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.870 9170
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.9 9170.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH2+CH3=CH2NH2+CH4 1.5E06 1.870 9170
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+CH3=CH3NH+CH4 1.60E+06 1.87 8837.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+CH3=CH3NH+CH4 1.60E+06 1.870 8842
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH2+CH3=CH3NH+CH4 1.60E+06 1.9 8842.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH2+CH3=CH3NH+CH4 1.6E06 1.870 8842
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+NH2=CH2NH2+NH3 2.80E+06 1.94 5491.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+NH2=CH2NH2+NH3 2.80E+06 1.940 5494
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH2+NH2=CH2NH2+NH3 2.80E+06 1.9 5494.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH2+NH2=CH2NH2+NH3 2.8E06 1.940 5494
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

CH3NH2+NH2=CH3NH+NH3 1.80E+06 1.94 7139.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH2+NH2=CH3NH+NH3 1.80E+06 1.940 7143
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH2+NH2=CH3NH+NH3 1.80E+06 1.9 7143.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH2+NH2=CH3NH+NH3 1.8E06 1.940 7143
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! !!
!! C2N1 Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CH3NCH=CH3+HCN 8.1E15 -2.375 14942
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw 0.04 bar

CH3NCH+H=CH2NCH2+H 2.0E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcnh+h

CH2NCH2=CH3NCH 1.3E45 -10.068 66111
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw 0.04 bar, 700-3000 K

CH2NCH2+H=CH3+NCH2 3.0E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

```

CH2NCH2+O=CH2O+NCH2	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2NCH2+OH=CH2OH+NCH2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2NCH2+H=CH3NCH2	5.8E13	0.180	-125	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2chch2+h
!** CH3NCH2+H=CH3+CH2NH	7.0E10	0.840	-238	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3no+h
CH3NCH2+H=CH2NCH2+H2	5.6E08	1.500	5464	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
CH3NCH2+H=CH3NCH+H2	3.0E08	1.500	6130	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+h
CH3NCH2+O=CH2NCH2+OH	4.0E08	1.500	5196	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
CH3NCH2+O=CH3NCH+OH	2.2E08	1.500	5404	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+o
CH3NCH2+OH=CH2NCH2+H2O	8.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh
CH3NCH2+OH=CH3NCH+H2O	2.4E06	2.000	457	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+oh
CH3NCH2+CH3=CH2NCH2+CH4	1.5E06	1.870	9170	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CH3NCH2+CH3=CH3NCH+CH4	5.3E05	1.870	9687	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+ch3
CH3NCH2+NH2=CH2NCH2+NH3	2.8E06	1.940	5494	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CH3NCH2+NH2=CH3NCH+NH3	1.8E06	1.940	6090	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+nh2
CH3NCH3=CH3NCH2+H	1.6E15	-7.544	38425	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
CH3NCH3+H=CH3NCH2+H2	3.2E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Curran
CH3NCH3+OH=CH3NCH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Curran
CH3NCH3+CH3=CH3NCH2+CH4	6.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				SEEKOS88
CH3NHCH2=CH3+CH2NH	9.8E43	-10.302	37459	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
CH3NHCH2=CH3NCH2+H	5.9E44	-10.314	46803	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
CH3NHCH2+H=CH3NCH2+H2	4.8E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+h
CH3NHCH2+O=CH2O+CH3NH	7.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+o

CH3NHCH2+O=CH3NCH2+OH	3.3E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+o
CH3NHCH2+OH=CH2OH+CH3NH	4.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+oh
CH3NHCH2+OH=CH3NCH2+H2O	2.4E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+oh
CH3NHCH2+CH3=C2H5+CH3NH	2.0E13	0.000	2702	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+ch3
CH3NHCH2+CH3=CH3NCH2+CH4	1.6E06	1.870	-626	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+ch3
! ** CH3NHCH2+O2=CH2O+CH3+HNO	2.5E11	0.000	-1700	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3och2+o2
CH3NHCH2+H (+M)=CH3NHCH3 (+M)	5.2E17	-0.990	1580	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h5+h (+m)
LOW /1.99E41 -7.08 6685/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
TROE /0.8422 125 2219 6882/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
CH3NCH3+H=CH3NHCH3	1.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH3NHCH3+H=CH3NHCH2+H2	5.6E08	1.500	5464	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
CH3NHCH3+H=CH3NCH3+H2	4.8E08	1.500	9706	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
CH3NHCH3+O=CH3NHCH2+OH	6.1E12	0.000	556	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78, est br ratio
CH3NHCH3+O=CH3NCH3+OH	3.0E12	0.000	556	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78, est br ratio
CH3NHCH3+OH=CH3NHCH2+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 (ktot),
GALALV08 (br)				
CH3NHCH3+OH=CH3NCH3+H2O	1.9E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 (ktot),
GALALV08 (br)				
CH3NHCH3+CH3=CH3NHCH2+CH4	1.5E06	1.870	9170	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CH3NHCH3+CH3=CH3NCH3+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CH3NHCH3+NH2=CH3NHCH2+NH3	2.8E06	1.940	5494	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CH3NHCH3+NH2=CH3NCH3+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CHCNH+H=CH2+HNC	1.5E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+h
CHCNH+O=H+CO+HNC	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+o



CHCNH+OH=HCO+CHNH 1.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcco+oh  
  
 CHCNH+O2=HNC+CO+OH 1.6E11 -0.020 1020  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcco+o2  
  
 CHCNH+O2=HNC+HCO+O 2.2E02 2.690 3540  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcco+o2  
  
 CH2SING+HCN=CH2CN+H 1.8E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KOC/WAG90  
 !CH2SING+HCN=CH2CN+H 1.80E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: KOC/WAG90  
  
 CH3+CN=CH2CN+H 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est  
 !CH3+CN=CH2CN+H 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 CH2CN+O=CH2O+CN 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !CH2CN+O=CH2O+CN 1.3E12 0.640 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HOYSEE95  
  
 CH2OH+CN=CH2CN+OH 5.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: JAM est  
 !CH2OH+CN=CH2CN+OH 5.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est  
  
 CH3CN=CH2CN+H 7.9E14 0.000 94940  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 !CH3CN(+M)=CH3NC(+M) 3.2E13 0.000 62000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SAIMUR84  
 ! LOW / 2.5E13 0.00 38000/  
  
 CH3CN+H=HCN+CH3 4.4E10 0.800 6800  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
 !CH3CN+H=HCN+CH3 4.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 CH3CN+H=HNC+CH3 2.8E15 -0.320 20030  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
  
 CH3CN+H=CH2CN+H2 6.0E04 3.010 8522  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
 !CH3CN+H=CH2CN+H2 3.00E+07 2.000 1000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 CH3CN+O=CH2CN+OH 4.7E08 1.180 14360  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SUNWAN10  
  
 CH3CN+OH=CH2CN+H2O 2.0E07 2.000 2000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est  
 !CH3CN+OH=CH2CN+H2O 2.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 CH3CN+CH3=CH2CN+CH4 5.0E12 0.000 7000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 CH3CN+CN=CH2CN+HCN 5.0E13 0.000 2000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 c-C2H3N=CH3CN 4.7E13 0.000 41500  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw

c-C2H3N+H=CH2NCH2	9.8E09	1.212	1969	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw
c-C2H3N+H=CH2CHNH	1.1E10	1.229	2422	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw
c-C2H3N+O=>NCH2+HCO	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
c-C2H3N+O=>C2H3+NO	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
c-C2H3N+OH=>NCH2+CH2O	5.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)+M=CH2CHN+M	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: H/0/				est
CH2CHN(S)+H=CH2CHN+H	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)+H=CH3+HCN	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)=c-C2H3N	3.0E13	0.000	4000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)=CH3CN	3.0E13	0.000	8000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)+O=>HCO+HCN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN(S)+OH=>CH2O+HCN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CNH=CH3CN	2.5E13	0.000	70300	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				DOUMAC94
CH2CNH+H=CH3CN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CNH+H=CH3+HNC	3.3E10	0.851	2840	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+h
CH2CNH+H=CHCNH+H2	3.0E07	2.000	10000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+h
CH2CNH+H=CH2CN+H2	2.4E08	1.500	7322	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+h
CH2CNH+O=CH2+HNCO	1.8E12	0.000	1350	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+o
CH2CNH+O=CHCNH+OH	2.0E07	2.000	10000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+o
CH2CNH+O=CH2CN+OH	1.7E08	1.500	4630	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+o
CH2CNH+OH=CH2OH+HNC	1.0E12	0.000	-1013	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+oh
CH2CNH+OH=CHCNH+H2O	1.0E07	2.000	3000	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+oh
CH2CNH+OH=CH2CN+H2O	1.2E06	2.000	-89	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+oh
CH2CNH+CH3=CH2CN+CH4	8.2E05	1.870	7123	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+ch3
CH2CNH+NH2=CH2CN+NH3	9.2E05	1.940	4441	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+nh2
CH2CHN+H=CH3+HCN	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CH2CHN+O=CH2O+HCN	5.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
CHCNH2+H=CHCNH+H2	4.8E08	1.500	9706	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
CHCNH2+O=CHCNH+OH	3.3E08	1.500	6348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
CHCNH2+O=HCCO+NH2	1.4E07	2.000	1900	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+o
CHCNH2+OH=CHCNH+H2O	2.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh
CHCNH2+CH3=CHCNH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CHCNH2+NH2=CHCNH+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CH3+HCN=CH3CHN	1.0E12	0.000	9900	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				Wang01, est
CH3CHN+H=CH3CN+H2	2.4E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+h
CH3CHN+H=CH2CHN+H2	9.0E13	0.000	15100	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+h
CH2CHN(S)+H2=CH3CHN+H	7.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CH2SING+h2
CH3CHN+O=CH3CN+OH	1.7E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+O
CH3CHN+OH=CH3CN+H2O	1.2E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+Oh
CH3CHN+OH=CH2CHN+H2O	1.1E03	3.000	2780	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+oh
CH3CHN+OH=CH2CHN(S)+H2O	4.4E13	-0.3485	-727	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+oh
CH3CHN+NH2=CH3CN+NH3	9.2E05	1.940	-1152	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+nh2
CH3CNH=CH3+HNC	6.5E18	-2.520	33000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co; Ea+17 (1 atm)
CH3CNH=CH3CN+H	7.7E25	-5.200	24000	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh; Ea+2 0.1 atm
CH3CNH+H=CH3+CHNH	2.1E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+h
CH3CNH+H=CH2CNH+H2	1.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+h
CH3CNH+H=CH3CN+H2	2.4E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+h
CH3CNH+O=CH2CNH+OH	5.3E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+o
CH3CNH+O=CH3CN+OH	1.7E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+o
CH3CNH+OH=CH2CNH+H2O	1.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+oh
CH3CNH+OH=CH3CN+H2O	1.2E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+oh
CH3CNH+O2=CH2O+CO+NH2	1.9E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+o2
CH3CNH+CH3=CH2CNH+CH4	5.3E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+ch3
CH3CNH+CH3=CH3CN+CH4	8.2E05	1.870	-1113	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+ch3
CH2CHNH+H=CH3+CHNH	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
CH2CHNH+H=CH3CNH+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
CH2CHNH+H=CH2CNH+H2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
CH2CHNH+O=CH2CNH+OH	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+o
CH2CHNH+OH=CH2CNH+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+oh
CH2CHNH+OH=CH2OH+CHNH	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+oh
CH2CHNH+O2=CH2O+CO+NH2	5.7E17	-1.757	11067	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+o2 (1 atm)
CHCNH2+H(+M)=CH2CNH2(+M)	1.7E10	1.266	2709	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+h(+m)
LOW /6.3E31 -4.664 3780 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
TROE /0.7878 -10212 1.E30 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
H2/2/ CO/2/ CO2/3/ H2O/5/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
CH2CNH2+H=CHCNH2+H2	4.5E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+h
CH2CNH2+O=CH2CO+NH2	3.0E13	0.000	0	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+o
CH2CNH2+OH=CHCNH2+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+oh
CH2CNH2+O2=OCHCHO+NH2	4.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				chchoh+o2
CH2CNH2+CH3=CHCNH2+CH4	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+ch3
NH2+C2H2=CHCHNH2	7.8E-18	8.310	7430	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				LINMOS98 ktot (350mbar)
CHCNH2+H(+M)=CHCHNH2(+M)	1.7E10	1.266	2709	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+h(+m)
LOW /6.3E31 -4.664 3780 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
TROE /0.7878 -10212 1.E30 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
H2/2/ CO/2/ CO2/3/ H2O/5/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
CHCHNH2+H=CHCNH2+H2	4.5E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+h
!CHCHNH2+O=OCCHNH2+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+o
CHCHNH2+OH=CHCNH2+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+oh
CHCHNH2+O2=OCHCHO+NH2	4.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				chchoh+o2
CHCHNH2+CH3=CHCNH2+CH4	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+ch3
CH2CHNH+H=CH3CHNH	5.8E13	0.180	-125	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2chch2+h Klippenstein v7
CH3+CHNH=CH3CHNH	1.8E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+hco
CH3CHNH+H=CH3CNH+H2	4.7E13	-0.350	3000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3hco+h
CH3CHNH+H=CH2CHNH+H2	1.9E12	0.400	5359	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3hco+h
CH3CHNH+H=CH3CHN+H2	2.4E08	1.500	7322	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+h
CH3CHNH+O=CH3CNH+OH	1.8E18	-1.900	2975	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3hco+o
CH3CHNH+O=CH2CHNH+OH	3.7E13	-0.200	3556	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3hco+o
CH3CHNH+O=CH3CHN+OH	1.7E08	1.500	4630	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+o
CH3CHNH+OH=CH3CNH+H2O	2.4E11	0.300	-1000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3hco+oh
CH3CHNH+OH=CH2CHNH+H2O	3.0E13	-0.600	800	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	ch3hco+oh
CH3CHNH+OH=CH3CHN+H2O !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	1.2E06 2.000 -89 ch2nh+oh
CH3CHNH+CH3=CH3CNH+CH4 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	3.9E-07 5.800 2200 ch3hco+ch3
CH3CHNH+CH3=CH2CHNH+CH4 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	2.5E01 3.150 5727 ch3hco+ch3
CH3CHNH+CH3=CH3CHN+CH4 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	8.2E05 1.870 7123 ch2nh+ch3
CH3CHNH+NH2=CH3CHN+NH3 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	9.2E05 1.940 4441 ch2nh+nh2
CHCHNH2+H(+M)=CH2CHNH2(+M) !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: LOW /2.10E24 -1.3 0/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TROE /0.5 1E-30 1E30 1E30/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	3.9E13 0.200 0 c2h3+h(+m)
CH2CNH2+H(+M)=CH2CHNH2(+M) !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: LOW /2.10E24 -1.3 0/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TROE /0.5 1E-30 1E30 1E30/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	3.9E13 0.200 0 c2h3+h(+m)
CH3CHNH=CH2CHNH2 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	5.0E18 -2.4965 67995 pw (0.04 bar, 1300-3000 K)
CH2CHNH2+H=CHCHNH2+H2 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	2.4E02 3.630 11266 c2h4+h
CH2CHNH2+H=CH2CNH2+H2 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	2.4E02 3.630 11266 c2h4+h
CH2CHNH2+H=CH2CHNH+H2 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	4.8E08 1.500 9700 ch3nh2+h
CH3CHNH+H=CH2CHNH2+H !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	3.0E13 0.000 0 est
CH2CHNH2+O=CH2CHNH+OH !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	3.3E08 1.500 6348 ch3nh2+o
CH2CHNH2+OH=CHCHNH2+H2O !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	1.3E-1 4.200 -860 c2h4+oh
CH2CHNH2+OH=CH2CNH2+H2O !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	1.3E-1 4.200 -860 c2h4+oh
CH2CHNH2+OH=CH2CHNH+H2O !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	2.4E06 2.000 447 ch3nh2+oh
!CH2CHNH2+O2=>p !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	*
CH2CHNH2+CH3=CHCHNH2+CH4 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:	6.0E07 1.560 16630 c2h4+ch3
CH2CHNH2+CH3=CH2CNH2+CH4	6.0E07 1.560 16630

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h4+ch3
CH2CHNH2+CH3=CH2CHNH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CH2CHNH2+NH2=CHCHNH2+NH3	5.3E12	0.000	10274	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h4+nh2
CH2CHNH2+NH2=CH2CNH2+NH3	5.3E12	0.000	10274	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h4+nh2
CH2CHNH2+NH2=CH2CHNH+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CH3CH2NH=CH2NH+CH3	1.9E10	0.000	23500	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: MATDIX07				C2H5O, 0.04 bar, Ea+8
CH3CH2NH=CH3CHNH+H	1.6E36	-7.920	36342	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh
CH3CH2NH+H=CH3+CH2NH2	1.4E12	0.701	346	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				C2H5O+h XULIN11
CH3CH2NH+H=CH3CHNH+H2	7.2E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+h
CH3CH2NH+O=CH3CHNH+OH	5.0E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+o
CH3CH2NH+OH=CH3CHNH+H2O	3.6E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+oh
CH3CH2NH+CH3=CH3CHNH+CH4	2.4E06	1.870	-1113	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+ch3
CH2CHNH2+H(+M)=CH3CHNH2(+M)	1.4E09	1.463	1355	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: LOW /2.0E39 -6.642 5769/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TROE /-0.569 299 9147 152.4/ !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h4+h(+m)
CH3CHNH2=CH3CHNH+H	1.1E45	-10.240	47817	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2
CH3CHNH2+H=CH2CHNH2+H2	4.9E08	1.700	588	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
CH3CHNH2+H=CH3+CH2NH2	8.4E16	-0.891	2903	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
CH3CHNH2+H=C2H4+NH3	4.7E21	-3.020	2845	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
CH3CHNH2+H=C2H5+NH2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
CH3CHNH2+O=CH2CHNH2+OH	2.5E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Hoyerermann
CH3CHNH2+OH=CH2CHNH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
CH3CHNH2+O2=CH2CHNH2+HO2	6.7E20	-3.020	2504	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 NIST

CH3CHNH2+CH3=CH2CHNH2+CH4	1.8E13	0.000	-769	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 NIST
C2H4+NH2=CH2CH2NH2	1.2E11	0.000	3955	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: close to hpl)				KHELES79 (addition,
CH2CH2NH2+H=CH2CHNH2+H2	1.8E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH2CH2NH2+O=CH2O+CH2NH2	9.6E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH2CH2NH2+OH=CH2CHNH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH2CH2NH2+HO2=>CH2O+OH+CH2NH2	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH2CH2NH2+O2=CH2CHNH2+HO2	3.7E16	-1.630	3418	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 NIST
CH2CH2NH2+CH3=CH2CHNH2+CH4	1.2E13	-0.320	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH3CH2NH2=C2H4+NH3	6.2E67	-15.944	99348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar, 1000-2500 K
C2H5+NH2 (+M)=CH3CH2NH2 (+M)	7.2E12	0.420	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: 400 Pa), est				ch3+nh2, DEMLES82 (298K
LOW /2.2E30 -3.85 0/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
CH3CHNH2+H=CH3CH2NH2	1.7E13	0.220	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7+h Klippenstein
CH2CH2NH2+H=CH3CH2NH2	5.4E13	0.160	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h5+h Klippenstein
CH3CH2NH2+H=CH2CH2NH2+H2	1.2E07	1.800	5100	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+h Marinov
CH3CH2NH2+H=CH3CHNH2+H2	2.6E07	1.650	2830	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+h Marinov
CH3CH2NH2+H=CH3CH2NH+H2	4.8E08	1.500	9700	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CH3CH2NH2+H=C2H5+NH3		*		
!CH3CH2NH2+H=C2H6+NH2		*		
CH3CH2NH2+O=CH2CH2NH2+OH	9.4E07	1.700	5460	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+o Marinov
CH3CH2NH2+O=CH3CHNH2+OH	6.8E12	0.000	1275	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78 (ktot)
CH3CH2NH2+O=CH3CH2NH+OH	3.3E08	1.500	6348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
CH3CH2NH2+OH=CH2CH2NH2+H2O	1.6E12	0.000	1300	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+oh CARSEA11



CH3CH2NH2+OH=CH3CHNH2+H2O	1.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 - ass dom ch as
for ch3ch2oh+oh Marinov				
CH3CH2NH2+OH=CH3CH2NH+H2O	2.4E06	2.000	447	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh - minor ch in
agr with GALALV08 theo				
CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.2E04	2.550	15750	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ho2 Marinov
CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.2E03	2.550	10750	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ho2 Marinov
CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.2E02	3.180	9620	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3 Marinov
CH3CH2NH2+CH3=CH3CHNH2+CH4	7.3E02	2.990	7950	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3 Marinov
CH3CH2NH2+CH3=CH3CH2NH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.2E02	3.180	9620	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3
CH3CH2NH2+NH2=CH3CHNH2+NH3	7.3E02	2.990	7950	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3
CH3CH2NH2+NH2=CH3CH2NH+NH3	1.8E06	1.940	7140	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
CH2CH2NH2+HCO=CH3CH2NH2+CO	6.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
CH3CHNH2+HCO=CH3CH2NH2+CO	1.2E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
!C2H2+NH2=NH2C2H2	4.6E06	8.310	7430	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				MOS/LIN98 (0.46 bar)
!C2+NO=CCN+O	5.2E13	0.000	8640	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				KRU/ROT99
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!!			!!	
!!	C1N2 Chemistry		!!	
!!			!!	
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!CH+N2=NCN+H	2.22E+07	1.48	23367.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML00				
!CH+N2=NCN+H	2.22E+07	1.5	23367.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid				
CH+N2=NCN+H	3.70E+07	1.420	20723	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/WAL97,MOS/LIN00				
!CH+N2=NCN+H	3.7E07	1.420	20723	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				MIL/WAL97,MOS/LIN00
H+NCN=HCN+N	1.89E+14	0.0	8425.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML00				
!H+NCN=HCN+N	1.89E+14	0.0	8425.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid				
!NCN+H=HCN+N	1.00E+14	0.000	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est				
!NCN+H=HCN+N	1.0E14	0.000	0	

```

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

!CN+NO=NCN+O                                1.80E+13    0.0      38190.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95, tst
calc
NCN+O=CN+NO                                1.00E+14    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!NCN+O=CN+NO                                1.0E14     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

NCN+OH=HCN+NO                               5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!NCN+OH=HCN+NO                              5.0E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

NCN+N=CN+N2                                 2.00E+13    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est.
!NCN+N=CN+N2                                 2.00E+13    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid

!CN+N2O=NCN+NO                              4.20E+11    0.0      7169.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+N2O=NCN+NO                              2.40E+13    0.0      13330.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Williams
etal1995, upp limb
CN+N2O=NCN+NO                              3.80E+03    2.6      3700.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+N2O=NCN+NO                              3.80E+03    2.600    3700
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92, WIL/NEL95
!CN+N2O=NCN+NO                              3.8E03     2.600    3700
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92, WIL/NEL95

!CH+N2=HCNN                                2.30E+27    -5.78    2443.
!0.1 atm                                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CH+N2=HCNN                                  3.60E+28    -5.84    2621.
!1.0 atm                                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N2=HCNN                                1.80E+30    -6.02    3445.
!10 atm                                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N2 (+M) <=>HCNN (+M)                    3.10E+12    0.150    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)
!   LOW/                                     1.30E+25    -3.160    740.00 /
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)
!   TROE/ 0.6670 235.00 2117.00 4536.00 /
!   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!   CO2/2.00/ C2H6/3.00/ AR/1.0/
!CH+N2=HCNN                                3.60E+28    -5.8     2623.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

HCNN+H<=>CH2+N2                             1.00E+14    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)

HCNN+O<=>CO+H+N2                            2.20E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)

HCNN+O<=>HCN+NO                             2.00E+12    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)

HCNN+OH<=>H+HCO+N2                          1.20E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)

HCNN+O2=H+CO2+N2                            4.00E+12    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HCNN+O2=HCO+N2O                             4.00E+12    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

HCNN+O2<=>O+HCO+N2 1.20E+13 0.000 0.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

!CH2+N2=CH2NN 9.30E+30 -7.01 19730.  
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
CH2+N2=CH2NN 1.60E+32 -7.07 19958.  
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH2+N2=CH2NN 4.30E+33 -7.18 20852.  
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH2+N2=CH2NN 1.60E+32 -7.1 19969.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NN=CH3+N2 3.00E+06 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96  
CH3NN+M=CH3+N2+M 1.00E+11 0.0 5900.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNH(+M)<=>CH3+NNH(+M) 3.30E+16 -0.1 55000.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 1.88E+31 -4.55 57500. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.97 250.59 1.0 401000 /

H2NN+CH3=CH3NNH+H 8.30E+05 1.93 6494.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH3NNH+O=CH3NN+OH 9.60E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH+OH=CH3NN+H2O 3.92E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NN+HO2=CH3NNH+O2 1.00E+06 2.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH+HO2=CH3NN+H2O2 1.00E+11 0.0 1987.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

!CH3NNH+CH3=CH4+CH3NN 4.60E+13 0.0 4850.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96  
CH3NNH+CH3=CH4+CH3NN 7.40E+13 0.0 5210.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NNH+NH2=NH3+CH3NN 4.60E+13 0.0 4850.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96  
CH3NNH+NH2=NH3+CH3NN 7.40E+13 0.0 5210.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNH+NO2=CH3NN+HONO 2.20E+11 0.0 5900.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 04

CH2NNH2+H=NCH2+NH3 1.76E+08 1.3 8801.1  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

H2NN+CH3=CH2NNH2+H 8.30E+05 1.93 6494.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NNH2+M=CH3NNH+H+M 1.00E+17 0.0 35770.

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96

CH3NNH2 (+M) <=> CH3NNH+H (+M)                    1.35E+08    1.7            47280.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    1.22E+53    -10.75       53560. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNH2 (+M) <=> CH2NNH2+H (+M)                    1.15E+09    1.2            50330.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    1.71E+49    -9.94       56000. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 331 10.0 47800 /

CH3NNH2+O=CH3NNH+OH                                    1.00E+08    2.0            0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH2+OH=CH3NNH+H2O                                1.00E+08    2.0            0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH2+O2=CH3NNH+HO2                                4.00E+12    0.0            0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH2+HO2=CH3NNH+HONO                             1.00E+08    2.0            0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NNH2+NO2=CH3NNH+HONO                             1.00E+08    2.0            0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 04

CH2NHNH2 (+M) <=> CH2NH+NH2 (+M)                    3.87E+12    0.2            12200.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    1.62E+27    -3.98       11800. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.866 298 10.0 280000 /

CH2NHNH2 (+M) <=> CH2NNH2+H (+M)                    5.92E+11    0.3            36300.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    5.25E+15    -0.72       34800. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 494 10.0 280000 /

CH3NHNH (+M) <=> CH3+N2H2 (+M)                    4.64E+09    1.6            35620.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    3.48E+48    -9.70       41200. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 233 10.0 308000 /

CH3NHNH (+M) <=> CH3NNH+H (+M)                    1.40E+07    2.0            44660.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    1.82E+36    -6.56       48600. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 134 10.0 51000 /

CH3NHNH2 (+M) <=> CH3NNH2+H (+M)                    4.66E+16    -0.2            77610.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    1.09E+49    -9.56       83400. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 169 13.7 40000 /

CH3NHNH2 (+M) <=> CH3NHNH+H (+M)                    4.69E+16    -0.2            80120.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/    4.44E+47    -9.19       85700. /

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 149 42.8 42400 /

CH3NHNH2 (+M) <=> CH2NHNH2+H (+M) 6.42E+16 -0.2 91800.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 1.80E+43 -7.98 96700. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.989 107 60.7 60100 /

!CH3NHNH2=CH3NNH+H2 3.16E+13 0.0 57000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Golden et al,  
72  
CH3NHNH2 (+M) <=> CH3NNH+H2 (+M) 9.70E+08 1.3 107500.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 1.05E+68 -13.84 115000. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 500000 10.0 41700 /

CH3NHNH2 (+M) <=> CH2NNH2+H2 (+M) 2.69E+09 1.2 105430.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 1.05E+68 -13.84 114.0 /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.195 4720 1.0 1.0 /

CH3NHNH2 (+M) <=> N2H3+CH3 (+M) 3.12E+16 -0.2 65180.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 7.34E+61 -13.01 72900. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 271 10.0 41700 /

CH3NHNH2 (+M) <=> H2NN+CH4 (+M) 1.36E+09 1.6 67110.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 2.47E+51 -10.4 74300. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 260 10.0 77500 /

CH3NHNH2 (+M) <=> N2H2+CH4 (+M) 1.61E+10 1.1 108880.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 4.382E+63 -12.62 116000. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 978 10.0 41700 /

!CH3NHNH2+M=CH3NH+NH2+M 2.50E+14 0.0 40940.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
96  
CH3NHNH2 (+M) <=> CH3NH+NH2 (+M) 2.40E+16 -0.1 63790.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 8.92E+64 -13.84 71900. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NHNH2=CH2NH+NH3 1.58E+13 0.0 54000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Golden et al,  
72  
CH3NHNH2 (+M) <=> CH2NH+NH3 (+M) 3.50E+08 1.4 68330.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 8.05E+48 -10.3 75300. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.0 242 10.0 41700 /

CH3NHNH2 (+M) <=> CH3N+NH3 (+M) 4.33E+09 1.2 62170.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
LOW/ 7.50E+69 -15.57 71600. /  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
TROE/ 0.355 293 10 41300 /

!CH3NHNH2+H=CH3NNH2+H2 1.30E+13 0.0 2500.

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96

CH3NHNH2+H=CH3NNH2+H2	2.08E+07	1.8	4488.1
-----------------------	----------	-----	--------

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+H=CH3NHNH+H2	1.68E+09	1.1	7289.0
-----------------------	----------	-----	--------

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+H=CH2NHNH2+H2	7.88E+07	1.7	11162.0
------------------------	----------	-----	---------

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NHNH2+H=CH3NH+NH3	4.46E+09	0.0	3100.
-----------------------	----------	-----	-------

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96

CH3NHNH2+H=CH3NH+NH3	1.37E+09	1.1	5526.4
----------------------	----------	-----	--------

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+O=CH3NNH+H2O	9.60E+12	0.0	0.
-----------------------	----------	-----	----

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NHNH2+O=CH3NNH2+OH	9.60E+12	0.0	0.
-----------------------	----------	-----	----

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NHNH2+O=CH3NHNH+OH	2.69E+12	0.0	0.
-----------------------	----------	-----	----

!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)

CH3NHNH2+O=CH2NHNH2+OH	1.30E+12	0.0	0.
------------------------	----------	-----	----

!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)

CH3NHNH2+OH=CH3NNH2+H2O	3.92E+13	0.0	0.
-------------------------	----------	-----	----

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NHNH2+OH=CH3NHNH+H2O	1.10E+13	0.0	0.
-------------------------	----------	-----	----

!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)

CH3NHNH2+OH=CH2NHNH2+H2O	5.30E+12	0.0	0.
--------------------------	----------	-----	----

!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)

CH3NNH2+HO2=CH3NHNH2+O2	1.00E+06	2.0	0.
-------------------------	----------	-----	----

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.
---------------------------	----------	-----	-------

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98

CH3NHNH2+HO2=CH3NHNH+H2O2	7.56E+10	0.0	1987.
---------------------------	----------	-----	-------

!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)

CH3NHNH2+HO2=CH2NHNH2+H2O2	3.65E+10	0.0	1987.
----------------------------	----------	-----	-------

!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)

!CH3NHNH2+CH3=CH4+CH3NNH2	1.00E+13	0.0	6990.
---------------------------	----------	-----	-------

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96

CH3NHNH2+CH3=CH4+CH3NNH2	4.79E+01	3.4	3578.3
--------------------------	----------	-----	--------

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+CH3=CH3NHNH+CH4	3.21E+02	3.1	5748.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+CH3=CH2NHNH2+CH4	2.27E+01	3.5	7669.4
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH3NNH2+NH2	1.45E+02	3.3	4435.5
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH3NHNH+NH2	6.20E+02	3.1	7062.4
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH2NHNH2+NH2	3.93E+01	3.6	10910.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!CH3NHNH2+NH2=NH3+CH3NNH2	1.00E+11	0.5	1990.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96			
CH3NHNH2+NH2=CH3NNH2+NH3	1.65E+02	3.0	870.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH2=CH3NHNH+NH3	5.98E+01	3.1	2110.2
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH2=CH2NHNH2+NH3	1.04E+00	3.6	1894.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NO2=CH3NNH2+HONO	2.20E+11	0.0	5900.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 04			
CH3NHNH2+NO2=CH3NHNH+HONO	7.87E+10	0.0	8839.
!NJL estimation off LFE relationships			
CH3NHNH2+NO2=CH2NHNH2+HONO	1.39E+09	0.0	9803.
!NJL estimation off LFE relationships			
CH3NHNH2+NO=CH3NNH2+HNO	1.85E+13	0.0	8524.
!NJL estimation off LFE relationships			
CH3NHNH2+NO=CH3NHNH+HNO	1.24E+12	0.0	9605.
!NJL estimation off LFE relationships			
CH3NHNH2+NO=CH2NHNH2+HNO	5.05E+12	0.0	11310.
!NJL estimation off LFE relationships			
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!!	!!		
!! C2N2 Chemistry	!!		
!!	!!		
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!NCCN(+M)=CN+CN(+M)	1.60E+34	-4.32	130005.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!CN+CN(+M)=NCCN(+M)	5.66E+12	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992			
! LOW/	3.43E+25	-2.61	0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
! TSA/ 0.5 0.0 /			
! N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/			
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed per Tsang;			
NCCN+M=CN+CN+M	1.10E+34	-4.3	130079.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust.2011.12.007			
N2/1.5/ O2/1.50/ H2/1.5/ H2O/10.0/			

CO2/3.0/

```
CN+HCN=NCCN+H 1.50E+07 1.71 1529.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCCN+H=HCN+CN 1.40E+14 0.0 7944.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+HCN=NCCN+H 1.51E+07 1.71 1530.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92, from
Yang et al 92;
!HCN+CN=NCCN+H 1.50E+07 1.7 1530.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+HCN=NCCN+H 1.50E+07 1.7 1530.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!HCN+CN=NCCN+H 1.50E+07 1.710 1530
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!HCN+CN=NCCN+H 1.5E07 1.710 1530
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

HNC+CN=NCCN+H 1.00E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+CN=NCCN+H 1.00E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PET/OSA04 est
!HNC+CN=NCCN+H 1.0E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PET/OSA04 est

!CH3NNCH3=CH3NN+CH3 6.90E+15 0.0 50880.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
CH3NNCH3=CH3NN+CH3 6.92E+15 0.0 50875.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNCH3=C2H6+N2 2.00E+11 0.0 33000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NNCH3=C2H6+N2 2.00E+11 0.0 33000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! all other !!
!! Non CNO Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! C2H4+CN=CH2CHCN+H 5.9E14 -0.240 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HER/SPE92
! C2H2+CN=C2HCN+H 3.6E15 -0.530 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HER/SPE92

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! !!
!! HCNO Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!NCO(+M)=N+CO(+M) 3.30E+14 0.0 54016.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+M=N+CO+M 1.14E+23 -1.95 59930.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992, N2
! N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.5/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 per
Tsang, others guessed
NCO+M=N+CO+M 2.20E+14 0.0 54050.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
N2/1.5/
```



```

!NCO+M=N+CO+M                2.20E+14    0.000    54050
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!   N2/1.5/
!NCO+M<=>N+CO+M                3.10E+14    0.000    54050.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!   CO2/2.00/ C2H6/3.00/ AR/0.70/
!NCO+M=N+CO+M                2.2E14    0.000    54050
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05
!   N2/1.5/

CN+OH=NCO+H                    4.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+OH=NCO+H                    4.00E+13    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,92;
!WHB95 confirm
!CN+OH=NCO+H                    1.00E+15   -0.4     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+OH=NCO+H                    1.00E+15   -0.437   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO96,DEC/MAC03
!CN+OH<=>NCO+H                    4.00E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+OH=NCO+H                    1.0E15   -0.437   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO96,DEC/MAC03

CH+NO=H+NCO                    2.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO<=>H+NCO                    1.62E+13    0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH+NO<=>H+NCO                    1.62E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH+NO=NCO+H                    1.8E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

!HCN+O=NCO+H                    2.00E+08    1.47     7586.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN+O=NCO+H                    1.38E+04    2.64     4980.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!MB89;Perry&Melius 85 similar
!HCN+O=NCO+H                    1.40E+04    2.6      4980.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCN+O=NCO+H                    1.40E+04    2.640    4980
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89
!HCN+O=NCO+H                    1.4E04     2.640    4980
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89
!HCN+O<=>NCO+H                    2.03E+04    2.640    4980.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

HNC+O=H+NCO                    1.60E+01    3.08     -224.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TDLLM, 1994

NCO+H=NH+CO                    5.20E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+H=NH+CO                    5.40E+13    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92
!NCO+H=CO+NH                    7.20E+13    0.0      1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+H=CO+NH                    7.20E+13    0.000    1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!NCO+H=CO+NH                    7.2E13     0.000    1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05
!NCO+H<=>NH+CO                    5.40E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!CN+O2=NCO+O                    1.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!CN+O2=NCO+O 2.60E+14 -0.5 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; S&S88  
 CN+O2=NCO+O 7.20E+12 0.0 -417.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 DUPLICATE  
 CN+O2=NCO+O -2.8E17 -2.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 DUPLICATE  
 !CN+O2=NCO+O 7.20E+12 0.000 -417  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05,RIM99  
 ! DUPLICATE  
 !CN+O2=NCO+O -2.80E+17 -2.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
 ! DUPLICATE  
 !CN+O2<=>NCO+O 6.14E+12 0.000 -440.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CN+O2=NCO+O 7.2E12 0.000 -417  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05,RIM99  
 ! DUP  
 !CN+O2=NCO+O -2.8E17 -2.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 ! DUP  
  
 !NCO+O=NO+CO 4.20E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+O=NO+CO 4.52E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992  
 NCO+O=NO+CO 2.00E+15 -0.5 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+O=NO+CO 2.00E+15 -0.500 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 GAO/MAC03  
 !NCO+O<=>NO+CO 2.35E+13 0.000 0.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !NCO+O=NO+CO 2.0E15 -0.500 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 GAO/MAC03  
  
 NCO+O=N+CO2 8.00E+12 0.0 2502.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+O=N+CO2 8.00E+12 0.0 2503.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
  
 NCO+OH=HON+CO 5.30E+12 -0.07 5124.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+OH=HON+CO 5.30E+12 -0.1 5126.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+OH=HON+CO 5.30E+12 -0.070 5126  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
 !NCO+OH=HON+CO 5.3E12 -0.070 5126  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00  
  
 NCO+OH=H+CO+NO 8.30E+12 -0.05 18032.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+OH=NO+CO+H 2.00E+13 0.0 7500.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
 !NCO+OH=H+CO+NO 8.30E+12 -0.1 18042.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+OH=H+CO+NO 8.30E+12 -0.050 18042  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
 !NCO+OH<=>NO+H+CO 0.25E+13 0.000 0.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !NCO+OH=H+CO+NO 8.3E12 -0.050 18042  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00  
  
 NCO+O2=NO+CO2 2.00E+12 0.0 20000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB91  
 !NCO+O2=NO+CO2 2.00E+12 0.0 20000.0

```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+O2=NO+CO2          1.00E+13    0.000    10000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: BEC/WIE00, est Ć!NCO+O2<=>NO+CO2
2.00E+12    0.000    20000.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+O2=NO+CO2          1.0E13    0.000    10000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          BEC/WIE00, est Ć
!CH3CN+O=NC+CH3          1.50E+04    2.640    4980
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
CH3CN+O=CH3+NCO          6.0E09    1.800    8130
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          SUNWAN10

CH3NCH+O=>CH3+NCO+H          7.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          hcnh+h

C2H2+NCO=HCCO+HCN          1.40E+12    0.000    1815
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/WIE95
!C2H2+NCO=HCCO+HCN          1.4E12    0.000    1815
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 BEC/WIE95

CN+CO2=NCO+CO          3.67E+06    2.16    26900.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WYL, IJCK 91
!CN+CO2=NCO+CO          3.70E+06    2.2    26900.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CO2+CN=NCO+CO          3.70E+06    2.160    26900
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WAN/LIN91
!CO2+CN=NCO+CO          3.7E06    2.160    26900
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WAN/LIN91

C2O+NO=CO+NCO          1.0E14    0.000    670
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          THW/HER04 (p)
!C2O+NO=CO+NCO          1.00E+14    0.000    670
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: THW/HER04 (p)

C2O+NO2=CO2+NCO          5.10E+13    0.000    125
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: THW/HER04 (p)
!C2O+NO2=CO2+NCO          5.1E13    0.000    125
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          THW/HER04 (p)

!NCO+N=N2+CO          3.30E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
NCO+N=N2+CO          2.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NCO+N=N2+CO          2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+N=N2+CO          2.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM est
!NCO+N<=>N2+CO          2.00E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+N=N2+CO          2.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM est

!CN+NO=NCO+N          5.50E+12    0.0    30620.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95 (Lin);
Shock Waves Symp.
CN+NO=NCO+N          9.60E+13    0.0    42100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+NO=NCO+N          9.60E+13    0.000    42100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 TSA92
!CN+NO=NCO+N          9.6E13    0.000    42100
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 TSA92

!CN+NO2=NCO+NO          6.20E+15    -0.75    348.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+NO2=NCO+NO          6.16E+15    -0.752    344.

```

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WMHB 25th ISC,
94
CN+NO2=NCO+NO          5.30E+15   -0.8     344.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+NO2=NCO+NO          5.30E+15   -0.752   344
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05
!CN+NO2<=>NCO+NO        6.16E+15   -0.752   345.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+NO2=NCO+NO          5.3E15    -0.752   344
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

!NCO+NO=CO2+N2          7.80E+17   -1.73    765.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+NO=CO2+N2          1.46E+21   -2.74    1824.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZL00, JPC
A104, 10807, 2000
NCO+NO=N2+CO2           1.50E+21   -2.7     1824.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+NO=N2+CO2           1.50E+21   -2.740   1824
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 ZHU/LIN04
!NCO+NO<=>N2+CO2        3.80E+18   -2.000   800.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+NO=N2+CO2           1.5E21    -2.740   1824
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 ZHU/LIN04

!NCO+NO=N2O+CO          6.20E+17   -1.73    765.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+NO=N2O+CO          3.98E+19   -2.19    1743.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZL00, JPC
A104, 10807, 2000
NCO+NO=N2O+CO           4.00E+19   -2.2     1743.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+NO<=>N2O+CO        1.90E+17   -1.520   740.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+NO=N2O+CO           4.0E19    -2.190   1743
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 ZHU/LIN04
!NCO+NO=N2O+CO           4.00E+19   -2.190   1743
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 ZHU/LIN04

NCN+O2=NO+NCO           4.40E+09    0.510   24580
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: ZHU/LIN05
!NCN+O2=NO+NCO           4.4E09    0.510   24580
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ZHU/LIN05

N2O+NCO=CO+N2+NO        9.00E+13    0.0     27800.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; TSA92
!NCO+NO2=CO+NO+NO       2.50E+11    0.000   -707
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR/HER93,WOO/BOW94
!NCO+NO2=CO+NO+NO       2.5E11    0.000   -707
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR/HER93,WOO/BOW94

!NCO+NO2=CO2+N2O        2.30E+12    0.0     -874.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+NO2=CO2+N2O        1.95E+13   -0.258   -620.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; see below
NCO+NO2=CO2+N2O         3.00E+12    0.0     -707.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+NO2=CO2+N2O         3.00E+12    0.000   -707
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR/HER93,WOO/BOW94
!NCO+NO2<=>N2O+CO2      3.25E+12    0.000   -705.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+NO2=CO2+N2O         3.0E12    0.000   -707
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR/HER93,WOO/BOW94

NCO+NO2=CO+NO+NO        2.10E+11    0.0     -874.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!NCO+NO2=CO+NO+NO          1.77E+12   -0.258   -620.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; see below
!NCO+NO2=CO+NO+NO          2.50E+11    0.0     -707.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

NCCN+O=NCO+CN              4.60E+12    0.0     8877.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCCN+O=NCO+CN              4.57E+12    0.0     8880.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NCCN+O=CN+NCO              4.60E+12    0.0     8880.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCCN+O=NCO+CN              4.57E+12    0.0     8880.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid

CN+NCO=NCN+CO              1.80E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+NCO=NCN+CO              1.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!CN+NCO=NCN+CO              1.8E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

NCO+NCO=CO+CO+N2           1.80E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+NCO=CO+CO+N2           1.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!NCO+NCO=CO+CO+N2           1.8E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

! C2H4+NCO=adduct
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          BEC/WIE95

!HCNO=HCN+O                 2.00E+30   -6.03    60698.
!0.1 atm                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HCNO=HCN+O                   4.20E+31   -6.12    61175.
!1.0 atm                     Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO=HCN+O                 5.90E+31   -5.85    61900.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO=HCN+O                 4.20E+31   -6.1     61210.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO=HCN+O                 2.00E+30   -6.030   60733
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2
!HCNO=HCN+O                 2.0E30    -6.030   60733
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2

CH2+NO=HCNO+H              3.80E+13   -0.36    576.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+NO=HCNO+H              3.10E+12    0.000   -378
!!CH2+NO<=>H+HCNO           3.80E+13   -0.360   580.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2+NO=HCNO+H              3.1E12     0.000   -378
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: ATA/WOL92,FIC/TEM01
!CH2+NO<=>H+HCNO            3.80E+13   -0.360   580.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH2+NO=HCNO+H              3.1E12     0.000   -378
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          ATA/WOL92,FIC/TEM01

CH2SING+NO<=>H+HCNO         3.80E+13   -0.360   580.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2SING+NO<=>H+HCNO         3.80E+13   -0.360   580.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

NCH2+O=HCNO+H              2.00E+13    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCNO+H=HCN+OH              2.70E+11    0.18    2115.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!HCNO+H<=>OH+HCN                2.70E+11    0.180    2120.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
HCNO+H=HCN+OH                      7.20E+10    0.8      8612.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+H=HCN+OH                      7.20E+10    0.841    8612
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+H<=>OH+HCN                2.70E+11    0.180    2120.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCNO+H=HCN+OH                      7.2E10    0.841    8612
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

HCNO+H=NH2+CO                      1.70E+14   -0.75    2889.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO+H<=>NH2+CO                  1.70E+14   -0.750    2890.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HCNO+H<=>NH2+CO                  1.70E+14   -0.750    2890.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HCNO+O=HCO+NO                     7.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HCNO+O=HCO+NO                       6.30E+13    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+O=HCO+NO                       6.30E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA98
!HCNO+O=HCO+NO                       6.3E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA98

HCNO+O=NCO+OH                       7.00E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+O=NCO+OH                       7.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+O=NCO+OH                       7.0E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

HCNO+OH=HCO+HNO                     4.50E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=HCO+HNO                     4.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=HCO+HNO                     4.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+OH=HCOH+NO                    4.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HCNO+OH=CH2O+NO                      1.00E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=CH2O+NO                      1.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03 (HCOH)
!HCNO+OH=CH2O+NO                      1.0E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03 (HCOH)

HCNO+OH=NO+CO+H2                    6.50E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NO+CO+H2                    6.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NO+CO+H2                    6.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

HCNO+OH=NCO+H2O                      3.50E+12    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NCO+H2O                      3.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NCO+H2O                      3.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

HCNO+OH=NCO+H+OH                     4.50E+12    0.0      0.0

```

```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NCO+H+OH          4.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NCO+H+OH          4.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

NO+HCCO=HCNO+CO          4.60E+13    0.0    695.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCCO+NO=HCNO+CO          2.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!HCCO+NO=HCNO+CO          5.90E+12    0.089    -457
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/GLA03
!HCCO+NO<=>HCNO+CO          0.90E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCCO+NO=HCNO+CO          5.9E12    0.089    -457
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          MIL/GLA03

HCCO+NO2=HCNO+CO2          1.60E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 TEM/WAG92/p
!HCCO+NO2=HCNO+CO2          1.6E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 TEM/WAG92/p

HCNO+CN=HCN+NCO          6.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: FEN/HER06,PAN/TAN08
!HCNO+CN=HCN+NCO          6.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          FEN/HER06,PAN/TAN08

!HNCO (+M)=NH+CO (+M)          1.30E+16    0.0    84320.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO (+M)=NH+CO (+M)          6.00E+13    0.0    99800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992
  LOW/          2.17E+28    -3.1    101900. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!  TSA/ 0.9 -2.0E-04 /
  TROE/0.4665 1000.0 1.0E6/
  N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed
per Tsang;
!HNCO+M=CO+NH+M          1.10E+16    0.0    86000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!  N2/1.5/
!HNCO+M=CO+NH+M          1.10E+16    0.000    86000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MER/HAN89
!  N2/1.5/
!HNCO+M<=>NH+CO+M          1.18E+16    0.000    84720.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!  H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!  CO2/2.00/ C2H6/3.00/ AR/0.70/
!HNCO+M=CO+NH+M          1.1E16    0.000    86000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MER/HAN89
!  N2/1.5/

HNCO+M=H+NCO+M          1.00E+17    0.0    112000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; WU90

HCNO+H<=>H+HNCO          2.10E+15    -0.690    2850.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HCNO+H=H+HNCO          2.10E+15    -0.69    2850.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO+H<=>H+HNCO          2.10E+15    -0.690    2850.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

CH2+NO=HNC+H          3.10E+17    -1.38    1271.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+NO<=>H+HNC          3.10E+17    -1.380    1270.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

```

```

!CH2+NO<=>H+HNCO          3.10E+17   -1.380   1270.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

CH2SING+NO<=>H+HNCO          3.10E+17   -1.380   1270.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2SING+NO<=>H+HNCO          3.10E+17   -1.380   1270.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!OH+HCN=HNCO+H              4.40E+03    2.26    6395.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
OH+HCN=HNCO+H              1.98E-03    4.0     1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!HCN+OH=HNCO+H              2.00E-03    4.0     1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCN+OH<=>HNCO+H            4.40E+03    2.260   6400.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCN+OH=HNCO+H              2.00E-03    4.000   1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89
!HCN+OH=HNCO+H              2.0E-03    4.000   1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

OH+HNC=HNCO+H               2.80E+13    0.0     3694.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNC+OH=HNCO+H              2.80E+13    0.0     3696.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLM, IJCK 24,
1103, (1992).
!HNC+OH=HNCO+H              2.80E+13    0.0     3700.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+OH=HNCO+H              2.80E+13    0.000   3700
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HNC+OH = HNCO+H            2.8E13    0.000   3700
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!NCH2+O=HNCO+H              6.00E+13    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CHNH+O=HNCO+H               7.00E+13    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+O=HNCO+H              7.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+O=HNCO+H              7.00E+13    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+O=HNCO+H              7.0E13    0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!NCO+H2=HNCO+H              7.60E+02    3.00    3972.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+H=NCO+H2              1.80E+05    2.40    9910.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+H2=HNCO+H              2.07E+06    2.0     6020.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992
HNCO+H=NCO+H2              9.00E+07    1.7     13900.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+H=NCO+H2              9.00E+07    1.660   13900
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!HNCO+H<=>H2+NCO            1.05E+05    2.500   13300.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+H=NCO+H2              9.0E07    1.660   13900
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

HNCO+H=NH2+CO                3.60E+04    2.49    2343.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+H=NH2+CO              2.25E+07    1.7     3800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Miller&Melius
IJCK92, TST,
!HNCO+H=NH2+CO                3.60E+04    2.5     2345.0

```



```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+H=NH2+CO 3.60E+04 2.490 2345
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!HNCO+H<=>NH2+CO 2.25E+07 1.700 3800.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+H=NH2+CO 3.6E04 2.490 2345
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

HNC+O2=HNCO+O 1.50E+12 0.01 4111.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNCO+O=HNO+CO 1.70E+06 2.08 0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO+O=HNO+CO 1.49E+08 1.57 44010.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC,
TST
!HNCO+O=HNO+CO 1.50E+08 1.6 44012.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O<=>HNO+CO 1.50E+08 1.570 44000.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=HNO+CO 1.50E+08 1.570 44012
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 HE/LIN92
!HNCO+O=HNO+CO 1.5E08 1.570 44012
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 HE/LIN92

!HNCO+O=NH+CO2 1.70E+06 2.08 0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO+O=CO2+NH 9.80E+07 1.41 8524.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC,
TST (Lin, p711)
!HNCO+O=NH+CO2 9.60E+07 1.4 8520.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O=NH+CO2 9.60E+07 1.410 8520
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92,CEC05
!HNCO+O<=>NH+CO2 9.80E+07 1.410 8500.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=NH+CO2 9.6E07 1.410 8520
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92,CEC05

!HNCO+O=NCO+OH 3.10E+06 1.94 6454.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+OH=HNCO+O 7.80E+04 2.27 -993.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO+O=NCO+OH 2.20E+06 2.11 11430.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC,
TST
!HNCO+O=NCO+OH 2.20E+06 2.1 11430.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O=NCO+OH 2.20E+06 2.110 11430
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92,CEC05
!HNCO+O<=>NCO+OH 2.20E+06 2.110 11400.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=NCO+OH 2.2E06 2.110 11430
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92,CEC05

HNCO+OH=NH2+CO2 6.30E+10 -0.06 11637.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=NH2+CO2 1.60E+05 2.0 2560.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
Tsang,1992/MB91
!HNCO+OH=NH2+CO2 6.30E+10 -0.1 11643.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!HNCO+OH<=>NH2+CO2 3.30E+06 1.500 3600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

HNCO+OH=NCO+H2O 3.60E+07 1.50 3594.

```

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=NCO+H2O 5.20E+10 -0.03 17555.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=H2O+NCO 4.79E+05 2.0 2560.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
Tsang,1992/MB91
!HNCO+OH=NCO+H2O 3.60E+07 1.5 3600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+OH=NCO+H2O 3.60E+07 1.500 3600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO/BOW95_hnco
!HNCO+OH<=>NCO+H2O 3.30E+07 1.500 3600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+OH=NCO+H2O 3.6E07 1.500 3600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO/BOW95_hnco

HNCO+O2=HNO+CO2 1.00E+12 0.0 35000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O2=HNO+CO2 1.00E+12 0.000 35000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 GLA/KRI94
!HNCO+O2=HNO+CO2 1.0E12 0.000 35000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 GLA/KRI94

NCO+HO2=HNCO+O2 2.00E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+HO2=HNCO+O2 2.00E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 mc lin est
!NCO+HO2=HNCO+O2 2.0E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 mc lin est

HNCO+HO2=NCO+H2O2 3.00E+11 0.0 23700.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HNCO+HO2=NCO+H2O2 3.00E+11 0.0 22000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+HO2=NCO+H2O2 3.00E+11 0.000 22000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM est
!HNCO+HO2=NCO+H2O2 3.0E11 0.000 22000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM est

NCO+CH4=HNCO+CH3 9.80E+12 0.0 8122.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+CH3=NCO+CH4 1.00E+12 0.0 9929.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+CH3=NCO+CH4 1.00E+12 0.0 9935.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH4+NCO=CH3+HNCO 9.80E+12 0.000 8120
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SCH/WOL94
!CH4+NCO=CH3+HNCO 9.8E12 0.000 8120
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SCH/WOL94

CH3CNH+O=CH3+HNCO 1.6E14 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3co+o

CH2CNH+OH=CH3+HNCO 6.7E11 0.000 -1013
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch2co+oh

C2H6+NCO=C2H5+HNCO 1.50E-09 6.890 -2910
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SCH/WOL94
!C2H6+NCO=C2H5+HNCO 1.5E-9 6.890 -2910
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SCH/WOL94

NCO+HCO=HNCO+CO 3.60E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCO+NCO=HNCO+CO 3.60E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!HCO+NCO=HNCO+CO 3.6E13 0.000 0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

```

CH2O+NCO=HNCO+HCO 6.00E+12 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92  
 !CH2O+NCO=HNCO+HCO 6.00E+12 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CH2O+NCO=HNCO+HCO 6.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92  
  
 CHCNH+O2=HNCO+HCO 4.9E12 -0.142 1150  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcco+o2  
  
 CH2CHN+O2=CH2O+HNCO 1.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est  
  
 HNCO+N=NH+NCO 2.32E+19 0.0 52500.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; XU99  
  
 !HNCO+NH=NH2+NCO 2.00E+13 0.0 19300.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est,  
 change due to new thermo  
 HNCO+NH=NH2+NCO 3.00E+13 0.0 23700.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HNCO+NH=NH2+NCO 3.00E+13 0.000 23700  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM lr  
 !HNCO+NH=NH2+NCO 3.0E13 0.000 23700  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM lr  
  
 NCO+NH3=HNCO+NH2 2.80E+04 2.48 983.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !HNCO+NH2=NCO+NH3 1.00E+12 0.0 8936.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+NH3=HNCO+NH2 2.80E+04 2.5 980.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+NH3=HNCO+NH2 2.80E+04 2.480 980  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 BEC/WIE97  
 !NCO+NH3=HNCO+NH2 2.8E04 2.480 980  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 BEC/WIE97  
  
 NCO+HNO=HNCO+NO 1.80E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+HNO=HNCO+NO 1.80E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92  
 !NCO+HNO=HNCO+NO 1.8E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92  
  
 HNC+NO2=HNCO+NO 1.00E+12 0.00 32000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TST result  
 from TDLLM, 1994  
  
 NCO+HONO=HNCO+NO2 3.60E+12 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+HONO=HNCO+NO2 3.60E+12 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92  
 !NCO+HONO=HNCO+NO2 3.6E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92  
  
 HNCO+NO2=HNNO+CO2 2.50E+12 0.0 26000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLLM93  
 !HNCO+NO2=CO2+HNNO 2.51E+12 0.0 26000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; HE93  
  
 CN+HNCO=HCN+NCO 1.00E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CN+HNCO=HCN+NCO 1.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92/1.5  
 !CN+HNCO=HCN+NCO 1.0E13 0.000 0

```

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92/1.5

!OH+HCN=HOCN+H                1.10E+06    2.03    13365.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HOCN+H=HCN+OH                2.00E+13   -0.04    2135.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!OH+HCN=HOCN+H                1.10E+06    2.03    13373
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MILLER/MELIUS
HCN+OH=HOCN+H                5.90E+04    2.4     12500.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCN+OH=HOCN+H                5.90E+04    2.400   12500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89
!HCN+OH<=>HOCN+H              1.10E+06    2.030   13370.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCN+OH=HOCN+H                5.9E04     2.400   12500
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

HCNO+H=HOCN+H                1.40E+11   -0.19    2482.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

HOCN+H=HNCO+H                3.10E+08    0.84    1916.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HOCN+H=HNCO+H                3.10E+08    0.84    1917
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HOCN+H=HNCO+H                3.10E+08    0.8     1917.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HOCN+H=HNCO+H                3.10E+08    0.840   1917
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HOCN+H<=>H+HNCO              2.00E+07    2.000   2000.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HOCN+H=HNCO+H                3.1E08     0.840   1917
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HOCN+H=NH2+CO                1.20E+08    0.61    2075.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HOCN+H=NH2+CO                1.20E+08    0.61    2076
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HOCN+H=NH2+CO                1.20E+08    0.6     2076.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HOCN+H=NH2+CO                1.20E+08    0.610   2076
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HOCN+H=NH2+CO                1.2E08     0.610   2076
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HOCN+H=H2+NCO                2.40E+08    1.50    6613.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HOCN+H=H2+NCO                2.40E+08    1.50    6617
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95
!HOCN+H=H2+NCO                2.40E+08    1.5     6617.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HOCN+H=H2+NCO                2.40E+08    1.500   6617
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HOCN+H=H2+NCO                2.4E08     1.500   6617
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HOCN+O=OH+NCO                1.70E+08    1.50    4131.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HOCN+O=OH+NCO                1.70E+08    1.5     4133.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HOCN+O=OH+NCO                1.70E+08    1.500   4133
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HOCN+O=OH+NCO                1.7E08     1.500   4133
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HOCN+OH=H2O+NCO              1.20E+06    2.00    -248.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HOCN+OH=H2O+NCO 1.20E+06 2.0 -248.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HOCN+OH=H2O+NCO 1.20E+06 2.000 -248  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!HOCN+OH=H2O+NCO 1.2E06 2.000 -248  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

HOCN+CH3=CH4+NCO 8.20E+05 1.87 6613.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH3+HOCN=CH3CN+OH 5.0E12 0.000 2000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM  
!CH3+HOCN=CH3CN+OH 5.00E+12 0.000 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM

HOCN+NH2=NCO+NH3 9.20E+05 1.94 3644.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HOCN+NH2=NCO+NH3 9.20E+05 1.9 3646.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HOCN+NH2=NCO+NH3 9.20E+05 1.940 3646  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!HOCN+NH2=NCO+NH3 9.2E05 1.940 3646  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

NCCN+OH=HOCN+CN 2.00E+12 0.0 18985.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCCN+OH=CN+HOCN 1.90E+11 0.0 2900.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

!CH2NO=HNCO+H 6.90E+41 -9.30 51673.  
!0.1 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
CH2NO=HNCO+H 2.30E+42 -9.11 53807.  
!1.0 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH2NO=HNCO+H 1.70E+38 -7.64 53549.  
!10 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+H=CH3+NO 4.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+H=HCNO+H2 4.80E+08 1.50 -894.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+O=CH2O+NO 7.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+O=HCNO+OH 3.30E+08 1.50 -894.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

NCH2+HO2=CH2NO+OH 3.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+OH=CH2OH+NO 4.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+OH=HCNO+H2O 2.40E+06 2.00 -1192.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+O2=CH2O+NO2 1.20E+15 -1.01 20117.  
!1000-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH2NO+O2=CH2O+NO2 2.90E+12 -0.31 17694.  
!300-1000K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+CH3=C2H5+NO 3.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+CH3=HCNO+CH4 1.60E+06 1.87 -1112.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+NH2=CH2NH2+NO 3.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH2NO+NH2=HCNO+NH3 1.80E+06 1.94 -1152.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!OH+HCN=NCHOH 1.70E+29 -6.31 5124.  
 !0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !OH+HCN=NCHOH 2.80E+30 -6.37 5342.  
 !1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !OH+HCN=NCHOH 1.10E+32 -6.53 6236.  
 !10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

H2NCO(+M)=CO+NH2(+M) 5.9E12 0.000 25000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: YOKBAC73  
 LOW / 1.0E14 0.00 21700/

H2NCO+H=HNCO+H2 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

H2NCO+O=HNCO+OH 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

H2NCO+OH=HNCO+H2O 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

CH2CHNH2+O=CH3+H2NCO 3.9E12 0.000 1494  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+o  
 DUPLICATE  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 CH2CHNH2+O=CH3+H2NCO 6.2E13 0.000 6855  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 DUPLICATE  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

!CH3+NO(+M)=CH3NO(+M) 9.00E+12 0.00 119.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 ! LOW/ 3.20E+23 -1.87 0. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 CH3+NO(+M)=CH3NO(+M) 9.00E+12 0.000 192  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAV/PIL91  
 ! LOW/ 2.50E+16 0.0 -2841 /  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
 TROE/ 5.0 1E-30 120 1E30 /  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d Fc=5.0exp(-T/120)  
 !CH3+NO(+N2)=CH3NO(+N2) 1.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 ! LOW/ 1.90E+18 0.0 0. /  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 ! SRI/ 0.03 790 1.0 /  
 !CH3+NO(+M)=CH3NO(+M) 9.0E12 0.000 192  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAV/PIL91  
 ! LOW /2.5E16 0.0 -2841/  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 ! TROE /5.0 1E-30 120 1E30/  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d Fc=5.0exp(-T/120)

!CH3+NO=CH3NO 3.60E+35 -8.25 4806.  
 !0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 CH3+NO=CH3NO 1.00E+37 -8.38 5223.  
 !1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NO=CH3NO 4.60E+41 -9.39 8261.

!10 atm                    Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH3NO+H=CH2NO+H2	4.40E+08	1.50	377.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+H=CH3+HNO	1.80E+13	0.0	2780.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+O=CH2NO+OH	3.30E+08	1.50	3614.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+O=CH3+NO2	1.70E+06	2.08	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+OH=CH2NO+H2O	3.60E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+OH=CH3+HONO	2.50E+12	0.0	993.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NO+CH3=CH2NO+CH4	7.90E+05	1.87	5412.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
CH3NCH3+O=CH3NO+CH3	5.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			est
CH3NCH3+O2=CH3NO+CH3O	1.0E09	1.000	6000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			LINSKA79,est (Ea,pr)
CH3NO+NH2=CH2NO+NH3	2.80E+06	1.94	1072.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
H2NCHO(+M)=CO+NH3(+M)	1.0E14	0.000	75514
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			KAKIMA85
LOW / 8.3E14 0.00 49084/			
H2NCHO+M=HCO+NH2+M	1.4E16	0.000	72900
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			KAKIMA85
H2NCHO+M=H2NCO+H+M	4.6E15	0.000	64200
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			KAKIMA85
H2NCHO+H=H2NCO+H2	1.3E13	0.000	6955
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			SYRTUR01
H2NCHO+H=HCO+NH3	1.0E13	0.000	19100
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			SYRTUR01,est
H2NCHO+O=H2NCO+OH	4.0E08	1.500	5196
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			ch3nh2+o
CH3CHNH2+O=CH3+H2NCHO	4.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			i-c3h7 Hoyermann
H2NCHO+OH=H2NCO+H2O	8.0E12	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			ch3nh2+oh
CH3CHNH2+HO2=>CH3+OH+H2NCHO	2.4E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			i-c3h7 TSA88
H2NCHO+CH3=H2NCO+CH4	7.0E05	2.000	9000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			BODBAC70,est
H2NCHO+NH2=H2NCO+NH3	2.0E06	2.000	5000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:			BACYOK73 (573K),est

!CH2NH2+O2=NH2CH2O+O 6.0E18 -1.590 30192  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

H2CNO2=CH2O+NO 1.00E+13 0.00 36000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3O+NO(+M)=CH3ONO(+M) 6.60E+14 -0.60 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 LOW/ 2.70E+27 -3.50 0. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2(+M)=CH3+NO2(+M) 1.80E+16 0.00 58500.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 LOW/ 1.30E+17 0.00 42000. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 ! TSA/ 0.183 0.0 /  
 TROE/0.1832 10.0 1.0E6/

CH3NO2+H=CH3+HONO 3.30E+12 0.00 3730.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+H=CH3NO+OH 1.40E+12 0.00 3730.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+H=H2CNO2+H2 5.40E+02 3.50 5200.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+O=H2CNO2+OH 1.50E+13 0.00 5350.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+OH=H2CNO2+H2O 5.00E+05 2.00 1000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+OH=CH3OH+NO2 2.00E+10 0.00 -1000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+CH2=H2CNO2+CH3 6.50E+12 0.00 7900.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+CH2SING=H2CNO2+CH3 1.20E+14 0.00 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CH3NO2+CH3=H2CNO2+CH4 5.50E-01 4.00 8300.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

CN+NO(+M)=NCNO(+M) 3.98E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992  
 LOW/ 1.56E+36 -6.2 4878. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 ! TSA/ 0.65 0.0 /  
 TROE/0.6508 10.0 1.0E6/  
 N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed  
 per Tsang;

CH3O+NO2(+M)=CH3ONO2(+M) 1.20E+13 0.00 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 LOW/ 1.40E+30 -4.50 0. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NNH2+NO2(+M)=CH3N(NH2)NO2(+M) 1.00E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 04  
 ! LOW/ 1.00E+17 0.0 0. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;



```

!CH3NNH2+NO2 (+M)=CH3N(NH2)ONO (+M)          1.00E+13   0.0   0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
04
!      LOW/          1.00E+17   0.0   0.   /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

! CH2CHO+NO2=CHOCH2NO2          8.0E22  -3.560  1930
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          DOU/HAY96 (i

```

## A.1.2 RedLabbe Model

### Kinetic parameters in CHEMKIN format

```

=====
REACTIONS
=====
!= Acetylene Mechanism Subset =
=====
!Reaction          A          n      Ea          ref.
!-----
!-----H2/O2 chemistry-----
!2O+M=O2+M          6.16E+15  -0.50   0.
!(1) TSA/HAM 86
! H2O/12.0/ H2/2.5/ AR/0.0/
!2O+AR=O2+AR          1.89E+13   0.00  -1790.
!(1) TSA/HAM 86
O+H+M=OH+M          4.71E+18  -1.00   0.
!(1) TSA/HAM 86
H2O/12.0/ H2/2.5/ !AR/0.75/
H2+M=2H+M          4.58E+19  -1.40  104380.
!(1) TSA/HAM 86
H2O/12.0/ H2/2.5/ !AR/0.0/
!H2+AR=2H+AR          5.84E+18  -1.10  104380.
!(1) TSA/HAM 86
H+OH+M=H2O+M          2.21E+22  -2.00   0.
!(45) Baulch 92
H2O/12.0/ H2/2.5/ !AR/0/
!H+OH+AR=H2O+AR          8.41E+21  -2.00   0.
!(1) TSA/HAM 86
!H2O2 (+M)=2OH (+M)          2.95E+14   0.00  48400.
!(2) BRO/COB 87
! LOW          /1.20E+17   0.00  45500./
!(3) Warnatz 84
! H2O/12.00/ H2/2.5/ AR/0.16/
H2O+O=OH+OH          2.97E+06   2.02  13400.
!(4) Sutherland 91
O+H2=H+OH          5.08E+04   2.67   6290.
!(5) Sutherland 86
OH+H2=H+H2O          2.16E+08   1.51   3430.
!(6) Michael/Sutherland 88
!H+O2 (+M)=HO2 (+M)          1.48E+12   0.60   0.
!(7) Cobos 85
! LOW          /3.50E+16  -0.41  -1120./
!(8) Mueller 99
! H2O/12.0/ H2/2.5/ AR/0.05/
!H+O2=O+OH          4.489E+08  1.257  16191.
!(9) Miller/Pilling 05
! DUPLICATE
!H+O2=O+OH          2.076E+16  -0.673  16191.

```

```

!(9) Miller/Pilling 05
! DUPLICATE
!O+HO2=OH+O2          3.25E+13  0.00    0.
!(10) Baulch 94
!H+HO2=O2+H2          1.66E+13  0.00   820.
!(8) Mueller 99
H+HO2=2OH             7.08E+13  0.00   300.
!(8) Mueller 99
!OH+HO2=O2+H2O        4.64E+13  0.00  -500.
!(11) GRI 1.2
!2HO2=O2+H2O2         1.30E+11  0.00 -1630.
!(12) HIP/TRO 90
! DUPLICATE
!2HO2=O2+H2O2         4.20E+14  0.00  11980.
!(12) HIP/TRO 90
! DUPLICATE
!O+H2O2=OH+HO2        9.55E+06  2.00   3970.
!(1) TSA/HAM 86
!H+H2O2=HO2+H2        4.82E+13  0.00   7950.
!(1) TSA/HAM 86
!H+H2O2=OH+H2O        2.41E+13  0.00   3970.
!(1) TSA/HAM 86
!OH+H2O2=HO2+H2O      1.00E+12  0.00    0.
!(13) HIP/TRO 92
! DUPLICATE
!OH+H2O2=HO2+H2O      5.80E+14  0.00   9560.
!(13) HIP/TRO 92
! DUPLICATE
!-----CO chemistry-----
!
!O+CO(+M)=CO2(+M)      1.80E+10  0.00   2385.
!(1) TSA/HAM 86
! LOW /6.02E+14  0.00  3000./
! H2/2./ O2/6./ H2O/6./ CH4/2./ CO/1.5/ CO2/3.5/ C2H6/3.0/ AR/0.5/
!O2+CO=O+CO2          2.50E+12  0.00  47800.
!(3) Warnatz 84
H2+CO(+M)=CH2O(+M)    4.30E+07  1.50  79600.
!(14) GRI-Mech 1.2
! LOW /5.07E+27  -3.42  84350./
! TROE /0.932 197 1540 10300/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !AR/0.7/ !C2H6/3.0/
OH+CO=H+CO2           4.10E+04  2.11  -1578.
!(15) Carriere 04
! Miller
! CO+OH=CO2+H 2.1370E05 1.9000 -1064.0
!JPS,SJK,&JAM 30th symp
! PLOG/ 0.01315 2.1370E05 1.9000 -1064.0/
! PLOG/ 0.1315 2.4537E05 1.8800 -1042.6/
! PLOG/ 1.315 8.7059E05 1.7300 -685.32/
! PLOG/ 13.158 6.7579E06 1.4800 48.483/
! PLOG/ 131.58 2.3432E07 1.3500 974.42/
! CO+OH=HOCO 1.6589E15 -2.6800 859.18
!JPS,SJK,&JAM 30th Symp
! PLOG/ 0.013158 1.6589E15 -2.6800 859.18/
! PLOG/ 0.13158 5.8859E18 -3.3500 887.00/
! PLOG/ 1.3158 2.5693E20 -3.5000 1309.0/
! PLOG/ 13.158 7.0764E20 -3.3200 1762.9/
! PLOG/ 131.58 1.1215E20 -2.7800 2055.6/
HO2+CO=OH+CO2         1.50E+14  0.00  23600.
!(16) Baulch 76
!O+HCO=OH+CO          3.00E+13  0.00    0.
!(1) TSA/HAM 86
O+HCO=H+CO2           3.00E+13  0.00    0.
!(1) TSA/HAM 86
H+HCO(+M)=CH2O(+M)    1.09E+12  0.48  -260.
!(17) Eiteneer 98

```

```

LOW /2.47E+24 -2.57 425./
TROE /0.7824 271 2755 6570/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !AR/0.7/ !C2H6/3.0/
H+HCO=H2+CO 7.30E+13 0.00 0.
!(18) TIMONEN 87a
OH+HCO=H2O+CO 3.00E+13 0.00 0.
!(1) TSA/HAM 86
HCO+M=H+CO+M 1.87E+17 -1.00 17000.
!(19) TIMONEN 87b
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !AR/0.7/ !C2H6/3.0/
!HCO+O2=HO2+CO 4.22E+12 0.00 0.
!(20) TIMONEN 88
HCO+HO2=CO2+OH+H 3.00E+13 0.00 0.
!(1) TSA/HAM 86
!
!-----CHxO chemistry-----
!
!O+CH2O=OH+HCO 1.81E+13 0.00 3078.
!(1) TSA/HAM 86
!O2+CH2O=HO2+HCO 2.05E+13 0.00 38920.
!(1) TSA/HAM 86
!Miller
!CH2O+O2=HCO+HO2 2.44E5 2.5 36461.
!Baulch 2004

H+CH2O=HCO+H2 5.18E+7 1.66 1834.
!(21) Hochgreb 92
!H+CH2O(+M)=CH2OH(+M) 5.40E+11 0.45 3600.
!(22) GRI 3.0
! LOW /1.27E+32 -4.82 6530./
! TROE /0.7187 103 1291 4160/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !C2H6/3.0/
H+CH2O(+M)=CH3O(+M) 5.40E+11 0.45 2600.
!(14) GRI-Mech 1.2
! LOW /2.20E+30 -4.80 5560./
! TROE /0.758 94 1555 4200/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !C2H6/3.0/
OH+CH2O=HCO+H2O 3.43E+09 1.18 -447.
!(1) TSA/HAM 86
!HO2+CH2O=HCO+H2O2 1.47E+13 0.00 15200.
!(21) Hochgreb 92
! Miller
! CH2O+HO2=HCO+H2O2 3.0E12 0.0 13000. !CEC 1994
!O+CH2OH=OH+CH2O 4.20E+13 0.00 0.
!(23) Tsang 87
!H+CH2OH=H2+CH2O 6.00E+12 0.00 0.
!(23) Tsang 87
!H+CH2OH=OH+CH3 9.63E+13 0.00 0.
!(1) TSA/HAM 86
!OH+CH2OH=H2O+CH2O 2.40E+13 0.00 0.
!(23) Tsang 87
!CH2OH+O2=HO2+CH2O 2.41E+14 0.00 5017.
!(24) Grotheer 88
! DUPLICATE
!CH2OH+O2=HO2+CH2O 1.51E+15 -1.00 0.
!(24) Grotheer 88
! DUPLICATE
!CH2OH+HO2=CH2O+H2O2 1.20E+13 0.00 0.
!(23) Tsang 87
!CH2OH+HCO=CH3OH+CO 1.20E+14 0.00 0.
!(23) Tsang 87
!CH2OH+HCO=CH2O+CH2O 1.80E+14 0.00 0.
!(23) Tsang 87
!2CH2OH=CH3OH+CH2O 3.00E+12 0.00 0.

```

```

!(23) Tsang 87
!CH2OH+CH3O=CH3OH+CH2O          2.40E+13    0.00    0.
!(23) Tsang 87
!O+CH3O=OH+CH2O                   6.00E+12    0.00    0.
!(1) TSA/HAM 86
H+CH3O=H2+CH2O                     2.00E+13    0.00    0.
!(3) Warnatz 84
H+CH3O=OH+CH3                      3.20E+13    0.00    0.
!(14) GRI-Mech 1.2
OH+CH3O=H2O+CH2O                   1.80E+13    0.00    0.
!(23) Tsang 87
!CH3O+O2=HO2+CH2O                  9.03E+13    0.00   11980.
!(26) Wantuck 87
! DUPLICATE
!CH3O+O2=HO2+CH2O                  2.20E+10    0.00   1748.
!(26) Wantuck 87
! DUPLICATE
!CH3O+HO2=CH2O+H2O2                 3.00E+11    0.00    0.
!(23) Tsang 87
CH3O+CO=CH3+CO2                     1.57E+13    0.00   11800.
!(23) Tsang 87
!CH3O+HCO=CH3OH+CO                 9.00E+13    0.00    0.
!(23) Tsang 87
!2CH3O=CH3OH+CH2O                  6.00E+13    0.00    0.
!(23) Tsang 87
!O+CH3OH=OH+CH2OH                  3.88E+05    2.50   3080.
!(23) Tsang 87
!H+CH3OH=CH2OH+H2                  1.44E+13    0.00   6095.
!(25) Held 98
!H+CH3OH=CH3O+H2                   3.60E+12    0.00   6095.
!(25) Held 98
!OH+CH3OH=CH2OH+H2O                7.10E+06    1.80   -596.
!(27) Bott 91
!OH+CH3OH=CH3O+H2O                 1.00E+06    2.10   496.5
!(27) Bott 91
!CH3+CH3OH=CH2OH+CH4               3.19E+01    3.17   7172.
!(23) Tsang 87
!O2+CH3OH=CH2OH+HO2                2.05E+13    0.00   44900.
!(23) Tsang 87
!HCO+CH3OH=CH2OH+CH2O              9.63E+03    2.90   13110.
!(23) Tsang 87
!HO2+CH3OH=CH2OH+H2O2              3.98E+13    0.00   19400.
!(28) Cathonnet 82
!CH3O+CH3OH=CH2OH+CH3OH            3.00E+11    0.00   4060.
!(23) Tsang 87
!CH3OH(+M)=CH3+OH(+M)              1.90E+16    0.00   91730.
!(25) Held 98
! LOW /2.95E+44 -7.35 95460./
! TROE /0.414 279 5459 /
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ AR/0.7/ !C2H6/3.0/
! Miller
! OH+CH3(+M)=CH3OH(+M) 4.34E15 -0.79 0.0
!BAULCH ET AL 2004
! LOW/3.85E37 -6.21 1333/
! TROE/0.25 210 1434/
! N2/1.43/ H2O/8.58/ CO2/3/ CO/2/ H2/2/

!CH3OH(+M)=CH2OH+H(+M)              2.69E+16   -0.08   98940.
!(25) Held 98
! LOW /2.34E+40 -6.33 103100.0/
! TROE /0.773 693 5333 /
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ AR/0.7/ !C2H6/3.0/
!
!-----CH4 (CHx) chemistry-----
!
O+CH4=OH+CH3                        1.02E+09    1.50   8600.

```

!(1) TSA/HAM 86				
H+CH4=CH3+H2	6.60E+08	1.62		10840.
!(22) GRI 3.0				
OH+CH4=CH3+H2O	1.00E+08	1.60		3120.
!(30) Cohen 91				
!CH+CH4=H+C2H4	6.00E+13	0.00		0.
!(31) Butler 80				
!CH2SING+CH4=2CH3	1.60E+13	0.00		-570.
!(22) GRI 3.0				
CH2+CH4=2CH3	2.46E+06	2.00		8270.
!(32) Bohland 85				
O+CH3=H+CH2O	5.06E+13	0.00		0.
!(22) GRI 3.0				
O+CH3=H+H2+CO	3.37E+13	0.00		0.
!(22) GRI 3.0				
! Used by Miller				
!CH3+O=CH2O+H	7.14E13	0.0	0.0	!Baulch 2004
!CH3+O=CO+H2+H	1.26E13	0.0	0.0	
!JAM ( 15% branching)				
H+CH3(+M)=CH4(+M)	1.39E+16	-0.53		536.
!(22) GRI 3.0				
LOW	/2.62E+33	-4.76		2440. /
TROE /0.783 74 2941 6964/				
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !AR/0.7/ !C2H6/3.0/				
OH+CH3=CH2+H2O	5.60E+07	1.60		5420.
!(22) GRI 3.0				
!OH+CH3=CH2SING+H2O	6.44E+17	-1.34		1417.
!(22) GRI 3.0				
! Miller				
! OH+CH3(+M)=CH2SING+H2O(+M)	6.4E-8	5.8		-964.
!BAULCH ET AL 2004				
! LOW/1.08E16 -0.91 546. /				
! TROE/0.336 3569. 108. 3240. /				
!OH+CH3=CH2OH+H	7.23E11	0.0		5484.
!BAULCH ET AL 2004				
!OH+CH3=CH3O+H	1.2E10	0.0		13889.
!BAULCH ET AL 2004				
!OH+CH3=CH2O+H2	3.19E9	0.0		5027.
!BAULCH ET AL 2004				
!OH+CH3(+M)=HCOH+H2(+M)	1.14E-17	8.0		-2464.
!BAULCH ET AL 2004				
! LOW/2.29E10 -0.12 -415. /				
! TROE/0.705 3704. 312. 1238. /				
!HO2+CH3=O2+CH4	1.00E+12	0.00		0.
!(33) Reid 84				
HO2+CH3=OH+CH3O	2.00E+13	0.00		0.
!(1) TSA/HAM 86				
!CH+CH3=H+C2H3	3.00E+13	0.00		0.
!(34) Miller 89				
!CH2SING+CH3=H+C2H4	1.20E+13	0.00		-570.
!(14) GRI-Mech 1.2				
!CH3+O2=O+CH3O	3.56E+13	0.00		30480.
!(22) GRI 3.0				
!CH3+O2=OH+CH2O	2.31E+12	0.00		20315.
!(22) GRI 3.0				
! Miller				
!CH3+O2=CH3O+O	6.08E7	1.54		27957.
!Herbon,etal (30th Symp)				
!CH3+O2=CH2O+OH	68.6	2.86		9474.
!Herbon,etal (30th Symp)				
!CH3+H2O2=HO2+CH4	2.45E+04	2.47		5180.
!(22) GRI 3.0				
!2CH3(+M)=C2H6(+M)	6.77E+16	-1.18		654.

```

!(22) GRI 3.0
! LOW /3.40E+41 -7.03 2763./
! TROE /0.619 73.2 1180 9999/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Below from Miller
! CH3+CH3(+M)=C2H6(+M) 9.22E16 -1.174 635.8
!PILL,WAG 23RD
! LOW/1.135E36 -5.246 1704.8/
! TROE/0.405 1120. 69.6/
! H2/2/ CO/2/ CO2/3/ H2O/5/

!2CH3=H+C2H5 6.84E+12 0.10 10600.
!(22) GRI 3.0
! Miller
! C2H5+H=CH3+CH3 3.47E13 0.205 -41.38
!SJK theory*0.9(recrossing)

CH3+HCO=CH4+CO 1.21E+14 0.00 0.
!(1) TSA/HAM 86
CH3+CH2O=HCO+CH4 3.32E+03 2.81 5860.
!(22) GRI 3.0
! Miller
! CH2O+CH3=HCO+CH4 7.8E-8 6.1 1967.
!CEC 1994

!CH2+CH3=H+C2H4 4.00E+13 0.00 0.
!(3) Warnatz 84
O+CH2=H+HCO 8.00E+13 0.00 0.
!(35) Herron 88
!O+CH2SING=H2+CO 1.50E+13 0.00 0.
!(1) TSA/HAM 86
!O+CH2SING=H+HCO 1.50E+13 0.00 0.
!(1) TSA/HAM 86
!H+CH2(+M)=CH3(+M) 6.00E+14 0.00 0.
!(22) GRI 3.0
! LOW /1.04E+26 -2.76 1600./
! TROE /0.562 91 5836 8552/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!H+CH2SING=CH+H2 3.00E+13 0.00 0.
!(1) TSA/HAM 86
OH+CH2=H+CH2O 2.00E+13 0.00 0.
!(1) TSA/HAM 86
!OH+CH2=CH+H2O 1.13E+07 2.00 3000.
!(1) TSA/HAM 86
!OH+CH2SING=H+CH2O 3.00E+13 0.00 0.
!(1) TSA/HAM 86
!HO2+CH2=OH+CH2O 2.00E+13 0.00 0.
!(1) TSA/HAM 86
!CH+CH2=H+C2H2 4.00E+13 0.00 0.
!(36) Braun 81
!CH2+O2=OH+H+CO 5.00E+12 0.00 1500.
!(37) Vinckier 79
!CH2+O2=CO2+2H 5.80E+12 0.00 1500.
!(37) Vinckier 79
!CH2+O2=O+CH2O 2.40E+12 0.00 1500.
!(37) Vinckier 79
CH2+H2=H+CH3 5.00E+05 2.00 7230.
!(22) GRI 3.0
!2CH2=H2+C2H2 1.60E+15 0.00 11944.
!(38) Bauerle 95
!2CH2=H+H+C2H2 2.00E+14 0.00 10989.
!(38) Bauerle 95
!CH2SING+CO=CH2+CO 9.00E+12 0.00 0.
!(22) GRI 3.0
!CH2SING+AR=CH2+AR 9.00E+12 0.00 600.
!(22) GRI 3.0

```

!CH2SING+CO2=CH2+CO2	7.00E+12	0.00	0.
!(39) Koch 90			
!CH2SING+CO2=CO+CH2O	1.40E+13	0.00	0.
!(39) Koch 90			
!CH2+CO(+M)=CH2CO(+M)	8.10E+11	0.50	4510.
!(22) GRI 3.0			
! LOW	/2.69E+33	-5.11	7095./
! TROE /0.5907 275 1226 5185/			
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.00/			
!CH2SING+O2=H+OH+CO	2.80E+13	0.00	0.
!(40) Langford 83			
!CH2SING+O2=CO+H2O	1.20E+13	0.00	0.
!(40) Langford 83			
!CH2SING+H2=CH3+H	7.00E+13	0.00	0.
!(22) GRI 3.0			
!CH2SING+H2O(+M)=CH3OH(+M)	4.82E+17	-1.16	1145.
!(22) GRI 3.0			
! LOW	/1.88E+38	-6.36	5040./
! TROE /0.6027 208 3922 10180/			
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ !C2H6/3.0/			
!CH2SING+H2O=CH2+H2O	3.00E+13	0.00	0.
!(41) Hack 88			
!CH2SING+H2O=H2+CH2O	6.82E+10	0.25	-935.
!(22) GRI 3.0			
!O+CH=H+CO	5.70E+13	0.00	0.
!(42) MESSING 80			
!OH+CH=H+HCO	3.00E+13	0.00	0.
!(43) Glarborg 86			
!CH+O2=O+HCO	6.71E+13	0.00	0.
!(22) GRI 3.0			
!CH+H2=H+CH2	1.08E+14	0.00	3110.
!(22) GRI 3.0			
!CH+H2O=H+CH2O	5.71E+12	0.00	-755.
!(10) Baulch 94			
!CH+CO(+M)=HCCO(+M)	5.00E+13	0.00	0.
!(14) GRI-Mech 1.2			
! LOW	/2.69E+28	-3.74	1936./
! TROE /0.5757 237 1652 5069/			
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/			
!CH+CO2=HCO+CO	1.90E+14	0.00	15792.
!(44) Markus 96			
!CH+CH2O=H+CH2CO	9.46E+13	0.00	-515.
!(45) Baulch 92			
!CH+HCCO=CO+C2H2	5.00E+13	0.00	0.
!(34) Miller 89			
!			
!-----C2H6 chemistry-----			
!			
!O+C2H6=OH+C2H5	3.00E+07	2.00	5115.
!(46) Miller 92			
!H+C2H6=C2H5+H2	5.40E+02	3.50	5210.
!(46) Miller 92			
!OH+C2H6=C2H5+H2O	7.26E+06	2.00	864.
!(45) Baulch 92			
!CH3+C2H6=C2H5+CH4	5.50E-01	4.00	8300.
!(46) Miller 92			
!CH2SING+C2H6=CH3+C2H5	4.00E+13	0.00	-550.
!(47) Wegener 90			
!C2H6+O2=C2H5+HO2	4.04E+13	0.00	50872.
!(1) TSA/HAM 86			
!C2H6+CH2OH=CH3OH+C2H5	1.99E+02	3.00	13976.
!(23) Tsang 87			
!C2H6+CH3O=CH3OH+C2H5	2.41E+11	0.00	7094.
!(1) TSA/HAM 86			
!C2H6+C2H=C2H2+C2H5	3.61E+12	0.00	0.
!(1) TSA/HAM 86			

```

!C2H6+C2H3=C2H4+C2H5          6.01E+02   3.30   10502.
!(1) TSA/HAM 86
!C2H6+CH3CO=CH3CHO+C2H5       1.81E+4    2.75   17527.
!(1) TSA/HAM 86
!C2H6+HCO=CH2O+C2H5           4.70E+04   2.72   18235.
!(1) TSA/HAM 86
!
!-----C2H5 chemistry-----
!
!O+C2H5=CH3+CH2O               2.24E+13   0.00    0.
!(22) GRI 3.0
! Miller
! C2H5+O=CH3+CH2O              4.2E13    0.0    0.0 !JAM&PG rbn (Slagle 1988)

!O+C2H5=H+CH3CHO               1.10E+14   0.00    0.
!(22) GRI 3.0
!H+C2H5=H2+C2H4               2.00E+12   0.00    0.
!(22) GRI 3.0
!H+C2H5(+M)=C2H6(+M)          5.21E+17  -0.99   1580.
!(22) GRI 3.0
! LOW /1.99E+41 -7.080 6685./
! TROE /0.8422 125 2219 6882/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!C2H5+O2=HO2+C2H4             1.92E+07   1.02  -2035.
!(48) Miller 00
! Miller
! C2H5+O2(+M)= C2H4+HO2(+M) 1.41E7 1.09 -1975.
! HIGH/6.85E-12 6.53 -834./
! TROE/0.45 1.E-10 1.E10/
! H2/2/ CO/2/ CO2/3/ H2O/5/
!not sure what this does
! C2H5+O2=C2H4+HO2            5.81E6    1.57  20578.
!Miller&Klipp 28th(abs)

!C2H5+HO2=C2H5O+OH            3.00E+13   0.00    0.
!(49) Bozzelli 90
!C2H5+HO2=C2H4+H2O2           3.01E+11   0.00    0.
!(1) TSA/HAM 86
!C2H5+OH=C2H4+H2O             2.41E+13   0.00    0.
!(1) TSA/HAM 86
!C2H5+CH3=CH4+C2H4            1.13E+12  -0.50    0.
!(1) TSA/HAM 86
!CH3+C2H5(+M)=C3H8(+M)        9.60E+14  -0.50    0.
!(50) Qin/Wan 00
! LOW /6.80E+61 -13.42 6000./
! TROE /1.00 1000 1433.9 5328.8/
!C2H5+CH2OH=C2H4+CH3OH        2.41E+12   0.00    0.
!(23) Tsang 87
!C2H5+CH2OH=C2H6+CH2O         2.41E+12   0.00    0.
!(23) Tsang 87
!C2H5+CH3O=C2H6+CH2O         2.41E+13   0.00    0.
!(1) TSA/HAM 86
!C2H5+C2H=C2H2+C2H4           1.81E+12   0.00    0.
!(1) TSA/HAM 86
!CH2+C2H5=C2H4+CH3            1.81E+13   0.00    0.
!(1) TSA/HAM 86
!CH2SING+C2H5=C2H4+CH3        9.00E+12   0.00    0.
!(1) TSA/HAM 86
!C2H5+CH2SING=C3H6+H          9.00E+12   0.00    0.
!(1) TSA/HAM 86
!C2H5+H2O2=C2H6+HO2           8.73E+09   0.00   974.
!(1) TSA/HAM 86
!
!-----C2H4 chemistry-----

```



```

!
!H+C2H4 (+M)=C2H5 (+M)                5.40E+11  0.45    1820.
!(22) GRI 3.0
!  LOW                                /6.00E+41  -7.62    6970./
!  TROE /0.9753 210 984 4374/
!  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
!H+C2H4 (+M)=C2H5 (+M)                1.367E9   1.463  1355.
!Miller&Klipp.
!  LOW/2.026E39 -6.642  5769./
!TROE/-0.569 299. -9147. 152.4/
!  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!  N2/1.2/ CO/1.5/ H2/2/ CO2/3/ H2O/10./

!H+C2H4=C2H3+H2                        1.12E+07  2.12    13366.
!(51) Bhargava 98
!OH+C2H4=C2H3+H2O                      5.53E+05  2.31    2900.
!(51) Bhargava 98
!OH+C2H4=C2H3+H2O                      1.31E-01  4.20   -860
!JPCA 110 6960-6970 (2006)
!OH+C2H4=CH3+CH2O                      3.19E+01  2.71  -1172.
!JPCA 110 6960-6970 (2006)
!OH+C2H4=CH3CHO+H                      8.73E-05  4.57   -618.
!JPCA 110 6960-6970 (2006)
! Miller OH+C2H4=H2O+C2H3  1.31E-01  4.20   -860
!JPCA 110 6960-6970 (2006)
! OH+C2H4=CH3+CH2O  5.35E+00  2.92  -1733
!JPCA 110 6960-6970 (2006)
! this reaction is in line 792-798
! 0  1.60E-01  3.34  -2776
! PLOG /0.01  5.35E+00  2.92  -1733./
! PLOG /0.025  3.19E+01  2.71  -1172./
! PLOG /0.1  5.55E+02  2.36  -181./
! PLOG /1.  1.78E+05  1.68  2061./
! PLOG /10.  2.37E+09  0.56  6007./
! PLOG /100.  2.76E+13  -0.50  11455./
! OH+C2H4=CH3CHO+H  2.37E-07  5.30  -2051
!JPCA 110 6960-6970 (2006)
! this reaction is in line 799-805
! 0  8.91E-09  5.69  -3209
! PLOG /0.01  2.37E-07  5.30  -2051./
! PLOG /0.025  8.73E-05  4.57  -618./
! PLOG /0.1  4.03E-01  3.54  1882./
! PLOG /1.  2.38E-02  3.91  1723./
! PLOG /10.  8.25E+08  1.01  10507./
! PLOG /100.  6.80E+09  0.81  13867./

!CH3+C2H4=C2H3+CH4                    2.27E+05  2.00    9200.
!(22) GRI 3.0
!CH3+C2H4 (+M)<=>nC3H7 (+M)            2.55E+06  1.600   5700.
!(52) Tsang 88
!  LOW                                /3.00E+63  -14.6   18170./
!  TROE /0.1894 277. 8748. 7891./
!  H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
!C2H4 (+M)=H2+C2H2 (+M)                8.00E+12  0.44   88770.
!(22) GRI 3.0
!  LOW                                /1.58E+51  -9.30   97800./
!  TROE /0.7345 180 1035 5417/
!  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! C2H4+CH2SING=C3H6                    9.03E+13  0.00    0.
!(1) TSA/HAM 86
!C2H4+CH2SING=AC3H5+H                  4.53E+13  0.00   -556.
!Baulch 2004
! Miller CH2SING+C2H4=CH2CHCH2+H        4.53E13  0.0   -556.
!Baulch 2004
!C2H4+HO2=C2H4O+OH                    6.03E+09  0.00   7949.

```

```

!(1) TSA/HAM 86
!C2H4+O=H+CH2CHO          7.33E+07   1.60   1260.
!(53) Westmoreland PC
!C2H4+O=CH3+HCO          1.13E+08   1.60   1020.
!(53) Westmoreland PC
! Miller
! C2H4+O=CH3+HCO          8.16E6     1.88   182.8
!BAULCH 2004 similar to CEC 94

!C2H4+O=C2H3+OH          2.15E+06   2.55   11900.
!(53) Westmoreland PC
!C2H4+O2=C2H3+HO2        4.22E+13   0.00   60800.
!(54) Wang 97
! Miller
! C2H4+O2=CH2HCO+OH      2.0E8     1.5    39000
!JAM /SWB 1996

!C2H4+CO=C2H3+HCO        1.51E+14   0.00   90616.
!(1) TSA/HAM 86
!C2H4+C2H=C4H4+H         1.21E+13   0.00    0.
!(1) TSA/HAM 86
!C2H4+C2H2=C2H3+C2H3     2.41E+13   0.00   68360.
!(1) TSA/HAM 86
!C2H4+C2H4=C2H5+C2H3     4.82E+14   0.00   71539.
!(1) TSA/HAM 86
!
!-----C2H3 chemistry-----
!
!H+C2H3 (+M)=C2H4 (+M)    6.08E+12   0.27    280.
!(22) GRI 3.0
! LOW /1.40E+30   -3.86   3320./
! TROE /0.782 207.5 2663 6095/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! C2H3 (+M)=C2H2+H (+M)   3.86E+08   1.62   37058.
!(55) Knyazev 96
! LOW /2.56E27   -3.40   35789.7/
! TROE /0.2134 36.643 7794.56 4007.66/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
!H+C2H2 (+M)=C2H3 (+M)   1.713E10   1.266   2709.
!Miller & Klipp.
! LOW/6.348E31   -4.6639 3780./
! TROE/ 0,78784 -1.021E4 1.0E-30 /
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! N2/1.2/ CO/1.5/ H2/2/ CO2/3/ H2O/10./

!H+C2H3=H2+C2H2          9.64E+13   0.00    0.
!(1) TSA/HAM 86
!OH+C2H3=H2O+C2H2        5.00E+12   0.00    0.
!(56) Lutz 88
!C2H3+O2=C2H2+HO2        1.34E+06   1.61   -383.
!(58) Mebel96
! DUPLICATE
!C2H3+O2=C2H2+HO2        1.37E+02   3.37   3663.
!(53) Westmoreland PC
! DUPLICATE
! C2H3+O2=HCO+CH2O        1.57E+08   1.32   -1953.9
!(15) Carriere 04 20Torr
! C2H3+O2=C2H3O           5.61E+19   -3.30   165.4
!(15) Carriere 04 20Torr
! C2H3+O2=O+CH2CHO        1.31E+01   3.55   2311.5
!(15) Carriere 04 20Torr
! Miller
!C2H3+O2=HCO+CH2O        9.33E13   -0.653  268.7
!Klipp.& Miller

```

!C2H3+O2=H+CO+CH2O	2.19E14	-0.653	268.7	
!Klipp. & Miller				
!C2H3+O2=CH2CHO+O	7.52E8	0.965	-137.4	
!Klipp.& Miller				
!C2H3+O2=CH2HCO+O	7.52E8	0.965	-137.4	
!Klipp.& Miller				
!C2H3+HO2=OH+CH2CO+H	3.01E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH3=C2H2+CH4	3.92E+11	0.00	0.	
!(1) TSA/HAM 86				
! C2H3+O=CH2CO+H	3.00E+13	0.00	0.	
!(57) Heinemann 86				
! Miller				
!C2H3+O=CH2CO+H	1.0E14	0.0	0.0	
!Harding&Klippenstein 2003				
!C2H3OO+H=CH2CHO+OH	1.00E+14	0.00	0.	
!(15) Carriere 04 20Torr				
!C2H3OO+CH2=CH2CHO+CH2O	2.00E+13	0.00	0.	
!(15) Carriere 04 20Torr				
!C2H3OO+OH=CH2CHO+HO2	2.00E+13	0.00	0.	
!(15) Carriere 04 20Torr				
!C2H3OO+O=CH2CHO+O2	2.00E+13	0.00	0.	
!(15) Carriere 04 20Torr				
!C2H3+CH2OH=C2H4+CH2O	3.01E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH3O=C2H4+CH2O	2.41E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH3OH=C2H4+CH3O	1.44E+01	3.10	6935.	
!(1) TSA/HAM 86				
!C2H3+CH3OH=C2H4+CH2OH	3.19E+01	3.20	7172.	
!(1) TSA/HAM 86				
!C2H3+CO=C2H3CO	1.51E+11	0.00	4809.	
!(1) TSA/HAM 86				
!C2H3+C2H=C4H4	1.00E+14	0.00	0.	
!(59) Duran 88				
!C2H3+C2H=C2H2+C2H2	9.64E+11	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH3CO=C2H3CO+CH3	1.81E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H5+C2H3=AC3H5+CH3	8.00E+25	-3.46	11775.	
!(1) TSA/HAM 86 0.1 atm				
!C2H3+C2H5 (+M)=IC4H8 (+M)	1.50E+13	0.00	0.	
!(60) Wang/Laskin 99				
! LOW	/1.55E+56	-11.79	8984.5/	
! TROE /0.198 2277.9 60000 5723.2/				
!C2H3+C2H5=C2H2+C2H6	4.82E+11	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH2SING=C2H2+CH3	1.81E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+CH2=C2H2+CH3	1.81E+13	0.00	0.	
!(1) TSA/HAM 86				
!C2H3+H2O2=C2H4+HO2	1.21E+10	0.00	-596.	
!(1) TSA/HAM 86				
!C2H3+CH2O=C2H4+HCO	5.43E+03	2.81	5862.	
!(1) TSA/HAM 86				
!C2H3+CH2=AC3H4+H	3.00E+13	0.00	0.	
!(61) Pauwels 95				
!C2H3+C2H3=i-C4H5+H	1.50E+30	-4.95	13000.	
!(54) Wang 97 20Torr				
!C2H3+C2H3=n-C4H5+H	1.10E+24	-3.28	12400.	
!(54) Wang 97 20Torr				
!				
!-----C2H2 chemistry-----				

```

!
!-----H2CC chemistry-----
!H2CC+C2H2 (+M)=C4H4 (+M)          3.50E+05    2.055  -2400.    !(141) Laskin/Wang 00
!  LOW                               /1.40E+60  -12.599  7417./
!  TROE /0.98 56.0 580.0 4164.0/
!  H2/2.0/ CH4/2.0/ H2O/6.0/ C2H2/3.0/ CO/1.5/ C2H4/3.0/ C2H6/3.0/ CO2/2.0/
!H2CC=C2H2                          1.0E7      0.00     0.        !JAM(10/02) Miller Est
!  USC_II
!C2H2 (+M)=H2CC (+M)                8.000E+14  -0.520  50750.00 !99LAS/WAN
!  LOW / 2.450E+15  -0.640  49700.00 /
!  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/C2H2/2.5/ C2H4/2.5/

!H2CC+C2H4=iiiC4H6                 1.0E12     0.00     0.        !(141) Laskin/Wang 00
!H2CC+O2=CH2+CO2                   1.00E+13   0.00     0.        !(141) Laskin/Wang 00
!H2CC+H=C2H2+H                      1.00E+14   0.00     0.        !(141) Laskin/Wang 00
!H2CC+OH=CH2CO+H                   2.00E+13   0.00     0.        !(141) Laskin/Wang 00
!-----
!
!O+C2H2=H+HCCO                      1.35E+07    2.00     1900.
!(22) GRI 3.0
!O+C2H2=CO+CH2                      6.94E+06    2.00     1900.
!(22) GRI 3.0
!O+C2H2=OH+C2H                      4.60E+19   -1.41    28950.
!(22) GRI 3.0
!Replaced by USC II as below
!C2H2+O=C2H+OH                      4.600E+19  -1.410  28950.00 !GRI
!C2H2+O=CH2+CO                      4.080E+06   2.000   1900.00 !GRI (0.2 branching
ratio)
!C2H2+O=HCCO+H                      1.632E+07   2.000   1900.00 !GRI (0.8 branching
ratio)
!O+C2H2=H+HCCO                      5.79E+06    2.09     1560.0
!Lindstedt 97
!O+C2H2=CO+CH2                      1.45E+06    2.09     1560.0
!Lindstedt 97
!O+C2H2=OH+C2H                      3.16E+15   -0.60    15000.
!MMSK
!C2H2+O=CH2+CO                      4.08E6      2.000   1900.000
!JAM, FONT, PEETERS
!C2H2+O=HCCO+H                      1.632E7     2.000   1900.000
!JAM, FONT, PEETERS
!C2H2+O=C2H+OH                      0.316E+16  -0.600  15000.000 !MMSK
!C2H2+O=CH2+CO                      2.350E+08   1.4     2204.50 !(0.2 branching ratio)
2005 Baulch Evaluation
!C2H2+O=HCCO+H                      9.400E+08   1.4     2204.50 !(0.8 branching ratio)
2005 Baulch Evaluation

!OH+C2H2=C2H+H2O                   3.37E+07    2.00     14000.
!(62) Miller 86
!OH+C2H2=H+CH2CO                   2.18E-04    4.50    -1000.
!(62) Miller 86
!OH+C2H2=CH3+CO                     4.83E-04    4.00    -2000.
!(62) Miller 86
!OH+C2H2=C2H+H2O                   2.63E6      2.14    17060. !SENOSIAIN, KLIPP., &
MILLER 2005
!OH+C2H2=H+CH2CO                   1.52E4      2.28    -292.
!SENOSIAIN, KLIPP., & MILLER 2005
!OH+C2H2=CH3+CO                     4.37E6      1.40     227.
!SENOSIAIN, KLIPP., & MILLER 2005
! Miller

```

```

! OH+C2H2=C2H+H2O          2.63E6    2.14   17060. !SENOSIAIN,KLIPP., & MILLER 2005
! OH+C2H2=HCCOH+H          2.77E5    2.28    12419.
!SENOSIAIN,KLIPP., & MILLER 2005
! PLOG /.01                2.77E5    2.28    12419./
! PLOG /.025               7.47E5    2.16    12547./
! PLOG /.1                  1.78E6    2.04    12669./
! PLOG / 1.0               2.415E6   2.0     12713./
! PLOG / 10.               3.21E6    1.97    12810./
! PLOG / 100.             7.35E6    1.89    13603./
! OH+C2H2=CH2CO+H         1.578E3    2.56    -844.
!SENOSIAIN,KLIPP., & MILLER 2005
! PLOG /.01                1.578E3    2.56    -844./
! PLOG /.025               1.52E4    2.28    -292. /
! PLOG / 0.1               3.02E5    1.92    598. /
! PLOG / 1.0               7.53E6    1.55    2106. /
! PLOG / 10.0              5.10E6    1.65    3400. /
! PLOG / 100.              1.46E4    2.45    4477. /
! OH+C2H2=CH3+CO          4.76E5    1.68    -330.
!SENOSIAIN,KLIPP., & MILLER 2005
! PLOG /.01                4.76E5    1.68    -330./
! PLOG /.025               4.37E6    1.40    227. /
! PLOG / 0.1               7.65E7    1.05    1115. /
! PLOG / 1.0               1.28E9    0.73    2579. /
! PLOG / 10.0              4.31E8    0.92    3736. /
! PLOG / 100.              8.25E5    1.77    4697. /
! OH+C2H2=C2H2OH          2.87E64   -18.57  10009
!SENOSIAIN,KLIPP., & MILLER 2005
! PLOG /.01                2.87E64   -18.57  10009. /
! PLOG /.01                2.64E33   -7.36   6392. /
! PLOG /.025               4.69E59  -16.87  9087. /
! PLOG /.025               4.38E32   -7.02   5933. /
! PLOG / 0.1               1.24E28   -5.56   3724. /
! PLOG / 0.1               6.38E42   -9.96  11737. /
! PLOG / 1.0               1.90E44  -11.38  6299. /
! PLOG / 1.0               3.49E31   -6.20   6635. /
! PLOG / 10.0              1.49E24   -4.06   3261. /
! PLOG / 10.0              4.51E31   -5.92   8761. /
! PLOG / 100.              6.20E20   -2.80   2831. /
! PLOG / 100.              1.60E29   -4.91   9734. /

!C2H2+CH=C3H2+H          1.10E+13   0.00    0.
!(63) Warnatz 82
!C2H2+CH2=C3H3+H          1.20E+13   0.000   6620.
!(64) Bohland 88
!C2H2+CH3=C2H+CH4          1.81E+11   0.00    17289.
!(1) TSA/HAM 86
!C2H2+O2=2HCO             1.00E+12   0.00    28000.
!(65) Hidaka 96
!C2H2+CH2OH=C2H3+CH2O     7.23E+11   0.00    9004.
!(23) Tsang 87
!C2H2+CO=C2H+HCO          4.82E+14   0.00    106713.
!(1) TSA/HAM 86
!C2H2+C2H=C4H2+H          3.00E+13   0.00    0.
!(10) Baulch94 uncertainty 3.16
!C2H2+C2H(+M)=nC4H3(+M)    8.30E+10   0.90    -363.
!(60) Wang/Laskin 99
! LOW                      /1.24E+31  -4.72   1871./
! TROE /1.0 100. 5613. 13387./
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
!C2H2+C2H(+M)=iC4H3(+M)    8.30E+10   0.90    -363.0
!(60) Wang/Laskin 99
! LOW                      /1.24E+31  -4.72   1871./
! TROE /1.0 100. 5613. 13387./
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
!C2H2+CH2SING=C3H3+H      3.42E15   -0.624  -230.7

```

```

!(66) Hansen/Miller 08
!C2H2+CH2SING=CH2+C2H2          8.55E14   -0.624   -230.7
!(66) Hansen/Miller 08
!HCCO+C2H2=C3H3+CO              1.00E+11    0.00    3000.
!(46) Miller 92
!C2H2+C2H3=n-C4H5                1.10E+32   -7.33    6200.
!(54) Wang 97 20Torr
!C2H2+C2H3=i-C4H5                2.10E+36   -8.78    9100.
!(54) Wang 97 20Torr
!C2H3+C2H2=C4H4+H                5.00E+14   -0.71    6700.
!(54) Wang 97 20Torr
!Miller These are fits from JAM&SJK 2002 30 Torr
!C2H3+C2H2=CH2CHCHCH   1.01E51   -12.778  15608.
!C2H3+C2H2=CH2CHCCH+H  1.54E16   -1.069   9566.
!
!-----C2H chemistry-----
!
!O+C2H=CH+CO                    1.00E+13    0.00    0.
!(3) Warnatz84
!H+C2H(+M)=C2H2(+M)            1.000E+17  -1.00    0.
!(22) GRI3.0
! LOW /3.750E+33 -4.80 1900./
! TROE /0.6464 132 1315 5566/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! Miller
! C2H2+M=C2H+H+M                9.08E30   -3.7  127138. !TSANG&HAMP (TAN&GARD)
! H2/2/ CO/2/ CO2/3/ H2O/5/
!OH+C2H=H+HCCO                  2.00E+13    0.00    0.
!(67) Frenklach 92
!C2H+O2=HCO+CO                  1.00E+13    0.00   -775.
!(22) GRI 3.0
!C2H+H2=H+C2H2                  5.68E+10    0.90   1993.
!(68) Farhat 93
! Miller
! H2+C2H=C2H2+H                  0.409E+06  2.390   864.300
!HARDING, SHATZ, CHILE

!C2H+HO2=HCCO+OH                1.81E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+CH3=C3H3+H                  2.41E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+O2=HCCO+O                   6.03E+11    0.00    0.
!(1) TSA/HAM 86
!C2H+CH2OH=C2H2+CH2O             3.61E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+CH2OH=C3H3+OH               1.21E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+CH3OH=C2H2+CH2OH            6.03E+12    0.00    0.
!(1) TSA/HAM 86
!C2H+CH3O=CH2O+C2H2              2.41E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+CH3OH=C2H2+CH3O             1.21E+12    0.00    0.
!(23) Tsang 87
!C2H+CH2=CH+C2H2                 1.81E+13    0.00    0.
!(1) TSA/HAM 86
!C2H+CH2SING=C2H2+CH             1.81E+13    0.00    0.
!(1) TSA/HAM 86
!
!-----C2HxOy chemistry-----
!
!O+HCCO=H+2CO                    1.00E+14    0.00    0.
!(69) Frank 88
!H+HCCO=CH2SING+CO              5.00E13    0.00    0.
!(3) Warnatz 84
!CH2+HCCO=C2H3+CO               3.00E+13    0.00    0.
!(62) Miller86

```

```

!HCCO+O2=CO2+CO+H          4.78E+12  -0.142  1150.
!(70) Klippenstain 02
!HCCO+O2=CO+CO+OH          1.91E+11  -0.02  1023.
!(70) Klippenstain 02
!HCCO+O2=O+CO+HCO          2.18E2    2.69  3541.
!(70) Klippenstain 02
! Miller
! HCCO+O2=CO2+CO+H          4.78E12  -0.142  1150.
!Klipp&JAM 29th
! HCCO+O2=CO +CO +OH        1.91E11  -0.02  1023.
! HCCO+O2=O+CO+HCO          2.18E2    2.69  3541.

!2HCCO=2CO+C2H2            1.00E+13  0.00  0.
!(34) Miller 89
!HCCO+CH3=C2H4+CO          5.00E+13  0.00  0.
!(54) Wang 97
!O+CH2CO=OH+HCCO           1.00E+13  0.00  8000.
!(34) Miller 89
!O+CH2CO=CH2+CO2           1.75E+12  0.00  1350.
!(71) Cvetanovic 87
!H+CH2CO=HCCO+H2           5.00E+13  0.00  8000.
!(34) Miller 89
! H+CH2CO=CH3+CO           3.28E+10  0.85  2839.
!(72) Hranislavljevic 98
! Miller
!CH2CO+H=CH3+CO            7.77E8    1.45  2780.
!SENOSIAN, KLIPP., & MILLER 2005

!H+CH2CO(+M)=CH2CHO(+M)     4.86E+11  0.42  -1755.
!(22) GRI 3.0
! LOW                        /1.01E+42  -7.63  3854./
! TROE /0.465 201 1773 5333.0/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!CH2CHO=H+CH2CO            2.48E+27  -5.23  44304.
!JPCA 110 5772 (2006)
!CH2CHO=CH3+CO              1.54E+31  -6.27  42478.
!JPCA 110 5772 (2006)
! Miller
! CH2HCO=H+CH2CO            2.39E+25  -4.8  43424.
!JPCA 110 5772 (2006)
! PLOG /0.01 2.39E+25 -4.80 43424./
! PLOG /0.025 2.48E+27 -5.23 44304./
! PLOG /0.1 2.37E+30 -5.86 46114./
! PLOG /1. 1.32E+34 -6.57 49454./
! PLOG /10. 3.46E+36 -6.92 52979./
! PLOG /100. 1.18E+36 -6.48 55171./
!
!inf 1.43E+15 -0.15 45606
! CH2HCO=CH3+CO            1.16E+30  -6.07  41332.
!JPCA 110 5772 (2006)
! this reaction is in line 976-977
! PLOG /0.01 1.16E+30 -6.07 41332./
! PLOG /0.025 1.54E+31 -6.27 42478./
! PLOG /0.1 6.37E+32 -6.57 44282./
! PLOG /1. 6.51E+34 -6.87 47191./
! PLOG /10. 2.15E+35 -6.76 49548./
! PLOG /100. 2.23E+33 -5.97 50448./
!
!inf 2.93E+12 0.29 40326.

!OH+CH2CO=HCCO+H2O          7.50E+12  0.00  2000.
!(34) Miller 89
!CH2CO+OH=CH2OH+CO          1.00E+13  0.00  0.
!(45) Baulch 92
!CH3CO+M=CH3+CO+M           8.74E+42  -8.62  22410.

```

```

!(1) TSA/HAM 86
!CH3CO=CH3+CO                2.40E+15   -2.00   14805.
!JPCA 110 5772 (2006)
! Miller
! CH3CO=CH3+CO                6.88E+14   -1.97   14585.
!JPCA 110 5772 (2006)
! PLOG /0.01    6.88E+14   -1.97   14585./
! PLOG /0.025  2.40E+15   -2.00   14805./
! PLOG /0.1    1.96E+16   -2.09   15197./
! PLOG /1.     6.45E+18   -2.52   16436./
! PLOG /10.    8.18E+19   -2.55   17263./
! PLOG /100.   1.26E+20   -2.32   18012./

!inf          1.07E+12    0.63   16895.

!CH2CHO+H=CH3CHO                6.40E35   -7.60    5215.
!(73) Hennessy 94
!CH2CHO+H=CH3+HCO              4.99E14   -0.32    912.
!(73) Hennessy 94
!CH2CHO+O=CH2O+HCO            5.00E13    0.00     0.
!(73) Hennessy 94
!CH2CHO+OH=H2O+CH2CO          1.20E+13    0.00     0.
!(22) GRI 3.0
!CH2CHO+OH=HCO+CH2OH          3.01E+13    0.00     0.
!(22) GRI 3.0
!CH2CHO+O2=CH2CO+HO2          1.57E11    0.00     0.
!(45) Baulch 92
!CH3CHO=CH3+HCO              9.59E+14    0.00   74180.
!(74) Dagaut 95
!CH3CHO+O2=CH3CO+HO2          2.00E+13    0.50   42200.
!(10) Baulch 94
!CH3CHO+H=CH2CHO+H2           4.10E+09    1.16    2405.
!(10) Baulch 94
!CH3CHO+OH=CH3CO+H2O          2.35E+10    0.73  -1113.
!(10) Baulch 94
!CH3CHO+O=CH2CHO+OH           5.85E+12    0.00    1808.
!(10) Baulch 94
!CH3CHO+HO2=CH3CO+H2O2        1.70E+12    0.00  10700.
!(75) Colket 77
!CH3CHO+CH3=CH3CO+CH4         1.70E+12    0.00    8440.
!(76) Wilk 89
!CH3CHO+HCO=CH3CO+CH2O        7.80E+13    0.00    8440.
!(74) Dagaut 95
! C2H5+O2=C2H5OO              2.24E+10    0.77   -568.
!(77) Wagner 90
! Miller
! C2H5+O2(+M)=C2H5OO(+M)      2.02E10  0.98  -63.6
!Miller&Klipp IJCK 33,654 (2001)
! LOW/8.49E29 -4.29 220./
!TROE/0.103 601. 1.0E-10/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! H2/2/ CO/2/ CO2/3/ H2O/5/
! C2H5OO(+M)=C2H4+HO2(+M)      7.14E4  2.32 27955.
! LOW/8.31E21 -0.651 22890./
! TROE/0.0 106. 106./
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
! H2/2/ CO/2/ CO2/3/ H2O/5/

!C2H5OO+HO2=C2H5O+OH+O2        1.75E+10    0.00  -3275.
!(78) Fischer 00
!C2H5O=CH3+CH2O               1.00E+15    0.00  21523.
!(79) Heicklen 88
!C2H5O=CH3CHO+H               2.00E+14    0.00  23215.
!(79) Heicklen 88
!C2H5O+O2=CH3CHO+HO2          6.03E+10    0.00   1643.
!(45) Baulch 92

```



!C2H4O+O2=CH2CHO+HO2	4.00E+13	0.00	61500.
!(80) Dagaut 96			
!C2H4O+H=CH2CHO+H2	2.00E13	0.00	8300.
!(81) Lifshitz 83			
!C2H4O+H=C2H3+H2O	5.00E+09	0.00	5000.
!(81) Lifshitz 83			
!C2H4O+H=C2H4+OH	9.51E+10	0.00	5000.
!(81) Lifshitz 83			
!C2H4O+OH=CH2CHO+H2O	4.79E+13	0.00	5955.
!(76) Wilk 89			
!C2H4O+O=CH2CHO+OH	1.91E+12	0.00	5250.
!(82) Bogan 78			
!C2H4O+HO2=CH2CHO+H2O2	4.00E+12	0.00	17000.
!(80) Dagaut 96			
!C2H4O=CH3CHO	6.00E+13	0.00	57167.
!(80) Dagaut 96			
!C2H4O=CH3+HCO	4.90E+13	0.00	57167.
!(80) Dagaut 96			
!C2H4O=CH4+CO	1.21E+13	0.00	57167.
!(80) Dagaut 96			
!			
!-----C3H8 chemistry-----			
!			
!C3H8+H=nC3H7+H2	1.30E+06	2.54	6756.
!(52) Tsang 88			
!C3H8+H=iC3H7+H2	1.30E+06	2.40	4471.
!(52) Tsang 88			
!C3H8+O=nC3H7+OH	1.90E+05	2.68	3716.
!(52) Tsang 88			
!C3H8+O=iC3H7+OH	4.76E+04	2.71	2106.
!(52) Tsang 88			
!C3H8+OH=iC3H7+H2O	1.40E+03	2.80	-310.
!(52) Tsang 88			
!C3H8+OH=nC3H7+H2O	1.37E+03	2.70	580.
!(52) Tsang 88			
!C3H8+O2=nC3H7+HO2	3.97E+13	0.00	50872.
!(52) Tsang 88			
!C3H8+O2=iC3H7+HO2	3.97E+13	0.00	47693.
!(52) Tsang 88			
!C3H8+HO2=nC3H7+H2O2	4.76E+04	2.55	16494.
!(52) Tsang 88			
!C3H8+HO2=iC3H7+H2O2	9.64E+03	2.60	13910.
!(52) Tsang 88			
!C3H8+CH3=nC3H7+CH4	9.04E-01	3.65	7154.
!(52) Tsang 88			
!C3H8+CH3=iC3H7+CH4	1.51E+00	3.46	5481.
!(52) Tsang 88			
!C3H8+CH2OH=nC3H7+CH3OH	1.99E+02	2.95	3976.
!(52) Tsang 88			
!C3H8+CH3O=nC3H7+CH3OH	4.34E+11	0.00	6458.
!(52) Tsang 88			
!C3H8+CH2SING=nC3H7+CH3	9.04E-01	3.65	7154.
!(52) Tsang 88			
!C3H8+C2H3=nC3H7+C2H4	6.03E+02	3.30	10502.
!(52) Tsang 88			
!C3H8+C2H=nC3H7+C2H2	3.61E+12	0.00	0.
!(52) Tsang 88			
!C3H8+C2H5=nC3H7+C2H6	9.04E-02	3.65	9141.
!(52) Tsang 88			
!C3H8+HCO=nC3H7+CH2O	2.05E+05	2.50	18431.
!(52) Tsang 88			
!C3H8+iC3H7=nC3H7+C3H8	8.40E-03	4.20	8716.
!(52) Tsang 88			
!C3H8+CH3CO=nC3H7+CH3CHO	4.22E+04	2.60	17658.
!(52) Tsang 88			
!C3H8+CH2=nC3H7+CH3	9.03E-01	3.65	7154.

!(52) Tsang 88			
!C3H8+CH2OH=iC3H7+CH3OH	6.03E+01	2.95	11989.
!(52) Tsang 88			
!C3H8+CH3O=iC3H7+CH3OH	1.45E+11	0.00	4571.
!(52) Tsang 88			
!C3H8+CH2SING=iC3H7+CH3	1.51E+00	3.46	7472.
!(52) Tsang 88			
!C3H8+C2H3=iC3H7+C2H4	1.02E+03	3.10	8829.
!(52) Tsang 88			
!C3H8+C2H=iC3H7+C2H2	1.21E+12	0.00	0.
!(52) Tsang 88			
!C3H8+C2H5=iC3H7+C2H6	1.21E+00	3.46	7468.
!(52) Tsang 88			
!C3H8+HCO=iC3H7+CH2O	1.08E+07	1.90	17006.
!(52) Tsang 88			
!C3H8+CH3CO=iC3H7+CH3CHO	5.30E+06	2.00	16241.
!(52) Tsang 88			
!C3H8+CH2=iC3H7+CH3	1.51E+00	3.46	7472.
!(52) Tsang 88			
!			
!-----C3H7 chemistry-----			
!			
!nC3H7+H=C3H6+H2	1.81E+12	0.00	0.
!(52) Tsang 88			
!nC3H7+H(+M)=C3H8(+M)	3.60E+13	0.00	0.
!(52) Tsang 88			
! LOW	/3.01E+58	-9.32	5833.6/
! TROE /0.498 1314 1314 50000/			
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/ 0.7/			
!nC3H7+H = C2H5+CH3	3.40E+18	-1.33	5386.
!(52) Tsang 88 0.1 atm			
!nC3H7+O=C2H5+CH2O	9.60E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+O2=C3H6+HO2	9.04E+10	0.00	0.
!(52) Tsang 88			
!nC3H7+HO2=C2H5+OH+CH2O	2.41E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+OH=C3H6+H2O	2.41E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH3=CH4+C3H6	1.14E+13	-0.32	0.
!(52) Tsang 88			
!nC3H7+C2H5=C3H6+C2H6	1.45E+12	0.00	0.
!(52) Tsang 88			
!nC3H7+C2H5=C3H8+C2H4	1.15E+12	0.00	0.
!(52) Tsang 88			
!nC3H7+C2H3=C3H8+C2H2	1.21E+12	0.00	0.
!(52) Tsang 88			
!nC3H7+C2H2=AC3H5+C2H4	7.23E11	0.00	9004.
!(52) Tsang 88			
!nC3H7+C2H=C3H3+C2H5	1.21E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+C2H=C3H6+C2H2	6.03E+12	0.00	0.
!(52) Tsang 88			
!nC3H7+iC3H7=C3H8+C3H6	5.13E+13	-0.35	0.
!(52) Tsang 88			
!nC3H7+HCO=CO+C3H8	6.03E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH3O=C3H8+CH2O	2.41E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH2SING=C2H5+C2H4	2.58E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH2SING=C3H6+CH3	1.03E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH2=C2H4+C2H5	1.81E+13	0.00	0.
!(52) Tsang 88			
!nC3H7+CH2=C3H6+CH3	1.81E+12	0.00	0.

```

!(52) Tsang 88
!nC3H7+CH2OH=C3H6+CH3OH          4.82E+11    0.00    0.
!(52) Tsang 88
!iC3H7=CH3+C2H4                    1.00E+14    0.00   45000.
!(83) Dagaut 92
!iC3H7+H=C3H6+H2                   3.61E+12    0.00    0.
!(52) Tsang 88
!iC3H7+H(+M)=C3H8(+M)              2.40E+13    0.00    0.
!(52) Tsang 88
! LOW                                /1.70E+58  -12.08  11263.7/
! TROE /0.649 1213.1 1213.1 13369.7/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!iC3H7+H = CH3+C2H5                 5.90E+23   -2.81   10009.
!(52) 88TSA RRKM 0.1 atm
!iC3H7+O=CH3CHO+CH3                9.60E+13    0.00    0.
!(52) Tsang 88
!iC3H7+O2=C3H6+HO2                 1.26E+11    0.00    0.
!(52) Tsang 88
!iC3H7+HO2=CH3CHO+OH+CH3           2.41E+13    0.00    0.
!(52) Tsang 88
!iC3H7+OH=C3H6+H2O                 2.41E+13    0.00    0.
!(52) Tsang 88
!iC3H7+CH3=CH4+C3H6                2.19E+14   -0.68    0.
!(52) Tsang 88
!iC3H7+C2H5=C3H6+C2H6              2.30E+13   -0.35    0.
!(52) Tsang 88
!iC3H7+C2H5=C3H8+C2H4              1.84E+13   -0.35    0.
!(52) Tsang 88
!iC3H7+C2H3=C2H4+C3H6              1.52E+14   -0.70    0.
!(52) Tsang 88
!iC3H7+C2H3=C3H8+C2H2              1.52E+14   -0.70    0.
!(52) Tsang 88
!iC3H7+C2H2=CH3+iiiC4H6            2.77E+10    0.00   6504.
!(52) Tsang 88
!iC3H7+C2H=C3H6+C2H2               3.60E+12    0.00    0.
!(52) Tsang 88
!iC3H7+iC3H7=C3H8+C3H6             2.11E+14   -0.70    0.
!(52) Tsang 88
!iC3H7+HCO=CO+C3H8                 1.20E+14    0.00    0.
!(52) Tsang 88
!iC3H7+CH3O=C3H8+CH2O              1.21E+13    0.00    0.
!(52) Tsang 88
!iC3H7+CH2SING=C3H6+CH3            1.04E+13    0.00    0.
!(52) Tsang 88
!iC3H7+CH2=C3H6+CH3                3.01E+13    0.00    0.
!(52) Tsang 88
!iC3H7+CH2OH=C3H6+CH3OH            2.89E+12    0.00    0.
!(52) Tsang 88
!iC3H7+CH2OH=C3H8+CH2O             2.35E+12    0.00    0.
!(52) Tsang 88
!
!-----C3H6 chemistry-----
!
!@CH3+C2H3(+M)=C3H6(+M)            2.50E+13    0.00    0.
!(50) Qin/Wan 00
! LOW                                /4.27E+58  -11.94  9770./
! TROE /0.175 1341 60000 10140/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H2/3.0/ AR/0.7/
!C3H6+H=H2+AC3H5                   1.70E+05    2.50   2492.
!(84) Tsang 91
!C3H6+H=C2H4+CH3                   8.80E+16   -1.05   6461.
!(84) Tsang 91 0.1 atm
!C3H6+H=SC3H5+H2                   7.81E+05    2.50  12285.
!(85) Tsang 92
!C3H6+H(+M)=nC3H7(+M)             1.33E+13    0.00   3260.7
!(84) Tsang 91

```

```

! LOW /6.26E+38 -6.66 7000./
! TROE /1.000 1000. 1310. 48097./
! H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
! C3H6+H(+M)=iC3H7(+M) 1.33E+13 0.00 1559.8
!(84) Tsang 91
! LOW /8.70E+42 -7.50 4721.8/
! TROE /1.000 1000. 645.4 6844.3 /
! H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
!C3H6+H=TC3H5+H2 3.90E+05 2.50 5821.
!(85) Tsang 92
!C3H6=H2+AC3H4 4.00E+13 0.00 80000.
!(87) Hidaka 92
!C3H6=CH4+C2H2 3.50E+12 0.00 70000.
!(87) Hidaka 92
!C3H6+O=C2H5+HCO 3.50E+07 1.65 -972.
!(84) Tsang 91
!C3H6+O=AC3H5+OH 1.75E+11 0.70 5884.
!(84) Tsang 91
!C3H6+O=SC3H5+OH 1.21E+11 0.70 8960.
!(84) Tsang 91
!C3H6+O=TC3H5+OH 6.03E+10 0.70 7633.
!(84) Tsang 91
!C3H6+O=CH3+H+CH2CO 1.20E+08 1.65 327.
!(84) Tsang 91
!C3H6+OH=AC3H5+H2O 3.12E+06 2.00 -298.
!(84) Tsang 91
!C3H6+OH=SC3H5+H2O 2.14E+06 2.00 2778.
!(84) Tsang 91
!C3H6+OH=TC3H5+H2O 1.11E+06 2.00 1451.
!(84) Tsang 91
!C3H6+HO2=AC3H5+H2O2 9.63E+03 2.60 13910.
!(84) Tsang 91
!C3H6+O2=AC3H5+HO2 6.03E+13 0.00 47590.
!(84) Tsang 91
!C3H6+CH3=AC3H5+CH4 2.20E+00 3.50 5675.
!(84) Tsang 91
!C3H6+CH3=TC3H5+CH4 8.40E-01 3.50 11660.
!(84) Tsang 91
!C3H6+C2H5=AC3H5+C2H6 2.23E+00 3.50 6637.
!(84) Tsang 91
!C3H6+C2H2=AC3H5+C2H3 4.04E+13 0.00 46818.
!(84) Tsang 91
!C3H6+C2H3=AC3H5+C2H4 2.21E+00 3.50 4682.
!(84) Tsang 91
!C3H6+C2H3=SC3H5+C2H4 1.35E+00 3.50 10842.
!(84) Tsang 91
!C3H6+C2H3=TC3H5+C2H4 8.40E-01 3.50 9670.
!(84) Tsang 91
!C3H6+C2H3=iiiC4H6+CH3 7.23E+11 0.00 5008.
!(84) Tsang 91
!C3H6+C2H4=AC3H5+C2H5 5.78E+13 0.00 51584.
!(84) Tsang 91
!C3H6+C2H4=nC3H7+C2H3 6.03E+13 0.00 75446.
!(84) Tsang 91
!C3H6+CH2OH=AC3H5+CH3OH 6.03E+01 2.95 12000.
!(84) Tsang 91
!C3H6+nC3H7=AC3H5+C3H8 2.23E+00 3.50 6637.
!(84) Tsang 91
!C3H6+nC3H7=IC4H8+C2H5 2.23E+00 3.50 -2000.
!(84) Tsang 91
!C3H6+iC3H7=C3H8+AC3H5 6.62E-02 4.00 8066.
!(84) Tsang 91
!C3H6+C3H6=AC3H5+nC3H7 2.53E+14 0.00 55179.
!(84) Tsang 91
!C3H6+C3H6=AC3H5+iC3H7 4.88E+13 0.00 52309.
!(84) Tsang 91

```

```

!
!-----C3H5 chemistry-----
!
!CH3+C2H3=AC3H5+H                1.50E+24   -2.83   18618.
!(88) Davis/Wang 99
!CH3+C2H3=SC3H5+H                3.20E+35   -7.76   13300.
!(88) Davis/Wang 99
!CH3+C2H3=TC3H5+H                4.99E+22   -4.39   18850.
!(88) Davis/Wang 99
!AC3H5+H(+M)=C3H6(+M)            2.00E14     0.00     0.
!(84) Tsang 91
! LOW                               /1.33E+60  -12.00   5967.8/
! TROE /0.02 1097 10967 6860/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!AC3H5+H=AC3H4+H2                1.80E+13     0.00     0.
!(84) Tsang 91
!TC3H5+H=AC3H4+H2                3.30E+12     0.00     0.
!(83) Dagaut 92
!SC3H5+H=AC3H4+H2                3.30E+12     0.00     0.
!(83) Dagaut 92
!AC3H5+O=C2H3CHO+H               6.00E+13     0.00     0.
!(84) Tsang 91
!AC3H5+O=C2H3+CH2O               1.80E+14     0.00     0.
!(89) Westmoreland PC
!SC3H5+O=CH2CO+CH3               1.81E+14     0.00     0.
!(83) Dagaut 92
!TC3H5+O=H+HCCO+CH3              1.81E+14     0.00     0.
!(83) Dagaut 92
!AC3H5+OH = C2H3CHO+H+H           5.30E+37   -6.71   29306.
!(84) Tsang 91 RRM 0.1atm
!AC3H5+OH=AC3H4+H2O              6.00E+12     0.00     0.
!(84) Tsang 91
!AC3H5+O2=AC3H4+HO2              4.99E+15   -1.40   22428.
!(90) Boz/Dean 93
!AC3H5+O2=CH2O+CH3CO             1.19E+15   -1.01   20128.
!(90) Boz/Dean 93
!AC3H5+O2=OH+C2H3CHO             1.82E+13   -0.41   22859.
!(90) Boz/Dean 93
!SC3H5+O2=CH3CHO+HCO             4.34E+12     0.00     0.
!(83) Dagaut 92
!TC3H5+O2=CH3CHO+HCO             4.34E+12     0.00     0.
!(83) Dagaut 92
!AC3H5+HO2=C2H3+CH2O+OH          6.60E+12     0.00     0.
!(10) Baulch 94
!AC3H5+CH3=AC3H4+CH4             3.00E+12   -0.32   -131.
!(84) Tsang 91
!AC3H5+CH3(+M)=IC4H8(+M)         1.00E+14   -0.32   -262.
!(84) Tsang 91
! LOW                               /3.51E+60  -12.97   6000./
! TROE /0.896 60000 1606 6118/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!SC3H5+CH3=AC3H4+CH4             1.00E+11     0.00     0.
!(83) Dagaut 92
!TC3H5+CH3=AC3H4+CH4             1.00E+11     0.00     0.
!(83) Dagaut 92
!AC3H5+C2H3=AC3H4+C2H4           1.00E+12     0.00     0.
!(83) Dagaut 92
!SC3H5+C2H3=AC3H4+C2H4           1.00E+11     0.00     0.
!(83) Dagaut 92
!TC3H5+C2H3=AC3H4+C2H4           1.00E+11     0.00     0.
!(83) Dagaut 92
!AC3H5+CH2O=C3H6+HCO             1.26E+08     1.90   18191.
!(83) Dagaut 92
!AC3H5+HCO=C3H6+CO               6.00E+13     0.00     0.
!(84) Tsang 91
!AC3H5+AC3H5=AC3H4+C3H6         8.43E+10     0.00   -262.

```

```

!(84) Tsang 91
!AC3H5+CH2=iiiC4H6+H          3.00E+13    0.00    0.
!(84) Tsang 91
!AC3H5+nC3H7=AC3H4+C3H8      7.23E+11    0.00   -131.
!(84) Tsang 91
!AC3H5+iC3H7=AC3H4+C3H8      4.58E+12   -0.35   -131.
!(84) Tsang 91
!AC3H5=TC3H5                   3.90E+59   -15.42  75400.
!(88) Davis/Wang 99
!AC3H5=SC3H5                   1.30E+55   -14.53  73800.
!(88) Davis/Wang 99
!TC3H5=SC3H5                   1.60E+44   -12.16  52200.
!(88) Davis/Wang 99
!
!-----C3H4 chemistry-----
!
!AC3H4=PC3H4                   6.0256E+53 -12.18  84276.
!(91) JAM/SJK 03

!AC3H4+H=AC3H5                 1.241E52  -12.02  17839.
!(92) JAM/JPS 08
! DUPLICATE
!AC3H4+H=AC3H5                 6.923E36   -8.19   7462.
!(92) JAM/JPS 08
! DUPLICATE
!AC3H4+H=TC3H5                 1.554E53  -13.10  14472.
!(92) JAM/JPS 08
! DUPLICATE
!AC3H4+H=TC3H5                 0.988E45  -11.21   8212.
!(92) JAM/JPS 08
! DUPLICATE
!PC3H4+H=TC3H5                 3.174E52  -12.69  14226.
!(92) JAM/JPS 08
! DUPLICATE
!PC3H4+H=TC3H5                 2.589E45  -11.23   8046.
!(92) JAM/JPS 08
! DUPLICATE
!PC3H4+H=AC3H5                 3.379E49  -12.75  14072.
!(92) JAM/JPS 08
! DUPLICATE
!PC3H4+H=AC3H5                 2.981E43  -11.43   8736.
!(92) JAM/JPS 08
! DUPLICATE
! Mistake above, should be SC3H5, fixed as below.
!PC3H4+H=SC3H5                 3.379E49  -12.75  14072.
!(92) JAM/JPS 08
! DUPLICATE
!PC3H4+H=SC3H5                 2.981E43  -11.43   8736.
!(92) JAM/JPS 08
! DUPLICATE
!AC3H4+H=PC3H4+H               1.476E13    0.26   4103.
!(92) JAM/JPS 08
!AC3H4+H=CH3+C2H2              2.722E9     1.20   6834.
!(92) JAM/JPS 08
!PC3H4+H=CH3+C2H2              3.891E10    0.989   4114.
!(92) JAM/JPS 08
!C2H2+CH3=AC3H5                -0.681E+49 -12.27  16642.
!(92) JAM/JPS 08
! DUPLICATE
!C2H2+CH3=AC3H5                1.524E+44  -10.73  15256.
!(92) JAM/JPS 08
! DUPLICATE
! Mistake above, should be SC3H5, fixed as below.
!C2H2+CH3=SC3H5                -0.681E+49 -12.27  16642.
!(92) JAM/JPS 08
! DUPLICATE

```

```

!C2H2+CH3=SC3H5                1.524E+44  -10.73  15256.
!(92) JAM/JPS 08
! DUPLICATE
!C2H2+CH3=CH3CHCH      1.4E+32  -7.14  10000.  !bpick jul03 actually from Wang Hai Davis/Wang
99 0.1 atm
! PLOG /0.1      1.4E+32  -7.14  10000./
! PLOG /1.      3.2E+35  -7.76  13300./
! PLOG /10.     2.4E+38  -8.21  17100./
! PLOG /100.    1.4E+39  -8.06  20200./
! PLOG /1.0E+5  1.5E+07  1.87   8200./
!C2H2+CH3=TC3H5                6.80E+20  -4.16  18000.
!(88) Davis/Wang 99 0.1 atm
! Miller
! C2H2+CH3=CH3CCH2      6.8E+20  -4.16  18000.  !bpick jul03 actually from Wang Hai
Davis/Wang 99 0.1 atm
! PLOG /0.1      6.8E+20  -4.16  18000./
! PLOG /1.      5.0E+22  -4.39  18800./
! PLOG /10.     9.3E+27  -5.55  22900./
! PLOG /100.    3.8E+36  -7.58  31300./
!C2H2+CH3=AC3H5                8.20E+53  -13.32  33200.
!(88) Davis/Wang 99 0.1 atm
!AC3H4+H=C3H3+H2                6.604E3   3.095  5522.
!(92) JAM/JPS 08
!AC3H4+OH=C3H3+H2O              1.00E+07   2.00   1000.
!(46) Miller 92
! Miller
! C3H4+H=H2CCCH+H2          6.604E3   3.095   5522. !JAM, SJK et al (2007)
! C3H4+OH=H2CCCH+H2O        2.0E7     2.0    5000. !JAM
! C3H4+OH=CH2O+C2H3          1.0E12    0.0    -198.7
!JAM/Liu(1988)/Butler(07)
! C3H4+OH=CH2CO+CH3          3.04E12   0.0    -198.7
!
!PC3H4+H=C3H3+H2              3.57E4    2.825  4821.
!(92) JAM/JPS 08
!AC3H4+O=C2H4+CO              2.00E+07   1.80   1000.
!(93) Davis/Wang 99
!AC3H4+C2H=C3H3+C2H2          1.00E+13   0.00    0.
!(54) Wang 97
!AC3H4+CH3=C3H3+CH4           1.30E+12   0.00   7700.
!(88) Davis/Wang 99
!PC3H4+O=HCCO+CH3            7.30E+12   0.00   2250.
!(94) Adusei 96
!PC3H4+O=C2H4+CO              1.00E+13   0.00   2250.
!(94) Adusei 96
!PC3H4+O=C3H3+OH              3.44E+04   2.16   4830.
!(94) Adusei 96
!PC3H4+OH=C3H3+H2O            1.00E+07   2.00   1000.
!(46) Miller 92
!PC3H4+C2H=C3H3+C2H2          1.00E+13   0.00    0.
!(54) Wang 97
!PC3H4+CH3=C3H3+CH4           1.80E+12   0.00   7700.
!(88) Davis/Wang 99
!
!-----C3H3 chemistry-----
!
!3H3+H=PC3H4                  3.6308E+36  -7.36  6039.
!(91) JAM/SJK 03
!C3H3+H=AC3H4                  3.3884E+36  -7.41  6337.
!(91) JAM/SJK 03
!C3H3+CH3(+M)=iiC4H6(+M)      1.50E+12   0.00    0.
!(54) Wang 97
! LOW                            /2.60E+57  -11.94  9770./
! TROE /0.175 1341 60000 9770/
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!C3H3+CH3=iiC4H6              3.61E13    0.0    0.0

```

![Fahr and Nayak '2000: 40% of total] MIT PAH

```
!C2H3+C2H3=iiiC4H6          7.00E+57   -13.82  17629.
!(54) Wang 97 RRKM 20 Torr
! C3H3+H=C3H2+H2            5.00E+13    0.00   3000.
!(46) Miller 92
!C3H3+H=C3H2+H2            2.14E+05    2.52   7453.
!JAM&SJK 2002 30 Torr
! Miller These reactions come from JAM&SJK 2002 30 Torr
! H2CCCH+H=C3H2+H2  2.14E5  2.52  7453.
!abstraction

!C3H3+O=>C2H2+HCO          1.385E+14    0.00    0.
!(95) Slagle 90
!C3H3+O=C2H3+CO            4.615E+13    0.00    0.
!(95) Slagle 90
!C3H3+O=C2H+CH2O           4.615E+13    0.00    0.
!(95) Slagle 90
!H2CCCH+O=CH2O+C2H        1.4E14  0.000  0.000
!GUTMAN 23RD (PRD JAM)
!C3H3+O=>C2H2+CO+H         4.615E+13    0.00    0.
!(95) Slagle 90

! C3H3+OH=C3H2+H2O         2.00E+13    0.00    0.
!(34) Miller 89
!C3H3+OH=C3H2+H2O         2.00E+13    0.00  8000.
!JAM 2007
! Miller H2CCCH+OH=C3H2+H2O  0.200E+14  0.000  8000.
!JAM 2007

!C3H3+HCO=AC3H4+CO         2.50E+13    0.00    0.
!(54) Wang 97
!C3H3+HCO=PC3H4+CO         2.50E+13    0.00    0.
!(54) Wang 97
!C3H3+CH=iC4H3+H           5.00E+13    0.00    0.
!(54) Wang 97
!C3H3+CH2=C4H4+H           5.00E+13    0.00    0.
!(46) Miller 92
! C3H3+O2=CH2CO+HCO        3.00E+10    0.00  2868.
!(99) Slagle 88
!C3H3+O2=CH2CO+HCO         1.70E+05    1.70   1500.
!JAM&SJK Faraday 119
! Miller
! H2CCCH+O2=CH2CO+HCO      1.70E5  1.7  1500. !JAM&SJK Faraday 119

!C3H3+HCCO=C4H4+CO         2.50E+13    0.00    0.
!(54) Wang 97
!C3H3+HO2=OH+CO+C2H3       8.00E+11    0.00    0.
!(93) Davis/Wang 99
!C3H3+HO2=AC3H4+O2         3.00E+11    0.00    0.
!(93) Davis/Wang 99
!C3H3+HO2=PC3H4+O2         2.50E+12    0.00    0.
!(93) Davis/Wang 99
!C3H2+O2=H+CO+HCCO         2.00E+12    0.00  1000.
!(61) Pauwels 95
! Miller
! C3H2+O2=CO2+C2H2         11.5E5  2.245  367.6
!JAM (based on ch2+O2)
! C3H2+O2=CO2+C2H+H        11.5E5  2.245  367.6
!JAM
! C3H2+O2=HCCO+CO+H        2.5E5  2.245  367.6
!JAM

!C3H2+O=C2H2+CO            6.80E+13    0.00    0.  !(100) Warnatz 83
```



```

!C3H2+OH=C2H2+HCO          6.80E+13   0.00   0.   !(100) Warnatz 83
!C3H2+H=C3H3                1.1E+40  -8.0   84700.  !(101) HAR/KLI
07,WestmQRRK
!C3H2+H=C3H3                7.60E+13  0.22  -86.84 !2007HAR/KLI3789-3801
!C3H2+CH=C4H2+H            5.00E+13   0.00   0.
!(54) Wang 97
!C3H2+CH2=nC4H3+H          5.00E+13   0.00   0.
!(54) Wang 97
!C3H2+CH3=C4H4+H           5.00E+12   0.00   0.
!(54) Wang 97
!C3H2+HCCO=nC4H3+CO        1.00E+13   0.00   0.
!(54) Wang 97
!
!-----C3HxO chemistry-----
!
!C2H3CO+M=>C2H3+CO+M        8.51E+15  0.00   23000.
!(76) Wilk 89
!C2H3+CO+M=>C2H3CO+M        1.58E+11  0.00   6000.
!(76) Wilk 89
!C2H3CHO+HO2=>C2H3CH2O+O2   1.29E+11  0.00   32000.
!(76) Wilk 89
!C2H3CH2O=>C2H3CHO+H        1.00E+14  0.00   19000.
!(76) Wilk 89
!C2H3CHO+H=>C2H3CH2O        1.00E+08  0.00   10000.
!(76) Wilk 89
!C2H3CHO+OH=>C2H3CO+H2O     1.00E+13  0.00   0.
!(76) Wilk 89
!C2H3CO+H2O=>C2H3CHO+OH     1.91E+13  0.00   36620.
!(76) Wilk 89
!C2H3CHO+H=>C2H3CO+H2       3.98E+13  0.00   4200.
!(76) Wilk 89
!C2H3CO+H2=>C2H3CHO+H       1.78E+13  0.00   23670.
!(76) Wilk 89
!C2H3CHO+O=>C2H3CO+OH       5.01E+12  0.00   1790.
!(76) Wilk 89
!C2H3CO+OH=>C2H3CHO+O       1.00E+12  0.00   19160.
!(76) Wilk 89
!C2H3CHO+HO2=>C2H3CO+H2O2   1.70E+12  0.00   10700.
!(76) Wilk 89
!C2H3CO+H2O2=>C2H3CHO+HO2   1.00E+12  0.00   14100.
!(76) Wilk 89
!C2H3CHO+CH3=>C2H3CO+CH4    1.74E+12  0.00   8440.
!(76) Wilk 89
!C2H3CO+CH4=>C2H3CHO+CH3    1.51E+13  0.00   28000.
!(76) Wilk 89
!C2H3CH2O+O2=>C2H3CHO+HO2   1.74E+11  0.00   1750.
!(76) Wilk 89
!C2H3CH2O=>CH2O+C2H3         1.00E+14  0.00   21600.
!(76) Wilk 89
!CH2O+C2H3=>C2H3CH2O        1.00E+11  0.00   0.
!(76) Wilk 89
!
! Miller C4H, only three reactions!
!C4H+H2=C4H2+H              2.0E13   0.0    5000. !JAM 6/01
!C4H+O2=CO+CO+C2H           1.2E12   0.0    0.0
!JAM 1996/CJP 092899
!C4H2+OH=H2O+C4H            9.15E+09  1.03   21746.
!Proc Comb Inst 31 185-193 (2007)
!
!-----C4H2 chemistry-----
!
!C4H2+OH=CO+C3H3            1.69E+28 -4.59   20140.  !(103) JPS/SJK/JAM 07
!C4H2+H=nC4H3                1.4375E+63 -15.66  24018   !(102) SJK/JAM 05
! DUPLICATE
!C4H2+H=nC4H3                4.165E+32 -6.4928  9726.1  !(102) SJK/JAM 05
! DUPLICATE

```

```

!C4H2+H(+M)=iC4H3(+M)          4.31E10   1.158      1752.9  !(102) SJK/JAM 05
!  LOW                          /2.30E45  -8.095      2506.6 /
!  TROE /0.0748 1.0E-50 -4215.9 1.0E50/
!  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
!C4H2+O=C3H2+CO                 2.70E+13   0.00        1720.
!(3) Warnatz 84
!
!-----C4H3 chemistry-----
!
!nC4H3=iC4H3                     3.70E+61  -15.81      54890.
!(54) Wang 97 20 Torr
!nC4H3+H=iC4H3+H                 2.40E+11   0.79        2410.
!(54) Wang 97 20 Torr
!nC4H3+H=C2H2+H2CC              1.60E+19  -1.60        2220.
!(54) Wang 97 20 Torr
!nC4H3+H=C4H4                   1.10E+42  -9.65       7000.
!(54) Wang 97 20 Torr
!nC4H3+H=C4H2+H2                3.00E+13   0.00         0.
!(54) Wang 97
!nC4H3+OH=C4H2+H2O             2.00E+12   0.00         0.
!(54) Wang 97
!iC4H3+H=C2H2+H2CC             2.40E+19  -1.60        2800.
!(54) Wang 97 20 Torr
!iC4H3+H=C4H4                   4.20E+44 -10.27      7890.
!(54) Wang 97 20 Torr
!iC4H3+H=C4H2+H2                5.00E+13   0.00         0.
!(46) Miller 92
!iC4H3+OH=C4H2+H2O             4.00E+12   0.00         0.
!(54) Wang 97
!iC4H3+O2=HCCO+CH2CO          7.86E+16  -1.80         0.
!(54) Wang 97
!
!-----C4H4 chemistry-----
!
!C4H4+H=n-C4H5                  4.20E+50 -12.34      12500.
!(54) Wang 97 20Torr
!C4H4+H=i-C4H5                   9.60E+52 -12.85      14300.
!(54) Wang 97 20Torr
!Miller These are fits from JAM&SJK 2002 30 Torr
!CH2CHCCH=CH2CHCCH+H          1.12E47  -10.997  48397.
!CH2CHCCH2=CH2CHCCH+H         3.15E58  -13.954  64898.
!C4H4+H=nC4H3+H2               6.65E+05   2.53       12240.
!(54) Wang 97
!C4H4+H=iC4H3+H2               3.33E+05   2.53       9240.
!(54) Wang 97
! CH2CHCCH+H=HCCHCCH+H2        2.0E7     2.0    15000.  !JAM
! CH2CHCCH+H=H2CCCCH+H2        3.0E7     2.0    5000.   !JAM
!C4H4+OH=nC4H3+H2O             3.10E+07   2.00       3430.
!(54) Wang 97
!C4H4+OH=iC4H3+H2O             1.55E+07   2.00       430.
!(54) Wang 97
! CH2CHCCH+OH=HCCHCCH+H2O      7.5E6     2.0    5000.   !JAM
! CH2CHCCH+OH=H2CCCCH+H2O      1.0E7     2.0    2000.   !JAM

!C4H4+O=C3H3+HCO               6.00E+08   1.45       -860.
!(54) Wang 97
!
!-----C4H5 chemistry-----
!
!n-C4H5=i-C4H5                   1.30E+62 -16.38     49600.
!(54) Wang 97 20Torr
!n-C4H5+H=i-C4H5+H              1.00E+36  -6.26     17486.
!(54) Wang 97 20Torr
!n-C4H5+H=C4H4+H2              1.50E+13   0.00         0.
!(54) Wang 97
!n-C4H5+OH=C4H4+H2O            2.00E+12   0.00         0.

```

!(54) Wang 97				
!n-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.00	0.	
!(54) Wang 97				
!n-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.00	0.	
!(54) Wang 97				
!n-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.00	-596.	
!(54) Wang 97				
!n-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.00	0.	
!(54) Wang 97				
!n-C4H5+O2=HCO+C2H3CHO	9.20E+16	-1.39	1010.	
!(54) Wang 97				
!i-C4H5+H=C4H4+H2	3.00E+13	0.00	0.	
!(54) Wang 97				
!i-C4H5+H=C3H3+CH3	1.0E14	0.00	0.	
!(66) Hansen/Miller 08				
!i-C4H5+OH=C4H4+H2O	4.00E+12	0.00	0.	
!(54) Wang 97				
!i-C4H5+HCO=iiiC4H6+CO	5.00E+12	0.00	0.	
!(54) Wang 97				
!i-C4H5+HO2=iiiC4H6+O2	6.00E+11	0.00	0.	
!(54) Wang 97				
!i-C4H5+HO2=C2H3+CH2CO+OH	6.60E+12	0.00	0.	
!(54) Wang 97				
!i-C4H5+H2O2=iiiC4H6+HO2	1.21E+10	0.00	-596.	
!(54) Wang 97				
!i-C4H5+O2=CH2CO+CH2CHO	2.16E+10	0.00	2500.	
!(54) Wang 97				
!!				
!-----C4H6 chemistry-----				
!				
!iiiC4H6=i-C4H5+H	8.20E+51	-10.92	118409.	
!(54) Wang 97 20Torr				
!iiiC4H6=n-C4H5+H	3.50E+61	-13.87	129677.	
!(54) Wang 97 20Torr				
! Miller CH2CHCHCH2=CH2CHCCH2+H		5.70E+36	-6.270	112353.2
!Laskin et al. 2000				
! Miller CH2CHCHCH2=CH2CHCHCH+H		5.30E+44	-8.620	123608.2
!Laskin et al. 2000				
!iiiC4H6=C4H4+H2	2.50E+15	0.00	94700.	!(106) Hidaka 96
!iiiC4H6+H=n-C4H5+H2	3.0E7	2.0	13000.	
!(66) Hansen/Miller 08 JAM Est				
!iiiC4H6+H=i-C4H5+H2	3.0E7	2.0	6000.	
!(66) Hansen/Miller 08 JAM Est				
!C2H4+C2H3=iiiC4H6+H	7.40E+14	-0.66	8420.	
!(54) Wang 97 20Torr				
!iiiC4H6+H=PC3H4+CH3	2.00E+12	0.00	7000.	
!(86) Wang USC_II 07				
!iiiC4H6+H=AC3H4+CH3	2.00E+12	0.00	7000.	
!(86) Wang USC_II 07				
!iiiC4H6+O=n-C4H5+OH	7.50E+06	1.90	3740.	
!(86) Wang USC_II 07				
!iiiC4H6+O=i-C4H5+OH	7.50E+06	1.90	3740.	
!(86) Wang USC_II 07				
!iiiC4H6+O=HCO+AC3H5	6.02E+08	1.45	-858.	
!(66) Hansen/Miller 08				
!iiiC4H6+OH=CH3CHO+C2H3	6.3E12	0.00	-874.	
!(66) Hansen/Miller 08 JAM Est				
!iiiC4H6+OH=AC3H5+CH2O	6.3E12	0.00	-874.	
!(66) Hansen/Miller 08				
! iiiC4H6+OH=n-C4H5+H2O	6.20E+06	2.00	3430.	!(107) Liu 88
! iiiC4H6+OH=i-C4H5+H2O	3.10E+06	2.00	430.	
!(86) Wang USC_II 07				
!iiiC4H6+OH=n-C4H5+H2O	2.0E7	2.0	5000.	
!JAM				
!iiiC4H6+OH=i-C4H5+H2O	2.0E7	2.0	2000.	
!JAM				

! CH2CHCHCH2+OH=CH2CHCHCH+H2O	2.0E7	2.0	5000.	
!JAM				
! CH2CHCHCH2+OH=CH2CHCCH2+H2O	2.0E7	2.0	2000.	
!JAM				
!iiiC4H6+CH3=n-C4H5+CH4	2.00E+14	0.00	22800.	!(106) Hidaka 96
!iiiC4H6+CH3=i-C4H5+CH4	1.00E+14	0.00	19800.	!(106) Hidaka 96
!iiiC4H6+C2H3=n-C4H5+C2H4	5.00E+13	0.00	22800.	!(106) Hidaka 96
!iiiC4H6+C2H3=i-C4H5+C2H4	2.50E+13	0.00	19800.	!(106) Hidaka 96
!iiiC4H6+C3H3=n-C4H5+AC3H4	1.00E+13	0.00	22500.	!(106) Hidaka 96
!iiiC4H6+C3H3=i-C4H5+AC3H4	5.00E+12	0.00	19500.	!(106) Hidaka 96
!iiiC4H6+AC3H5=n-C4H5+C3H6	1.00E+13	0.00	22500.	
!(86) Wang USC_II 07				
!iiiC4H6+AC3H5=i-C4H5+C3H6	5.00E+12	0.00	19500.	
!(86) Wang USC_II 07				
!iiC4H6=i-C4H5+H	4.20E+15	0.00	92600.	!(108) Leung/Linstedt 95
!iiC4H6+H=iiiC4H6+H	2.00E+13	0.00	4000.	
!(86) Wang USC_II 07				
!iiC4H6+H=i-C4H5+H2	1.70E+05	2.50	2490.	
!(86) Wang USC_II 07				
!iiC4H6+H=AC3H4+CH3	2.00E+13	0.00	2000.	
!(86) Wang USC_II 07				
!iiC4H6+H=PC3H4+CH3	2.00E+13	0.00	2000.	
!(86) Wang USC_II 07				
!iiC4H6+CH3=i-C4H5+CH4	7.00E+13	0.00	18500.	
!(86) Wang USC_II 07				
!iiC4H6+O=CH2CO+C2H4	1.20E+08	1.65	327.	
!(86) Wang USC_II 07				
!iiC4H6+O=i-C4H5+OH	1.80E+11	0.70	5880.	
!(86) Wang USC_II 07				
!iiC4H6+OH=i-C4H5+H2O	3.10E+06	2.00	-298.	
!(86) Wang USC_II 07				
!iiC4H6=iiiC4H6	3.00E+13	0.00	65000.	
!(86) Wang USC_II 07				
!				
!-----1-C4H8 1-butene chemistry-----				
!				
!IC4H8+H=C2H4+C2H5	1.60E+22	-2.39	11180.	
!(86) Wang USC_II 07				
!IC4H8+H=C3H6+CH3	3.20E+22	-2.39	11180.	
!(86) Wang USC_II 07				
!IC4H8+H=C4H7+H2	6.50E+05	2.54	6756.	
!(86) Wang USC_II 07				
!IC4H8+O=nC3H7+HCO	3.30E+08	1.45	-402.	!(109) Ko/Adusei 91
!IC4H8+O=C4H7+OH	1.50E+13	0.00	5760.	!(109) Ko/Adusei 91
! DUPLICATE				
!IC4H8+O=C4H7+OH	2.60E+13	0.00	4470.	!(109) Ko/Adusei 91
! DUPLICATE				
!IC4H8+OH=C4H7+H2O	7.00E+02	2.66	527.	
!(86) Wang USC_II 07				
!IC4H8+O2=C4H7+HO2	2.00E+13	0.00	50930.	
!(86) Wang USC_II 07				
!IC4H8+HO2=C4H7+H2O2	1.00E+12	0.00	14340.	
!(86) Wang USC_II 07				
!IC4H8+CH3=C4H7+CH4	4.50E-01	3.65	7153.	
!(86) Wang USC_II 07				
!C4H7=iiiC4H6+H	1.27E24	-4.752	23777.	
!(133) Kiefer 09				
!C4H7+H(+M)=IC4H8(+M)	3.60E+13	0.00	0.	
!(86) Wang USC_II 07				
! LOW	/3.01E+48	-9.32	5833.6/	
! TROE /0.498 1314 1314 50000/				
! H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/				
!C4H7+H=CH3+AC3H5	2.00E+21	-2.00	11000.	
!(86) Wang USC_II 07				
!C4H7+H=iiiC4H6+H2	1.80E+12	0.00	0.	
!(86) Wang USC_II 07				

```

!C4H7+O2=iiiC4H6+HO2          1.00E+11    0.00    0.
!(86) Wang USC_II 07
!C4H7+HO2=CH2O+OH+AC3H5        2.40E+13    0.00    0.
!(86) Wang USC_II 07
!C4H7+HCO=IC4H8+CO              6.00E+13    0.00    0.
!(86) Wang USC_II 07
!C4H7+CH3=iiiC4H6+CH4          1.10E+13    0.00    0.
!(86) Wang USC_II 07
!C2H4+C2H3=C4H7                 1.23E+35    -7.76    9930.
!(54) Wang 97 RRKM 0.1 atm
!
!-----1-butyl nC4H9 chemistry from USC_Mech_II:          (86) Wang USC_II 07
! (86) 2007 Hai Wang USC_II
!IC4H8+H(+M) = nC4H9(+M)        1.33E+13    0.00    3260.7    !=(C3H6+H) TS5 600 cm-1
! LOW /6.26E+38 -6.66 7000./
! TROE /1.000 1000. 1310. 48097. /
! H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
!C2H4+C2H5 = nC4H9              1.50E+11    0.00    7300.
!KP, P
!nC4H9+H = IC4H8+H2             1.80E+12    0.00    0.
!=(nC3H7+H) TS4
!nC4H9+O = nC3H7+CH2O           9.60E+13    0.00    0.
!=(nC3H7+O) TS3 ka+kb
!nC4H9+OH = IC4H8+H2O           2.40E+13    0.00    0.
!=(nC3H7+OH) TS3
!nC4H9+O2 = IC4H8+HO2           2.70E+11    0.00    0.
!BB75
!nC4H9+HO2 = nC3H7+OH+CH2O      2.40E+13    0.00    0.
!=(nC3H7+HO2) TS3 ?
!pC4H9+HCO = C4H10+CO           9.00E+13    0.00    0.
!=(nC3H7+HCO) TS3
!nC4H9+CH3 = IC4H8+CH4          1.10E+13    0.00    0.
!=(nC3H7+CH3) TS3
!C4H10+H = pC4H9+H2             9.20E+05    2.54    6756.
!=(C3H8+H scaled to BBW at 753K)
!
!=====
! = DME and EtOH Subset =
!=====

!C2H5OH=CH3+CH2OH 1.26E+51 -10.59 100869 !Juan's RRKM_v0.6 for 1 atm
!C2H5OH=C2H4+H2O 8.80E+25 -3.68 70799 !Juan's RRKM_v0.6 for 1 atm
!C2H5OH+OH=C2H4OH+H2O 1.81E+11 0.39 716.5 !temp
!C2H5OH+OH=CH3CHOH+H2O 3.09E+10 0.49 -379.8 !temp
!C2H5OH+OH=C2H5O+H2O 1.05E+10 0.79 716.9 !temp
!C2H5OH+H=C2H4OH+H2 1.90E+7 1.8 5098.0 !temp
!C2H5OH+H=CH3CHOH+H2 2.58E+7 1.65 2827.0 !MARINOV 1998
!C2H5OH+H=C2H5O+H2 1.50E+7 1.60 3038.0 !MARINOV 1998
!C2H5OH+O=C2H4OH+OH 9.41E+7 1.70 5459.0 !MARINOV 1998
!C2H5OH+O=CH3CHOH+OH 1.88E+7 1.85 1824.0 !MARINOV 1998
!C2H5OH+O=C2H5O+OH 1.58E+7 2.00 4448.0 !MARINOV 1998
!C2H5OH+CH3=C2H4OH+CH4 2.19E+2 3.18 9622.0 !MARINOV 1998
!C2H5OH+CH3=CH3CHOH+CH4 7.28E+2 2.99 7948.0 !MARINOV 1998
!C2H5OH+CH3=C2H5O+CH4 1.45E+2 2.99 7649.0 !MARINOV 1998
!C2H5OH+HO2=CH3CHOH+H2O2 8.20E+3 2.55 10750.0 !temp
!C2H5OH+HO2=C2H4OH+H2O2 2.43E+4 2.55 15750.0 !temp
!C2H5OH+HO2=C2H5O+H2O2 3.80E+12 0.0 24000.0 !temp
!C2H5O+M=CH3CHO+H+M 0.56E+35 -5.89 25274.0
!temp
!C2H5O+M=CH3+CH2O+M 5.35E+37 -6.96 23800.0 !temp
!C2H5O+CO=C2H5+CO2 4.68E+2 3.16 5380.0 !MARINOV 1998
!C2H5O+H=CH3+CH2OH 3.00E+13 0.0 0.0 !MARINOV 1998
!C2H5O+H=C2H4+H2O 3.00E+13 0.0 0.0 !MARINOV 1998
!C2H5O+OH=CH3CHO+H2O 1.00E+13 0.0 0.0 !MARINOV 1998
!CH3CHOH+O2=CH3CHO+HO2 4.82E+13 0.0 5017.0 !MARINOV 1998

```

```

!DUP
!CH3CHOH+O2=CH3CHO+HO2      8.43E+14  -1.2      0.0 !MARINOV 1998
!DUP
!CH3CHOH+O=CH3CHO+OH         1.00E+14   0.0      0.0 !MARINOV 1998
!CH3CHOH+H=C2H4+H2O          3.00E+13   0.0      0.0 !MARINOV 1998
!CH3CHOH+H=CH3+CH2OH         3.00E+13   0.0      0.0 !MARINOV 1998
!CH3CHOH+HO2=CH3CHO+OH+OH    4.00E+13   0.0      0.0 !MARINOV 1998
!CH3CHOH+OH=CH3CHO+H2O       5.00E+12   0.0      0.0 !MARINOV 1998
!CH3CHOH+M=CH3CHO+H+M        1.00E+14   0.0     25000.0 !MARINOV 1998
!C2H4+OH=C2H4OH              2.41E+11   0.0    -2385.0
!Diau, 1992
!C2H4OH+O2=HOC2H4O2          1.00E+12   0.0    -1100.0
!MARINOV 1999
!HOC2H4O2=CH2O+CH2O+OH       1.80E+11   0.0    24500.0
!temp
!CH3OCH3 = CH3+CH3O          1.87637E+49 -1.04002E+01  9.34535E+04
!P = 0.04atm
!CH3OCH3+OH = CH3OCH2+H2O    6.71E+06   2.0  -6.2988E+02
!PCCP 2001, 3, 4722-4732
!CH3OCH3+H = CH3OCH2+H2      2.97E+07   2.0  4033.61
!PCCP 2001, 3, 4722-4732
!CH3OCH3+O = CH3OCH2+OH      1.855E-03   5.29 -1.090E+02
!CH3OCH3+HO2 = CH3OCH2+H2O2  1.680E+13   0.00  1.769E+04
!CH3OCH3+CH3 = CH3OCH2+CH4   3.86E-08   6.2464 2513.9
!CH3OCH3+O2 = CH3OCH2+HO2    4.100E+13   0.00  4.491E+04
!CH3OCH3+CH3O = CH3OCH2+CH3OH 6.020E+11   0.00  4.074E+03
!CH3OCH2 = CH2O+CH3          1.600E+13   0.00  2.550E+04
!CH3OCH2+CH3O = CH3OCH3+CH2O 2.410E+13   0.00  0.000E+00
!CH3OCH2+CH2O = CH3OCH3+HCO  5.490E+03   2.80  5.862E+03
!CH3OCH2+O2 => CH2O + CH2O + OH 5.02345E+23 -3.80666E+00  3.10000E+03
!p=0.04atm
!CH3OCH2 + HO2 = CH3OCH2O + OH 9.000E+12   0.00  0.000E+00
!CH3OCH2O = CH3OCHO+H        1.745E+16  -0.66  1.172E+04
!CH3OCHO = CH3+OCHO          1.392E+18  -0.99  7.914E+04
!CH3OCHO+O2 = CH3OCO+HO2     1.000E+13   0.00  4.970E+04
!CH3OCHO+OH = CH3OCO+H2O     2.340E+07   1.61 -3.500E+01
!CH3OCHO+HO2 = CH3OCO+H2O2   1.220E+12   0.00  1.700E+04
!CH3OCHO+O = CH3OCO+OH       2.350E+05   2.50  2.230E+03
!CH3OCHO+H = CH3OCO+H2       4.550E+06   2.00  5.000E+03
!CH3OCHO+CH3 = CH3OCO+CH4    7.550E-01   3.46  5.481E+03
!CH3OCHO+CH3O = CH3OCO+CH3OH 5.480E+11   0.00  5.000E+03
!CH3OCO = CH3O + CO          7.451E+12  -1.76  1.715E+04
!CH3OCO = CH3 + CO2          1.514E+12  -1.78  1.382E+04
!OCHO + M = H + CO2 + M      2.443E+15  -0.50  2.650E+04

=====
!= HNO Mechanism Subset =
=====
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   NH Chemistry               !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH+M=N+H+M                    2.65E+14   0.0     75500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH+M=N+H+M                    2.65E+14   0.0     75510.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91 keyed
to Ar=1.0

!NH+H=N+H2                     3.50E+13   0.0     1728.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+H=N+H2                     3.200E+13   0.000   330.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+H=N+H2                     3.00E+13   0.000   0

```

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90,rv
!NH+H=N+H2          3.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N+H2=NH+H          2.33E+14    0.0    30830.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZT00 (JCP 113,
6152, 2000)
NH+H=N+H2          3.20E+13    0.0    325.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH+H=N+H2          3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DAV/HAN90,rv
!NH+H=N+H2          3.20E+13    0.00    325
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NH+H=N+H2          3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90,rv
!NH+H=N+H2          3.0E+13    0.0    0.0
!Miller personal communication; Original comments: DAVIDSON&HANSON 1990

!NH+O=N+OH          1.70E+08    1.5    3368.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
!NH+O=N+OH          3.72E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91
!N+OH=NH+O          6.40E+12    0.10    21249.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O=N+OH          1.70E+08    1.50    3366.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O=N+OH          7.00E+12    0.00    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

!NH+OH=N+H2O        1.20E+06    2.00    -487.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+OH=N+H2O        2.000E+09    1.200    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+OH=N+H2O        5.00E+11    0.500    2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH+OH=N+H2O        5.00E+11    0.5    2000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+OH=N+H2O        5.00E+11    0.5    2000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
NH+OH=N+H2O        1.60E+07    1.733    -576
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!NH+OH=N+H2O        2.00E+09    1.20    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NH+OH=N+H2O        5.0E+11    0.500    2000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH+OH=N+H2O        0.500E+12    0.500    2000.000
!Miller personal communication; Original comments: NH3 CST

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!          !!
!!   NH2 Chemistry   !!
!!          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2+M=NH+H+M        3.16E+23    -2.0    91400.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH2+M=NH+H+M        3.16E+23    -2.0    91400
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

!NH2+H=NH+H2        4.80E+08    1.50    7934.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+H=NH+H2        7.20E+05    2.320    799
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG95
!NH2+H=NH+H2        4.00E+13    0.0    3650.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

!NH2+H=NH+H2	4.000E+13	0.000	3650.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH2+H=NH+H2	4.00E+13	0.0	3650.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90			
!NH+H2=NH2+H	1.00E+14	0.0	20070.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186. [EDIT TEST]			
!NH2+H=NH+H2	7.20E+05	2.320	799
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG95			
!NH2+H=NH+H2	1.00E+06	2.32	799
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+H=NH+H2	7.2E+05	2.320	799
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG95			
NH2+H=NH+H2	4.0E+13	0.0	3650.
!Miller personal communication; Original comments: NH2-NO2 paper [EDIT TEST]			
!NH2+O=NH+OH	7.00E+12	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+O=NH+OH	3.30E+08	1.50	5074.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+O=OH+NH	3.000E+12	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
NH2+O=NH+OH	7.00E+12	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: INO/WAS99,DRA/WAG84,ADA/PHI94			
DUPLICATE			
NH2+O=NH+OH	8.60E-01	4.010	1673
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DUA/PAG95			
DUPLICATE			
!NH2+O=NH+OH	6.80E+12	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+O=NH+OH	7.00E+12	0.00	0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00			
! DUPLICATE			
!NH2+O=NH+OH	3.33E+08	1.50	5077
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00			
! DUPLICATE			
!NH2+O=NH+OH	7.00E+12	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09			
INO/WAS99,DRA/WAG84,ADA/PHI94			
! DUPLICATE			
!NH2+O=NH+OH	8.60E-01	4.010	1673
!Klippenstein et al. C&F 158 (2011) 774-789.			
! DUPLICATE			
!NH2+O=NH+OH	7.00E+12	0.00	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+O=NH+OH	7.0E+12	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:			
INO/WAS99,DRA/WAG84,ADA/PHI94			
! DUPLICATE			
!NH2+O=NH+OH	8.6E-1	4.010	1673
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: DUA/PAG95			
! DUPLICATE			
!NH2+O=NH+OH	0.675E+13	0.000	0.000
!Miller personal communication; Original comments:			
!NH2+OH=NH+H2O	2.40E+06	2.00	50.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+OH=NH+H2O	9.000E+07	1.500	-460.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH2+OH=NH+H2O	4.00E+06	2.000	1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NH2+OH=NH+H2O	4.00E+06	2.0	1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+OH=NH+H2O	4.00E+06	2.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
NH2+OH=NH+H2O	3.30E+06	1.949	-217
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09,adj			



!NH2+OH=NH+H2O	9.00E+07	1.50	-460
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+OH=NH+H2O	4.0E+06	2.000	1000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH2+OH=NH+H2O	0.400E+07	2.000	1000.000
!Miller personal communication; Original comments: JAM,9/87			
!NH2+O2=NH+HO2	1.00E+14	0.0	49997.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94			
!NH+NH=NH2+N	5.95E+02	2.9	-2030.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+NH=NH2+N	5.70E-01	3.880	342
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!!			!!
!!	NH3 Chemistry		!!
!!			!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!NH3(+M)=NH2+H(+M)	3.60E+16	0.0	93733.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH3+M=NH2+H+M	2.20E+16	0.000	93470
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90			
!NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH3(+M)=NH2+H(+M)	5.50E+15	0.00	107792.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)			
!	LOW/	2.20E+16	0.00 93470. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)			
!NH3+M=NH2+H+M	2.20E+16	0.0	93470.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH3+M=NH2+H+M	2.20E+16	0.000	93470
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DAV/HAN90			
!NH3+M=NH2+H+M	2.20E+16	0.00	93500
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH3+M=NH2+H+M	2.2E+16	0.000	93470
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90			
!NH3+M=NH2+H+M	2.2E+16	0.0	93470.
!Miller personal communication; Original comments: NH2-NO2 paper			
!	CO/2/ H2/2/ CO2/3/ H2O/5/		
!NH3+M=NH+H2+M	6.30E+14	0.0	93390.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH3+H=NH2+H2	5.40E+05	2.40	9910.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH3+H=NH2+H2	5.400E+05	2.400	9915.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH3+H=NH2+H2	6.40E+05	2.390	10171
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIC/SUT86			
!NH3+H=NH2+H2	6.40E+05	2.4	10171.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH3+H=NH2+H2	5.42E+05	2.40	9917.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; KMF90 (Ko, Marshall...) [EDIT TEST]			
!NH3+H=NH2+H2	5.42E+05	2.4	9920.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH3+H=NH2+H2	6.40E+05	2.390	10171
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIC/SUT86			
!NH3+H=NH2+H2	5.42E+05	2.40	9920
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011			
!NH3+H=NH2+H2	6.4E+05	2.390	10171

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIC/SUT86  
NH3+H=NH2+H2 0.636E+06 2.390 10171.000  
!Miller personal communication; Original comments: MICHAEL [EDIT TEST]

!NH3+O=NH2+OH 9.40E+06 1.94 6454.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH3+O=NH2+OH 9.40E+06 1.940 6460.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NH3+O=NH2+OH 9.40E+06 1.940 6460  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SUT/KLE90  
!NH3+O=NH2+OH 9.40E+06 1.9 6460.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH3+O=NH2+OH 9.40E+06 1.94 6460.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
SUT/PAT/KLEMM90  
NH3+O=NH2+OH 2.80E+02 3.290 4471  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09  
!NH3+O=NH2+OH 1.10E+06 2.10 5210  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH3+O=NH2+OH 9.4E+06 1.940 6460  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SUT/KLE90  
!NH3+O=NH2+OH 9.4E+6 1.90 6460.  
!Miller personal communication; Original comments: NH2-NO2 paper

!NH3+OH=NH2+H2O 5.00E+07 1.60 953.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH3+OH=NH2+H2O 5.00E+07 1.600 955.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NH3+OH=NH2+H2O 2.00E+06 2.040 566  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SAL/HAN84  
NH3+OH=NH2+H2O 2.00E+06 2.0 566.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH3+OH=NH2+H2O 2.04E+06 2.04 566.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!NH3+OH=NH2+H2O 2.00E+06 2.040 566  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 SAL/HAN84  
!NH3+OH=NH2+H2O 3.683E+03 2.86 -197.  
!Corchado et al. J. Phys Chem 99 (1995) 687-694. ; NIST Fit.  
!NH3+OH=NH2+H2O 5.00E+07 1.60 950  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH3+OH=NH2+H2O 2.0E+06 2.040 566  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SAL/HAN84  
!NH3+OH=NH2+H2O 0.204E+07 2.040 566.000  
!Miller personal communication; Original comments: LOUGE

!NH2+HO2=NH3+O2 9.20E+05 1.94 -1152.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+HO2=NH3+O2 9.20E+05 1.940 -1152  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!NH2+HO2=NH3+O2 9.20E+05 1.9 -1152.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+HO2=NH3+O2 2.0E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97,  
298 K  
!NH2+HO2=NH3+O2 9.20E+05 1.940 -1152  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!NH2+HO2=NH3+O2 9.2E+05 1.940 -1152  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
!NH2+HO2=NH3+O2 1.0E+13 0.0 0.0  
!Miller personal communication; Original comments: JAM/PG

!NH3+HO2=NH2+H2O2 3.00E+11 0.000 22000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!NH3+HO2=NH2+H2O2 3.00E+11 0.0 22000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

!NH3+HO2=NH2+H2O2	3.00E+11	0.000	22000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			
!NH3+HO2=NH2+H2O2	3.0E+11	0.000	22000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH3+HO2=NH2+H2O2	3.0E+11	0.0	22000.
!Miller personal communication; Original comments: MILLER&BOWMAN IJCK			
!NH2+NH=NH3+N	9.20E+05	1.94	2443.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+NH=NH3+N	9.20E+05	1.940	2444
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!NH2+NH=NH3+N	9.20E+05	1.9	2444.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+NH=NH3+N	1.00E+13	0.0	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+NH=NH3+N	9.60E+03	2.460	107
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!NH2+NH=NH3+N	1.00E+13	0.00	2000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NH=NH3+N	9.2E+05	1.940	2444
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!NH2+NH2=NH3+NH	5.00E+13	0.0	9929.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+NH2=NH3+NH	5.00E+13	0.000	10000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DAV/HAN90			
!NH2+NH2=NH3+NH	5.00E+13	0.0	10000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+NH2=NH+NH3	5.00E+13	0.0	10000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90			
!NH3+NH=NH2+NH2	3.16E+14	0.0	26770.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
NH2+NH2=NH3+NH	5.60E+00	3.530	552
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!NH3+NH=NH2+NH2	3.16E+14	0.00	26800
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NH2=NH3+NH	5.0E+13	0.000	10000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DAV/HAN90			
!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!!		!!	
!!	N2 Chemistry	!!	
!!		!!	
!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!N2+M=N+N+M	3.71E+21	-1.6	225000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Baulch et al, 1973			
!N2+M=N+N+M	1.00E+28	-3.3	225000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+N=N2+H	1.50E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+N=N2+H	1.500E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+N=N2+H	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NH+N=N2+H	3.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+N=N2+H	3.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NH+N=N2+H	9.00E+11	0.5	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH+N=N2+H	3.00E+13	0.000	0

```

!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH+N=N2+H          9.00E+11    0.50    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH+N=N2+H          3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH+N=N2+H          0.300E+14   0.000    0.000
!Miller personal communication; Original comments: JAM

!NH+NH=N2+H+H      5.10E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+NH=N2+H+H      2.50E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH+NH=N2+H+H      2.50E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+NH=N2+H+H      5.10E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB89
!NH+NH=N2+H+H      2.5E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH+NH=N2+H+H      0.254E+14   0.000    0.000
!Miller personal communication; Original comments: NH3 CST

!NH2+N=N2+H+H      7.10E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+N=N2+H+H      7.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 WHY/PHI83
!NH2+N=N2+H+H      7.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+N=N2+H+H      7.20E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NH2+N=N2+H+H      6.90E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH2+N=N2+H+H      7.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 WHY/PHI83
!NH2+N=N2+H+H      6.90E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+N=N2+H+H      7.0E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 WHY/PHI83
!NH2+N=N2+H+H      0.720E+14   0.000    0.000
!Miller personal communication; Original comments: JAM/PG

!NH+NH=N2+H2        1.00E+08    1.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                      !!
!!   NNH Chemistry     !!
!!                      !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NNH=N2+H           3.300E+08   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+M=N2+H+M      1.300E+14   -0.110  4980.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!   CO2/2.00/ C2H6/3.00/ AR/ .70/
!NNH=N2+H           6.50E+07   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99
!NNH=N2+H           6.50E+07   0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH(+M)=N2+H(+M)  4.10E+09   1.13   5186.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D95; high P
limit [EDIT TEST]
!   LOW/           1.00E+13   0.5    3060. /

```

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D95; low P
limit
!      N2O/5.0/ H2O/9.0/ N2/1.0/ O2/0.82/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; like N2O+M
!      HNO3/5.0/ NH3/5.0/ NO3/5.0/
!
!      DUPLICATE
!NNH=N2+H                                3.00E+08    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; tunneling
term, B&D95 [EDIT TEST]
!      DUPLICATE
!NNH=N2+H                                3.00E+08    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!      DUPLICATE
!NNH+M=N2+H+M                            1.00E+13    0.5    3060.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!      DUPLICATE
NNH=N2+H                                1.00E+09    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST]
!NNH=N2+H                                3.00E+08    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH+M=N2+H+M                            1.00E+13    0.50    3060
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH=N2+H                                6.5E+07    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99
!NNH=N2+H                                6.5E+7     0.0     0.0
!Miller personal communication; Original comments: JAM 6/98

!NNH+H=N2+H2                            2.40E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+H=H2+N2                            5.00E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+H=N2+H2                            1.00E+14    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NNH+H=N2+H2                            1.00E+14    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+H=N2+H2                            1.00E+14    0.0     0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NNH+H=N2+H2                            1.00E+14    0.0     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NNH+H=N2+H2                            1.00E+14    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+H=N2+H2                            1.0E+14    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+H=N2+H2                            0.100E+15  0.000    0.000
!Miller personal communication; Original comments: JAM,9/87

!NH+NH=NNH+H                            5.10E+13    0.0     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NH+NH=NNH+H                            5.10E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

!NNH+O=N2+OH                            1.70E+16    -1.23    496.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+O=N2+OH                            1.70E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+O=OH+N2                            2.500E+13  0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+O=N2+OH                            8.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NNH+O=N2+OH                            8.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+O<=>OH+N2                          2.500E+13  0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)
!NNH+O=N2+OH                            1.20E+13    0.145    -217
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw

```

!NNH+O=N2+OH	8.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NNH+O=N2+OH	8.0E+13	0.0	0.0
!Miller personal communication; Original comments:			
!NNH+OH=N2+H2O	2.40E+22	-2.88	2453.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+OH=N2+H2O	1.20E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+OH=H2O+N2	2.000E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+OH=N2+H2O	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NNH+OH=N2+H2O	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+OH=N2+H2O	5.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NNH+OH=N2+H2O	5.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			
!NNH+OH=N2+H2O	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NNH+OH=N2+H2O	0.500E+14	0.000	0.000
!Miller personal communication; Original comments:			
!NNH+O2=N2+HO2	1.20E+12	-0.34	149.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+O2=HO2+N2	5.000E+12	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NNH+O2=N2+HO2	2.00E+14	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+HO2	2.00E+14	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O2<=>HO2+N2	5.000E+12	0.000	0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)			
!NNH+O2=N2+HO2	5.60E+14	-0.385	-13
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NNH+O2=N2+HO2	2.0E+14	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+HO2	2.0E+14	0.0	0.0
!Miller personal communication; Original comments: JAM			
!NNH+O2=N2+H+O2	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+H+O2	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+O2=N2+H+O2	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99			
!NNH+O2=N2+O2+H	5.0E+13	0.0	0.0
!Miller personal communication; Original comments: JAM			
!NNH+HO2=N2+H2O2	1.40E+04	2.69	-1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NNH+N=NH+N2	3.00E+13	0.0	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NNH+NH=N2+NH2	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NNH+NH=N2+NH2	5.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NNH+NH=N2+NH2	5.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NNH+NH=N2+NH2	2.00E+11	0.5	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NNH+NH=N2+NH2	5.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			

```

!NNH+NH =N2+NH2          5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NH=N2+NH2          0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

!NNH+NH2=N2+NH3          9.20E+05    1.94    -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+NH2=N2+NH3          5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NNH+NH2=N2+NH3          5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+NH2=N2+NH3          5.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NNH+NH2=N2+NH3          1.00E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NNH+NH2=N2+NH3          5.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+NH2=N2+NH3          5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NH2=N2+NH3          0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  N2H2 Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!N2H2=NNH+H              5.60E+36    -7.75    70211.
!0.1 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H              1.80E+40    -8.41    73348.
!1.0 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H              3.10E+41    -8.42    76000.
!10 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H              1.60E+37    -7.94    70717.
!0.1 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H              2.60E+40    -8.53    72882.
!1.0 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=NNH+H              1.30E+44    -9.22    77032.
!10 atm                 Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2+M=NNH+H+M          1.90E+27    -3.050    66107
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 M=N2
!  H2O/7/
!N2H2+M=NNH+H+M          5.00E+16    0.0    50000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: MB89
N2H2+M=NNH+H+M          5.00E+16    0.0    50000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
  H2O/15.0/ N2/2.0/ H2/2.0/ !O2/2.0/
!N2H2+M=NNH+H+M          5.00E+16    0.0    50000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!  N2/2.00/ H2/2.00/
!N2H2+M=NNH+H+M          1.90E+27    -3.050    66107
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 M=N2
!  H2O/7/
!N2H2+M=NNH+H+M          5.00E+16    0.00    50000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!  H2/2/ H2O/15/ O2/2/ N2/2/
!N2H2+M=NNH+H+M          1.9E+27    -3.050    66107
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
M=N2
!  H2O/7/
!N2H2+M=NNH+H+M          0.500E+17    0.000    50000.000
!Miller personal communication; Original comments: NH3 CST
!  H2O/15/ O2/2/ N2/2/ H2/2/

```

!N2H2+M=NH+NH+M	3.16E+16	0.0	99400.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
! N2/2.00/ H2/2.00/			
!NH2+NH=N2H2+H	1.50E+15	-0.50	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+NH=N2H2+H	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!NH2+NH=N2H2+H	1.50E+15	-0.5	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!NH2+NH=N2H2+H	1.50E+15	-0.50	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DKCH90			
!NH2+NH=N2H2+H	1.50E+15	-0.5	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186. [EDIT TEST]			
!NH2+NH=N2H2+H	4.30E+14	-0.272	-77
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09 [EDIT TEST]			
!NH2+NH=N2H2+H	1.50E+15	-0.50	0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NH=N2H2+H	5.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			
!NH2+NH=N2H2+H	0.500E+14	0.000	0.000
!Miller personal communication; Original comments: NH3CST			
!N2H2+H=NNH+H2	4.80E+08	1.50	1579.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
N2H2+H=NNH+H2	8.50E+04	2.630	230
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+H=NNH+H2	4.80E+08	1.5	1580.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+H=NNH+H2	5.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+H=NNH+H2	8.50E+04	2.6	-230.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+H=NNH+H2	8.50E+04	2.630	230
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+H=NNH+H2	8.50E+04	2.63	-230
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+H=NNH+H2	8.5E+04	2.630	230
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+H=NNH+H2	0.500E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!2NH2=N2H2+H2	5.00E+11	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DAV90			
!NH2+NH2=N2H2+H2	1.00E+13	0.0	1500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
NH2+NH2=N2H2+H2	1.70E+08	1.620	11783
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09			
!NH2+NH2=N2H2+H2	5.00E+13	0.00	1500
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+NH2=N2H2+H2	8.5E+11	0.0	0.0
!Miller personal communication; Original comments: NH2-NO2 paper			
!N2H2+O=NNH+OH	3.30E+08	1.50	496.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+O=NNH+OH	3.30E+08	1.500	497
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+O=NNH+OH	3.30E+08	1.5	497.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N2H2+O=NNH+OH	2.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+O=NNH+OH	3.30E+08	1.500	497
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			



!N2H2+O=NNH+OH	2.00E+13	0.00	1000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+O=NNH+OH	3.3E+08	1.500	497
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+O=NNH+OH	0.200E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!N2H2+OH=NNH+H2O	2.40E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
N2H2+OH=NNH+H2O	5.90E+01	3.400	1360
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	2.40E+06	2.0	-600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+OH=NNH+H2O	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+OH=NNH+H2O	5.90E+01	3.400	1360
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	5.92E+01	3.40	-1360
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+OH=NNH+H2O	5.9E+01	3.400	1360
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+OH=NNH+H2O	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!N2H2+N=NNH+NH	1.00E+06	2.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH=NNH+NH2	2.40E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+NH=NNH+NH2	2.40E+06	2.000	-1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	2.40E+06	2.0	-1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+NH=NNH+NH2	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+NH=NNH+NH2	1.00E+13	0.0	6000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH=NNH+NH2	2.40E+06	2.000	-1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	2.4E+06	2.000	-1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H2+NH=NNH+NH2	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			
!N2H2+NH2=NH3+NNH	1.80E+06	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H2+NH2=NNH+NH3	8.80E-02	4.050	1610
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+NH2=NH3+NNH	1.80E+06	1.9	-1152.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000			
!N2H2+NH2=NH3+NNH	1.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N2H2+NH2=NH3+NNH	8.80E-02	4.0	-1610.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H2+NH2=NNH+NH3	8.80E-02	4.050	1610
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+NH2=NH3+NNH	8.80E-02	4.05	-1610
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N2H2+NH2=NNH+NH3	8.8E-2	4.050	1610
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 LIN/PAG96			
!N2H2+NH2=NH3+NNH	0.100E+14	0.000	1000.000
!Miller personal communication; Original comments: NH3 CST			

```

!NNH+NNH=N2H2+N2                                1.00E+13    0.0    4000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
!! H2NN Chemistry !!
!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!H2NN=NNH+H                                5.90E+32    -6.99    51762.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                9.60E+35    -7.57    54810.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                5.00E+36    -7.43    57263.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                7.20E+28    -7.77    50729.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                3.20E+31    -6.22    52288.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                5.10E+33    -6.52    54185.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN=NNH+H                                3.40E+26    -4.830   46228
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM
!H2NN=NNH+H                                3.40E+26    -4.830   46228
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM
!H2NN=NNH+H                                3.4E+26    -4.830   46228
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1
ATM

!N2H2=H2NN                                9.20E+38    -9.01    67689.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=H2NN                                2.00E+41    -9.38    68413.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H2=H2NN                                1.30E+45    -10.13   70717.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!H2NN+H=N2H2+H                            1.80E+10    0.97    4468.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+H=N2H2+H                            7.00E+13    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+H=N2H2+H                            7.00E+13    0.000   0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+H=N2H2+H                            7.0E+13    0.000   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+H=NNH+H2                            4.80E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+H=NNH+H2                            4.80E+08    1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+H=NNH+H2                            4.80E+08    1.500   -894
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+H=NNH+H2                            4.8E+08    1.500   -894
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2+NH2=H2NN+H2                          2.40E+20    -2.91    2135.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                          1.20E+21    -3.08    3366.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                          2.30E+19    -2.54    4180.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=H2NN+H2                          1.20E+21    -3.080   3368
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2
!NH2+NH2=H2NN+H2                          7.20E+04    1.880   8802
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

```

```

!NH2+NH2=H2NN+H2                1.2E+21   -3.080   3368
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1
ATM N2

!H2NN+O=OH+NNH                    3.30E+08   1.50   -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+O=NNH+OH                    3.30E+08   1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NNH+OH                    3.30E+08   1.500   -894
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NNH+OH                    3.3E+08    1.500   -894
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+OH=NNH+H2O                  2.40E+06   2.00   -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+OH=NNH+H2O                  2.40E+06   2.000   -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=NNH+H2O                  2.40E+06   2.000   -1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=NNH+H2O                  2.4E+06    2.000   -1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+HO2=NNH+H2O2                2.90E+04   2.69   -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+HO2=NNH+H2O2                2.90E+04   2.690   -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=NNH+H2O2                2.90E+04   2.690   -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=NNH+H2O2                2.9E+04    2.690   -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+NH2=NH3+NNH                 1.80E+06   1.94   -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+NH2=NNH+NH3                 1.80E+06   1.940   -1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+NH2=NNH+NH3                 1.80E+06   1.940   -1152
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+NH2=NNH+NH3                 1.8E+06    1.940   -1152
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  N2H3 Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2H3=N2H2+H                       2.30E+43   -9.55   64432.
!0.1 atm                            Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3=N2H2+H                       3.60E+47   -10.38   68970.
!1.0 atm                            Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3=N2H2+H                       1.80E+45   -9.39    70101.
!10 atm                             Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3=N2H2+H                       3.60E+47   -10.380   69009
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2 600-
2500K
!N2H3+M=N2H2+H+M                   1.00E+16   0.0     37000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H3=N2H2+H                       3.60E+47   -10.380   69009
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2
600-2500K
!N2H3=N2H2+H                       3.6E+47   -10.380   69009
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
1ATM N2 600-2500K

!N2H3+M=NH2+NH+M                   5.00E+16   0.0     60000.0

```

!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!NH2+NH2=N2H3+H	9.20E+11	-0.01	10009.
!0.1 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!NH2+NH2=N2H3+H	1.20E+12	-0.03	10078.
!1.0 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!NH2+NH2=N2H3+H	4.70E+12	-0.20	10615.
!10 atm	Dean & Bozzelli	"Gas-Phase Combustion Chemistry"	Ch. 2 (2000)
!NH2+NH2=N2H3+H	1.20E+12	-0.030	10084
!Tian et al. C&F 156 (2009) 1413-1426;	Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !		
!NH2+NH2=N2H3+H	1.79E+13	-0.35	11320.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D93, AMD, priv. comm.			
!N2H3+H=NH2+NH2	5.00E+13	0.0	2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH2+NH2=N2H3+H	1.20E+12	-0.030	10084
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !			
!NH2+NH2=N2H3+H	1.2E+12	-0.030	10084
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00 1 ATM N2 !			
!N2H3+H=N2H2+H2	2.40E+08	1.50	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+H=N2H2+H2	2.40E+08	1.500	-10
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+H=N2H2+H2	2.40E+08	1.50	-10
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION 1/15/96 (DB00)			
!N2H3+H=N2H2+H2	1.00E+13	0.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H3+H=N2H2+H2	2.40E+08	1.500	-10
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+H=N2H2+H2	2.4E+08	1.500	-10
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+H=NH+NH3	1.00E+11	0.0	0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NH3+NH2=N2H3+H2	1.00E+11	0.5	21600.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!N2H3+O=N2H2+OH	1.70E+08	1.50	-645.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+O=N2H2+OH	1.70E+08	1.500	-646
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+O=N2H2+OH	1.70E+08	1.50	-646
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION 1/15/96 (DB00)			
!N2H3+O=N2H2+OH	1.70E+08	1.500	-646
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+O=N2H2+OH	1.7E+08	1.500	-646
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+OH=N2H2+H2O	1.20E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+OH=N2H2+H2O	1.20E+06	2.000	-1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+OH=N2H2+H2O	1.20E+06	2.00	-1192
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION 1/15/96 (DB00)			
!N2H3+OH=N2H2+H2O	1.20E+06	2.000	-1192
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+OH=N2H2+H2O	1.2E+06	2.000	-1192
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			

```

!N2H3+OH=H2NN+H2O          3.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3+OH=H2NN+H2O          3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+OH=H2NN+H2O          3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+OH=H2NN+H2O          3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H3+HO2=N2H2+H2O2         2.90E+04    2.69   -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3+HO2=N2H2+H2O2         1.40E+04    2.690   -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+HO2=N2H2+H2O2         2.90E+04    2.69   -1600
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; UPDATE
10/18/97 (DB00)
!N2H3+HO2=N2H2+H2O2         1.40E+04    2.690   -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+HO2=N2H2+H2O2         1.4E+04    2.690   -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H3+N=N2H2+NH            1.00E+06    2.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H3+NH=N2H2+NH2          2.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!N2H3+NH=N2H2+NH2          2.00E+13    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H3+NH=N2H2+NH2          2.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!N2H3+NH=N2H2+NH2          2.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

!N2H3+NH2=N2H2+NH3         9.20E+05    1.94   -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3+NH2=N2H2+NH3         9.20E+05    1.940   -1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+NH2=N2H2+NH3         9.20E+05    1.94   -1152
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
1/15/96 (DB00)
!N2H3+NH2=NH3+N2H2          1.00E+11    0.5    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H3+NH2=N2H2+NH3         9.20E+05    1.940   -1152
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+NH2=N2H2+NH3         9.2E+05    1.940   -1152
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H3+NH2=H2NN+NH3         3.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3+NH2=H2NN+NH3         3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+NH2=H2NN+NH3         3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+NH2=H2NN+NH3         3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H3+NNH=N2H2+N2H2         1.00E+13    0.0    4000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H3+N2H3=NH3+NH3+N2       3.00E+12    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!

```

```

!! N2H4 Chemistry    !!
!!                  !!
!!!!!!!!!!!!!!!!!!!!

!NH2+NH2=N2H4                2.00E+46   -10.93   9989.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                5.60E+48   -11.30   11876.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                3.20E+49   -11.18   13981.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NH2=N2H4                5.60E+48   -11.300  11882
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00 1ATM N2(600-2500K)!
!NH2+NH2+M=N2H4+M           2.98E+47   -9.44    9680.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B&D93, AMD,
priv. comm.
!N2H4(+M)=NH2+NH2(+M)       5.00E+14    0.0     60000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   LOW/                      1.50E+15    0.0     39000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.40/ NH3/3.00/ N2H4/4.00/
!NH2+NH2(+M)=N2H4(+M)       5.60E+14   -0.414   66
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!   LOW/                      1.60E+34   -5.49    1987 /
!Klippenstein et al. C&F 158 (2011) 774-789.
!   TROE/ 0.31 1E-30 1E30 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: (Fc=0.31) ??
!NH2+NH2=N2H4                5.6E+48   -11.300  11882
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
1ATM N2(600-2500K)!

!N2H4+M=N2H3+H+M           1.00E+15    0.0     63600.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   N2/2.40/ NH3/3.00/ N2H4/4.00/

!N2H4=H2NN+H2                4.00E+44   -9.85    71313.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4=H2NN+H2                5.30E+39   -8.35    69267.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4=H2NN+H2                2.50E+39   -8.19    69625.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!N2H4+H=N2H3+H2             9.60E+08    1.50    4836.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4+H=N2H3+H2             7.00E+12    0.000   2500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 VAG95
!N2H4+H=N2H3+H2             4.90E+12    0.00    2130.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; fit to data
from 6 sources in NIST (WRA)
!N2H4+H=N2H3+H2             7.00E+12    0.0     2500.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H4+H=N2H3+H2             7.00E+12    0.000   2500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 VAG95
!N2H4+H=N2H3+H2             7.0E+12     0.000   2500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 VAG95

!N2H4+H=NH2+NH3             2.40E+09    0.0     3100.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H4+O=N2H3+OH             6.70E+08    1.50    2850.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4+O=N2H3+OH             1.50E+11    0.000  -1270
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG96,VAG01
!N2H4+O=N2H3+OH             6.70E+08    1.50    2851
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95                      (DB00)

```

```

!N2H4+O=N2H3+OH                6.70E+08    1.500    2851
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H4+O=N2H3+OH                1.5E+11    0.000   -1270
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG96,VAG01

!N2H4+O=N2H2+H2O                4.40E+11    0.000   -1270
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 VAG96

!N2H4+OH=N2H3+H2O              4.80E+06    2.00    -645.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4+OH=N2H3+H2O              1.30E+13    0.000   -318
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG01
!N2H4+OH=N2H3+H2O              4.80E+06    2.00    -646
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95 (DB00)
!N2H4+OH=N2H3+H2O              4.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HAR/ATK79
!N2H4+OH=N2H3+H2O              1.3E+13    0.000   -318
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG01

!N2H3+HO2=N2H4+O2              9.20E+05    1.94    2125.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H3+HO2=N2H4+O2              9.20E+05    1.940   2126
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+HO2=N2H4+O2              9.20E+05    1.94    2126
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; NH2 WITH
ADJUSTED THERMO (DB00)
!N2H3+HO2=N2H4+O2              9.20E+05    1.940   2126
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+HO2=N2H4+O2              9.2E+05    1.940   2126
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H4+N=N2H3+NH                1.00E+10    1.0     2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H4+NH=NH2+N2H3              1.00E+09    1.5     2000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H4+NH2=N2H3+NH3             3.70E+06    1.94    1628.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2H4+NH2=N2H3+NH3             3.90E+12    0.000   1500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 GEH/WAG71,JAM est
!N2H4+NH2=N2H3+NH3             1.80E+06    1.7     -1380.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!N2H4+NH2=N2H3+NH3             3.90E+12    0.000   1500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 GEH/WAG71,JAM est
!N2H4+NH2=N2H3+NH3             3.9E+12    0.000   1500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 GEH/WAG71,JAM
est

!N2H3+N2H2=N2H4+NNH            1.00E+13    0.0     6000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!N2H3+N2H3=N2H4+N2H2            1.20E+13    0.0     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   NO Chemistry               !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NO(+M)=N+O(+M)                 1.45E+15    0.0     148345.
!1.4      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663

```

```

!NO(+M)=N+O(+M) 1.40E+15 0.0 148345.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO+M=N+O+M 1.40E+15 0.0 148429.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ
2000
!NO+M=N+O+M 1.40E+15 0.0 148430.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
! N2/1.0/ H2/2.2/ H2O/6.7/ CO2/3.0/
! N2O/2.2/

!NO+H=N+OH 1.69E+14 0.0 48773.
!1.5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!NO+H=N+OH 1.70E+14 0.0 48800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HS85
!N+OH=NO+H 1.10E+14 0.0 1122.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N+OH=NO+H 3.360E+13 0.000 385.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
N+OH=NO+H 3.80E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 FLO/HAN77,HOW/SMI80
!N+OH=NO+H 3.80E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N+OH=NO+H 3.80E+13 0.000 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04
FLO/HAN77,HOW/SMI80
!N+OH=NO+H 2.80E+13 0.00 0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!N+OH=NO+H 3.8E+13 0.000 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04
FLO/HAN77,HOW/SMI80
!N+OH=NO+H 0.380E+14 0.000 0.000
!Miller personal communication; Original comments: SMITH,FLOWER

!NH+O=NO+H 6.00E+13 0.0 0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O=NO+H 4.000E+13 0.000 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+O=NO+H 9.20E+13 0.000 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 CEC94
NH+O=NO+H 9.20E+13 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+O=NO+H 5.50E+13 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MCHB91
!NH+O=NO+H 9.20E+13 0.000 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 CEC94
!NH+O=NO+H 7.00E+13 0.00 0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NH+O=NO+H 9.2E+13 0.000 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 CEC94
!NH+O=NO+H 9.2E+13 0.0 0.0
!Miller personal communication; Original comments: MERTENS

!NH2+O=NO+H2 5.00E+12 0.0 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: COH91
!NH2+O=H2+NO 5.00E+12 0.00 0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

NH+OH=NO+H2 2.00E+13 0.00 0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

!NO+O=O2+N 1.81E+09 1.0 38725.
!1.5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!O+NO=N+O2 3.80E+09 1.0 41375.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
!N+O2=NO+O 9.00E+09 1.00 6494.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```



!N+O2=NO+O	9.000E+09	1.000	6500.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N+O2=NO+O	6.40E+09	1.000	6280
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	6.40E+09	1.0	6280.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N+O2=NO+O	6.40E+09	1.000	6280
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	9.00E+09	1.00	6500
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N+O2=NO+O	6.4E+09	1.000	6280
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 BAU/DRY73			
!N+O2=NO+O	0.640E+10	1.000	6280.000
!Miller personal communication; Original comments:			
!NH+O2=NO+OH	7.60E+10	0.0	1529.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+O2=NO+OH	1.280E+06	1.500	100.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+O2=NO+OH	1.30E+06	1.500	100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=NO+OH	1.30E+06	1.5	100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+O2=NO+OH	1.28E+06	1.5	100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC, 92			
!NH+O2=NO+OH	1.30E+06	1.500	100
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=NO+OH	4.50E+08	0.790	1190
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH+O2=NO+OH	1.3E+06	1.500	100
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=NO+OH	1.28E+6	1.5	100.
!Miller personal communication; Original comments: MILL&MEL 24TH			
!O+N2=N+NO	2.00E+14	0.0	76774.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N+NO=N2+O	2.700E+13	0.000	355.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!N+NO=N2+O	2.10E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05			
!N+NO=N2+O	3.30E+12	0.3	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!N+NO=N2+O	3.27E+12	0.3	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!N+NO=N2+O	2.10E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09 CEC05			
!N2+O=NO+N	1.80E+14	0.00	76100
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!N+NO=N2+O	2.1E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: CEC05			
!N+NO=N2+O	0.327E+13	0.300	0.000
!Miller personal communication; Original comments: LEEDS,MONAT			
!NH+NO=N2+OH	1.40E+17	-1.49	1311.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+NO=N2+OH	2.160E+13	-0.230	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+NO=N2+OH	2.20E+13	-0.230	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
!NH+NO=N2+OH	2.20E+13	-0.2	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+NO=N2+OH	2.16E+13	-0.23	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC, 92			
!NH+NO=N2+OH	2.70E+12	-0.0721	-512

```

!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw
!NH+NO=N2+OH          6.10E+13   -0.50   120
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH+NO=N2+OH          2.2E+13   -0.230   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92
!NH+NO=N2+OH          2.16E+13   -0.23   0.0
!Miller personal communication; Original comments: MILL&MEL 24TH

!NH+NO=NNH+O          1.70E+14   -0.20   12193.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+O=NH+NO          7.000E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NNH+O=NH+NO          5.00E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92
!NNH+O=NH+NO          5.00E+13   0.0   0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+O=NO+NH          3.30E+14   -0.23   -1013.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ditto
NNH+O=NH+NO          5.20E+11   0.381   -409
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw
!NNH+O=NH+NO          2.00E+14   0.00   4000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH+O=NH+NO          5.0E+13   0.000   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92
!NNH+O=NH+NO          5.0E+13   0.0   0.0
!Miller personal communication; Original comments: JAM&CFM 24TH

!NH2+NO=N2+H2O        4.70E+12   -0.25   -1201.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NO=N2+H2O        2.80E+20   -2.654   1258
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99
NH2+NO=N2+H2O        2.80E+20   -2.7   1258.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+NO=N2+H2O        2.77E+20   -2.65   1258.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99
!NH2+NO=N2+H2O        1.30E+16   -1.25   0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: MILKLI00,fit
!
!   DUPLICATE
!NH2+NO=N2+H2O        -3.1E+13   -0.48   1180
!Klippenstein et al. C&F 158 (2011) 774-789.
!
!   DUPLICATE
!NH2+NO=N2+H2O        2.77E+20   -2.65   1260
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+NO=N2+H2O        2.8E+20   -2.654   1258
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99
!NH2+NO=N2+H2O        2.77E+20   -2.654   1258.3
!Miller personal communication; Original comments: JAM 3/98

!NH2+NO=NNH+OH        3.50E+10   0.34   -765.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NO=NNH+OH        2.30E+10   0.425   -814
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/GLA99
!NH2+NO=NNH+OH        2.30E+10   0.4   -814.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+NO=NNH+OH        2.29E+10   0.425   -815.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99 [EDIT
TEST]
!NH2+NO=NNH+OH        3.10E+13   -0.48   1180
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: MILKLI00,fit [EDIT TEST]
[EDIT TEST]
NH2+NO=NNH+OH        2.29E+10   0.425   -814
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NH2+NO=NNH+OH        2.3E+10   0.425   -814
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/GLA99
!NH2+NO=NNH+OH        2.294E+10   0.425   -813.56
!Miller personal communication; Original comments: JAM 6/98

```

```

!N2H2+O=NH2+NO                1.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!N2H2+O=NH2+NO                1.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94
!N2H2+O=NH2+NO                1.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!N2H2+O=NH2+NO                1.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!N2H2+O=NH2+NO                1.00E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!N2H2+O=NH2+NO                1.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!N2H2+O=NH2+NO                0.100E+14    0.000    0.000
!Miller personal communication; Original comments: NH3 CST

!H2NN+O=NH2+NO                7.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NH2+NO                3.20E+09    1.03    2701.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H2NN+O=NH2+NO                7.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+O=NH2+NO                7.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+OH=>NH2+NO+H            2.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=>NH2+NO+H            2.00E+12    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+OH=>NH2+NO+H            2.0E+12    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!N2H3+O=>NH2+NO+H            3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=>NH2+NO+H            3.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!N2H3+O=>NH2+NO+H            3.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!H2NN+HO2=>NH2+NO+OH          9.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=>NH2+NO+OH          9.00E+12    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!H2NN+HO2=>NH2+NO+OH          9.0E+12    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   HNO Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NO+H(+M)=HNO(+M)              1.52E+15    -0.41    0.
!4   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!   LOW/                          8.96E+19    -1.32    735. /
!1.5-3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!   TROE/ 0.167 12.94 100000 /
!   DUPLICATE

!HNO(+M)=H+NO(+M)              1.20E+16    -0.43    49492.
!4   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!   LOW/                          6.02E+21    -1.61    50808. /
!1.5-3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663 [EDIT TEST]
!   TROE/ 0.157 12.94 100000 /
!   DUPLICATE

```

```

!HNO(+M)=H+NO(+M)                2.60E+16    0.0    48654.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!H+NO+M=HNO+M                    4.480E+19   -1.320   740.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!   CO2/2.00/ C2H6/3.00/ AR/ .70/
!NO+H(+M)=HNO(+M)                1.50E+15   -0.410    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 NBS91
!   LOW/                          2.40E+14    0.206   -1550 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 RIL/FON03
!   TROE/ 0.82 1E-30 1E30 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.82 (NBS91)
!   N2/1.6/
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 RIL/FON03
!H+NO(+M)=HNO(+M)                1.50E+15   -0.4    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   LOW/                          0.23E+15    0.206   -1550.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   N2/1.0/ H2O/10.0/ O2/1.5/ H2/2.0/
!   CO2/3.0/
!H+NO(+M)=HNO(+M)                1.52E+15   -0.41    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Fall-off, TH91
!   LOW/                          4.00E+20   -1.75    0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Glarborg et
al, ISC 1998
!   N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.3/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 from
TH91
NO+H(+M)=HNO(+M)                1.50E+15   -0.410    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 NBS91 [EDIT
TEST]
!   LOW/                          2.40E+14    0.206   -1550 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 RIL/FON03 [EDIT
TEST]
!   TROE/ 0.82 1E-30 1E30 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.82 (NBS91)
[EDIT TEST]
!   N2/1.6/
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 RIL/FON03 [EDIT
TEST]
!H+NO(+M)=HNO(+M)                1.52E+15   -0.41    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!   LOW/                          4.00E+20   -1.75    0.0 /
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!   H2/2/ H2O/10/ O2/1.5/ AR/0.75/
!NO+H(+M)=HNO(+M)                1.5E+15   -0.410    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 NBS91
!   LOW/                          2.4E+14    0.206   -1550 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 RIL/FON03
!   TROE/ 0.82 1E-30 1E+30 1E+30/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.82
(NBS91)
!   N2/1.6/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 RIL/FON03
!H+NO+M=HNO+M                    4.0E+20   -1.75    0.0
!Miller personal communication; Original comments: Glarborg,et al 27th
!   H2O/10/ O2/1.5/ H2/2/ CO2/3/ N2/0.0/

!NO+H2=HNO+H                    1.39E+13    0.0    56498.
!3   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!H+HNO=H2+NO                    1.81E+13    0.0    993.
!4   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
HNO+H=H2+NO                    4.50E+11    0.72    655.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+H=H2+NO                    9.000E+11    0.720    660.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

```

```

!HNO+H=NO+H2                4.40E+11    0.720    650
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=NO+H2                4.40E+11    0.7    650.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!H+HNO=H2+NO                4.46E+11    0.72    655.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SP92
!HNO+H=NO+H2                4.40E+11    0.720    650
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=NO+H2                4.46E+11    0.72    655
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!HNO+H=NO+H2                4.4E+11    0.720    650
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 SOT/PAG92
!HNO+H=H2+NO                4.46E+11    0.720    655.
!Miller personal communication; Original comments: SOTO&PAGE JCP 1992

!NH+OH=HNO+H                2.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+OH=HNO+H                2.00E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+OH=HNO+H                2.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH+OH=HNO+H                2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
NH+OH=HNO+H                3.20E+14    -0.376    -46
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!H+HNO=NH+OH                3.00E+14    0.0    18000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, 1993
jannaf est
!NH+OH=HNO+H                2.00E+13    0.00    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NH+OH=HNO+H                2.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH+OH=HNO+H                0.200E+14    0.000    0.000
!Miller personal communication; Original comments: NH3 CST

!HNO+H=O+NH2                3.50E+15    -0.30    29252.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+H=O+NH2                3.50E+15    -0.30    29252.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+O=HNO+H                4.60E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+O=H+HNO                3.900E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH2+O=HNO+H                6.60E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: INO/WAS99,DRA/WAG84,ADA/PHI94
!NH2+O=HNO+H                6.60E+14    -0.5    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2+O=HNO+H                4.60E+13    0.00    0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DB00 [EDIT
TEST]
!NH2+O=HNO+H                6.60E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: TIA/QI09
DRA/WAG84,ADA/PHI94
!NH2+O=HNO+H                4.50E+13    0.00    0.0
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011
!NH2+O=HNO+H                6.6E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
INO/WAS99,DRA/WAG84,ADA/PHI94
!NH2+O=HNO+H                0.663E+15    -0.500    0.000
!Miller personal communication; Original comments: [EDIT TEST]

NH+H2O=HNO+H2                2.000E+13    0.000    13850.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+H2O=HNO+H2                2.00E+13    0.00    13900
!Duynslaeagher et al. Proceedings of the European Combustion Meeting 2011

```

HNO+O=OH+NO	1.81E+13	0.0	0.
!3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!HNO+O=OH+NO	4.50E+11	0.72	655.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HNO+O=NO+OH	2.500E+13	0.000	0.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HNO+O=NO+OH	2.30E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 INO/WAS99			
!HNO+O=NO+OH	2.30E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNO+O=OH+NO	3.61E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91			
!HNO+O=NO+OH	2.30E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 INO/WAS99			
!HNO+O=OH+NO	5.00E+11	0.50	2000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!HNO+O=NO+OH	2.3E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 INO/WAS99			
!HNO+O=OH+NO	1.0E+13	0.0	0.0
!Miller personal communication; Original comments: NH2-NO2 paper			
!NH+O2=HNO+O	4.60E+05	2.00	6494.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH+O2=HNO+O	4.610E+05	2.000	6500.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NH+O2=HNO+O	4.60E+05	2.000	6500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=HNO+O	4.60E+05	2.0	6500.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH+O2=HNO+O	4.61E+05	2.0	6500.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&M, 24th ISC, 92			
!NH+O2=HNO+O	4.60E+05	2.000	6500
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=HNO+O	4.00E+13	0.00	17900
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH+O2=HNO+O	4.6E+05	2.000	6500
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92			
!NH+O2=HNO+O	4.61E+5	2.0	6500.
!Miller personal communication; Original comments: MILL&MEL 24TH			
!OH+HNO=H2O+NO	4.82E+13	0.0	993.
!3-<10 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!HNO+OH=NO+H2O	1.30E+07	1.88	-953.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HNO+OH=NO+H2O	1.300E+07	1.900	-950.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HNO+OH=NO+H2O	3.60E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 BAU73			
HNO+OH=NO+H2O	3.60E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNO+OH=NO+H2O	1.295E+07	1.884	-958.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SPM91			
!HNO+OH=NO+H2O	3.60E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 BAU73			
!HNO+OH=NO+H2O	1.30E+07	1.88	-956
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!HNO+OH=NO+H2O	3.6E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 BAU73			
!HNO+OH=NO+H2O	0.360E+14	0.000	0.000
!Miller personal communication; Original comments: NH3 CST			
!NH2+O2=HNO+OH	6.20E+07	1.23	35081.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+O2=HNO+OH	6.20E+07	1.230	35100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			

!NH2+O2=HNO+OH	6.20E+07	1.2	35100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NH2+O2=HNO+OH	4.50E+12	0.0	25000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NH2+O2=HNO+OH	2.90E-02	3.764	18185
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw			
!NH2+O2=HNO+OH	1.00E+13	0.00	26300
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+O2=HNO+OH	6.2E+07	1.230	35100
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!NH2+HO2=HNO+H2O	5.68E+15	-1.12	707
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!HNO+O2=NO+HO2	2.00E+13	0.0	15887.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HNO+O2=HO2+NO	1.000E+13	0.000	13000.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HNO+O2=HO2+NO	2.00E+13	0.000	16000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!HNO+O2=HO2+NO	2.00E+13	0.0	16000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNO+O2=HO2+NO	1.00E+13	0.0	25000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB91			
!HNO+O2=HO2+NO	2.00E+13	0.000	16000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!HNO+O2=HO2+NO	2.0E+13	0.000	16000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!HNO+O2=HO2+NO	2.0E+12	0.0	25000.
!Miller personal communication; Original comments: JAM 3/98			
!HNO+NH2=NH3+NO	9.20E+05	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NH2+HNO=NH3+NO	3.60E+06	1.630	-1250
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96			
!NH2+HNO=NH3+NO	3.60E+06	1.6	-1250.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNO+NH2=NH3+NO	2.00E+13	0.0	1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!NH2+HNO=NH3+NO	3.60E+06	1.630	-1250
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN96			
!HNO+NH2=NH3+NO	2.00E+13	0.00	1000
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NH2+HNO=NH3+NO	3.6E+06	1.630	-1250
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96			
!HNO+NH2=NH3+NO	3.63E+6	1.63	-1252
!Miller personal communication; Original comments: Lin,Morokuma JPC 1996			
!N2H3+O=NH2+HNO	3.00E+13	0.0	0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!N2H3+O=NH2+HNO	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+O=NH2+HNO	3.00E+13	0.00	0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; (DB00)			
!N2H3+O=NH2+HNO	3.00E+13	0.000	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+O=NH2+HNO	3.0E+13	0.000	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00			
!N2H3+OH=NH3+HNO	1.00E+12	0.000	15000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est			
!N2H3+OH=NH3+HNO	1.00E+12	0.000	15000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est			
!N2H3+OH=NH3+HNO	1.0E+12	0.000	15000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est			

```

!NNH+NO=N2+HNO                1.20E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NNH+NO=N2+HNO                5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
NNH+NO=N2+HNO                5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NNH+NO=N2+HNO                2.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, est,
040596
!NNH+NO=N2+HNO                5.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NNH+NO=N2+HNO                5.00E+13    0.00    0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NNH+NO=N2+HNO                5.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NNH+NO=N2+HNO                0.500E+14    0.000    0.000
!Miller personal communication; Original comments:

H+NO+N2=HNO+N2                4.0E+20    -1.75    0.0
!Miller personal communication; Original comments: Glarborg,et al 27th

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  HON Chemistry               !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!HON(+M)=NO+H(+M)              5.10E+19    -1.73    16036.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+M=NO+H+M                  5.10E+19    -1.7    16045.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   AR/0.7/ H2O/7.0/ CO2/2.0/

!HON+H=HNO+H                   2.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+H=HNO+H                   2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

!HON+H=OH+NH                   2.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+H=OH+NH                   2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

!HON+O=OH+NO                   7.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HON+O=OH+NO                   7.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !! !!! change NHOH to HNOH
!!  HNOH Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!HNOH+M=H+HNO+M               2.00E+24    -2.84    58901.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+M=HNO+H+M               2.00E+24    -2.840    58934
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/
!HNOH+M=HNO+H+M               2.00E+24    -2.8    58934.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   H2O/10.0/

```



```

!HNOH+M=HNO+H+M                2.00E+24   -2.840   58934
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/
!HNOH+M=HNO+H+M                2.0E+24   -2.840   58934
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!   H2O/10/

!HNOH+H=NH2+OH                  4.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+H=NH2+OH                  4.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=NH2+OH                  4.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+H=NH2+OH                  4.00E+13    0.00     0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION
!HNOH+H=NH2+OH                  4.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=NH2+OH                  4.0E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNOH+H=HNO+H2                 4.80E+08    1.50    377.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNOH+H=HNO+H2                 4.80E+08    1.500    378
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=HNO+H2                 4.80E+08    1.5     378.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+H=HNO+H2                 4.80E+08    1.50     378
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!HNOH+H=HNO+H2                 4.80E+08    1.500    378
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!HNOH+H=HNO+H2                 4.8E+08     1.500    378
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNOH+O=HNO+OH                 7.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!   DUPLICATE
!HNOH+O=HNO+OH                 3.30E+08    1.50    -357.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!   DUPLICATE
!HNOH+O=HNO+OH                 7.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                 3.30E+08    1.500    -358
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                 7.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+O=HNO+OH                 3.30E+08    1.5     -358.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNOH+O=HNO+OH                 7.00E+13    0.00     0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION
!   DUPLICATE
!HNOH+O=HNO+OH                 3.30E+08    1.50    -358
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!   DUPLICATE
!HNOH+O=HNO+OH                 7.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                 3.30E+08    1.500    -358
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                 7.0E+13     0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!   DUPLICATE
!HNOH+O=HNO+OH                 3.3E+08     1.500    -358
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

```

! DUPLICATE

!HNOH+OH=HNO+H2O 2.40E+06 2.00 -1192.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNOH+OH=HNO+H2O 2.40E+06 2.000 -1192  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+OH=HNO+H2O 2.40E+06 2.0 -1192.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNOH+OH=HNO+H2O 2.40E+06 2.00 -1192  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
!HNOH+OH=HNO+H2O 2.40E+06 2.000 -1192  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+OH=HNO+H2O 2.4E+06 2.000 -1192  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
  
!HNOH+O2=HNO+HO2 3.00E+12 0.000 25000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!HNOH+O2=HNO+HO2 3.00E+12 0.0 25000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNOH+O2=HNO+HO2 3.00E+12 0.000 25000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!HNOH+O2=HNO+HO2 3.0E+12 0.000 25000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
  
!HNOH+HO2=HNO+H2O2 2.90E+04 2.69 -1599.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNOH+HO2=HNO+H2O2 2.90E+04 2.690 -1600  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+HO2=HNO+H2O2 2.90E+04 2.7 -1600.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNOH+HO2=HNO+H2O2 2.90E+04 2.690 -1600  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+HO2=HNO+H2O2 2.9E+04 2.690 -1600  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
  
!HNOH+NH2=N2H3+OH 6.70E+06 1.82 715.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNOH+NH2=N2H3+OH 1.00E+01 3.460 -467  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=N2H3+OH 1.00E+01 3.460 -467  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=N2H3+OH 1.0E+01 3.460 -467  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
  
!HNOH+NH2=H2NN+H2O 4.60E+19 -1.94 1926.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNOH+NH2=H2NN+H2O 8.80E+16 -1.080 1113  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=H2NN+H2O 8.80E+16 -1.080 1113  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=H2NN+H2O 8.8E+16 -1.080 1113  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
  
!HNOH+NH2=HNO+NH3 1.80E+06 1.94 -1152.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNOH+NH2=NH3+HNO 1.80E+06 1.940 -1152  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=NH3+HNO 1.80E+06 1.9 -1152.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNOH+NH2=NH3+HNO 1.80E+06 1.940 -1152  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!HNOH+NH2=NH3+HNO 1.8E+06 1.940 -1152  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!\*\* change H2NO to NH2O

```

!!          !!
!!  NH2O Chemistry  !!
!!          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2O(+M)=HNO+H(+M)                2.80E+24   -2.83   64879.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+M=HNO+H+M                    2.80E+24   -2.83   64915
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNO+H+M                    2.80E+24   -2.8   64915.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!  H2O/10.0/
!NH2O+M=HNO+H+M                    2.80E+24   -2.830   64915
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNO+H+M                    2.8E+24   -2.830   64915
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNO+H+M                    7.5E+15    0.0    50000.0
!Miller personal communication; Original comments: JAM 12/96
!  H2O/5/  N2/2/

!NH2O=HNOH                          8.20E+25   -4.94   43769.
!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O=HNOH                          1.30E+27   -4.99   43957.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O=HNOH                          2.60E+28   -5.06   44742.
!10 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O(+M)=HNOH(+M)                  1.10E+29   -3.99   43957.
!T>1000K          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+M=HNOH+M                      1.10E+29   -4.000   44000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNOH+M                      1.10E+29   -4.0   44000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!  H2O/10.0/
!NH2O+M=HNOH+M                      1.10E+29   -4.000   44000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/
!NH2O+M=HNOH+M                      1.1E+29   -4.000   44000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00
!  H2O/10/

!NH2O+H=NH2+OH                      4.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+H=NH2+OH                      5.00E+13    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2O+H=NH2+OH                      5.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+H=NH2+OH                      4.00E+13    0.00   0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; RECOMBINATION
!NH2O+H=NH2+OH                      5.00E+13    0.000   0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+H=NH2+OH                      5.0E+13    0.000   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+H=NH2+OH                      5.0E+13    0.0    0.0
!Miller personal communication; Original comments:

!NH2O+H=HNO+H2                      4.80E+08    1.50   1559.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+H=HNO+H2                      3.00E+07    2.000   2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2O+H=HNO+H2                      3.00E+07    2.0    2000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+H=HNO+H2                      4.80E+08    1.50   1560

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
!NH2O+H=HNO+H2 3.00E+07 2.000 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH2O+H=HNO+H2 3.0E+07 2.000 2000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
!NH2O+H=HNO+H2 3.0E+7 2.0 2000.  
!Miller personal communication; Original comments: JAM,PG EST

!NH2O+O=HNO+OH 3.30E+08 1.50 487.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2O+O=HNO+OH 3.00E+07 2.000 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!NH2O+O=HNO+OH 3.00E+07 2.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2O+O=HNO+OH 3.30E+08 1.50 487  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
!NH2O+O=HNO+OH 3.00E+07 2.000 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH2O+O=HNO+OH 3.0E+07 2.000 2000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
!NH2O+O=HNO+OH 3.0E+7 2.0 2000.  
!Miller personal communication; Original comments:

!NH2+O2=NH2O+O 2.50E+11 0.48 29570.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+O2=NH2O+O 2.50E+11 0.480 29586  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!NH2+O2=NH2O+O 2.50E+11 0.5 29586.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+O2=NH2O+O 2.60E+11 0.4872 29050  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw  
!NH2+O2=NH2O+O 2.5E+11 0.480 29586  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2O+OH=HNO+H2O 2.40E+06 2.00 -1192.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2O+OH=HNO+H2O 1.00E+14 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SUN/CUR01  
!NH2O+OH=HNO+H2O 2.00E+07 2.0 1000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2O+OH=HNO+H2O 2.40E+06 2.00 -1192  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION  
!NH2O+OH=HNO+H2O 2.00E+07 2.000 1000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH2O+OH=HNO+H2O 1.0E+14 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SUN/CUR01  
!NH2O+OH=HNO+H2O 2.0E+7 2.0 1000.  
!Miller personal communication; Original comments:

!NH2+HO2=NH2O+OH 2.50E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+HO2=NH2O+OH 5.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!NH2+HO2=NH2O+OH 5.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+HO2=NH2O+OH 5.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH2+HO2=NH2O+OH 5.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
!NH2+HO2=NH2O+OH 5.0E+13 0.0 0.0  
!Miller personal communication; Original comments: JAM/PG

!NH2O+O2=HNO+HO2 3.00E+12 0.000 25000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!NH2O+O2=HNO+HO2 3.00E+12 0.0 25000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

!NH2O+O2=HNO+HO2                3.00E+12    0.000    25000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+O2=HNO+HO2                3.0E+12    0.000    25000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+O2=HNO+HO2                3.0E+12    0.0      25000.
!Miller personal communication; Original comments: JAM

!NH2O+HO2=HNO+H2O2                2.90E+04    2.69    -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+HO2=HNO+H2O2                2.90E+04    2.690    -1600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00
!NH2O+HO2=HNO+H2O2                2.90E+04    2.7      1600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+HO2=HNO+H2O2                2.90E+04    2.690    -1600
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00
!NH2O+HO2=HNO+H2O2                2.9E+04    2.690    -1600
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!NH2O+NH2=HNO+NH3                1.80E+06    1.94    -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2O+NH2=HNO+NH3                3.00E+12    0.000    1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2O+NH2=HNO+NH3                3.00E+12    0.0      1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+NH2=HNO+NH3                1.80E+06    1.94    -1152
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ABSTRACTION
!NH2O+NH2=HNO+NH3                3.00E+12    0.000    1000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+NH2=HNO+NH3                3.0E+12    0.000    1000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+NH2=NH3+HNO                3.0E+12    0.0      1000.
!Miller personal communication; Original comments:

!NH2O+NO=HNO+HNO                2.00E+04    2.000    13000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est
!NH2O+NO=HNO+HNO                2.00E+04    2.0      13000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH2O+NO=HNO+HNO                2.00E+04    2.000    13000
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est
!NH2O+NO=HNO+HNO                2.0E+04    2.000    13000
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est
!NH2O+NO=HNO+HNO                2.0E+7     2.0      13000.
!Miller personal communication; Original comments:

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  NH2OH Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH2+OH=NH2OH                    1.80E+32    -6.91    4111.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+OH=NH2OH                    3.90E+33    -7.00    4438.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+OH=NH2OH                    5.60E+34    -7.02    5362.
!10 atm                           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2OH(+M)=NH2+OH(+M)            1.40E+20    -1.310   64080
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09
!  LOW/                            5.40E+37    -5.96    66783 /
!Klippenstein et al. C&F 158 (2011) 774-789.
!  TROE/ 0.31 1E-30 1E30 1E30 /

!NH2OH+H=HNOH+H2                4.80E+08    1.50     6246.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2OH+H=HNOH+H2                4.80E+08    1.50     6249

```

!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!NH2OH+H=NH2O+H2 2.40E+08 1.50 5064.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+H=NH2O+H2 2.40E+08 1.50 5067  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!NH2OH+O=HNOH+OH 3.30E+08 1.50 3863.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+O=HNOH+OH 3.30E+08 1.50 3865  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!NH2OH+O=NH2O+OH 1.70E+08 1.50 3009.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+O=NH2O+OH 1.70E+08 1.50 3010  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!NH2OH+OH=HNOH+H2O 2.40E+06 2.00 -328.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+OH=HNOH+H2O 1.50E+04 2.61 -3537  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+OH=NH2O+H2O 1.20E+06 2.00 -596.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+OH=NH2O+H2O 1.50E+05 2.28 -1296  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2O+HO2=O2+NH2OH 2.90E+04 2.69 -1599.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNOH+HO2=NH2OH+O2 2.90E+04 2.69 -1599.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2OH+HO2=HNOH+H2O2 2.90E+04 2.69 9552.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+HO2=HNOH+H2O2 2.90E+04 2.69 9557  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!NH2OH+HO2=NH2O+H2O2 1.40E+04 2.69 6414.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+HO2=NH2O+H2O2 1.40E+04 2.69 6418  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: DB HTRANS

!N2H4+O=NH2OH+NH 2.90E+11 0.000 -1270  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: VAG96,VAG01  
!N2H4+O=NH2OH+NH 2.9E+11 0.000 -1270  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: VAG96,VAG01

!NH2OH+NH=HNOH+NH2 2.90E-03 4.40 1564  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+NH=NH2O+NH2 1.50E-03 4.60 2424  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+NH2=HNOH+NH3 1.80E+06 1.94 3227.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+NH2=HNOH+NH3 1.10E-01 4.00 -97  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!NH2OH+NH2=NH2O+NH3 9.20E+05 1.94 1887.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2OH+NH2=NH2O+NH3 9.50E+00 3.42 -1013  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: KLIMIC09

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! HNNNH2 Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!H2NN+NH2=HNNNH2+H 7.90E+06 1.90 -1331.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! N2O Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!N2O(+M)=N2+O(+M) 1.30E+11 0.0 59576.  
 !2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! LOW/ 7.23E+17 -0.73 62754. /  
 !Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! TROE/ 0.0175 12.94 100000 /  
 !N2O(+M)=N2+O(+M) 5.70E+14 0.0 56061.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !N2O(+M)=N2+O(+M) 7.910E+10 0.000 56020.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 ! LOW/ 6.370E+14 0.000 56640.00 /  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 ! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/  
 ! CO2/2.00/ C2H6/3.00/ AR/ .625/  
 !N2O(+M)=N2+O(+M) 1.30E+12 0.000 62570  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JOH/GLA92,ROH/HAN96  
 ! LOW/ 4.00E+14 0.0 56600 /  
 ! N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/  
 !N2O(+M)=N2+O(+M) 1.30E+12 0.0 62570.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! LOW/ 0.40E+15 0.0 56600.0 /  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 ! N2/1.70/ O2/1.40/ CO2/3.00/ H2O/12.00/  
 !N2O(+M)=N2+O(+M) 1.26E+12 0.0 62620.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Rohrig et al,  
 1996 preprint [EDIT TEST]  
 ! LOW/ 5.97E+14 0.0 56640. /  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; to appear in  
 IJCK; rekeyed to N2  
 ! N2O/5.0/ H2O/9.0/ N2/1.0/ CO2/3.2/  
 ! O2/0.82/  
 !N2O(+M)=N2+O(+M) 1.30E+12 0.000 62570  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04  
 JOH/GLA92,ROH/HAN96 [EDIT TEST]  
 ! LOW/ 4.00E+14 0 56600 /  
 ! N2/1.7/ CO2/3.0/ H2O/12/ !O2/1.4/  
 !N2O(+M)=N2+O(+M) 1.26E+12 0.00 62600  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 ! LOW/ 4.00E+14 0.00 56600 /  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 ! NO/3/ N2O/3.5/ O2/1.4/ N2/1.7/  
 ! H2O/12/  
 !N2O(+M)=N2+O(+M) 1.3E+12 0.000 62570  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04  
 JOH/GLA92,ROH/HAN96  
 ! LOW/ 4.0E+14 0 56600 /  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
 ! N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
 !N2O+M=N2+O+M 4.0E+14 0.0 56100.

```

!Miller personal communication; Original comments: PG,ET AL 24TH [EDIT TEST]
! N2/1.7/ O2/1.4/ H2O/12/ CO/1.5/ CO2/3/
!Miller personal communication; Original comments: PG,et al 25th except CO [EDIT TEST]

!N2O+H=N2+OH 9.64E+13 0.0 15093.
!1.7 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!N2O+H=N2+OH 2.20E+14 0.0 16741.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!N2O+H=N2+OH 3.870E+14 0.000 18880.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
N2O+H=N2+OH 3.30E+10 0.000 4729
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MAR/FON87
DUPLICATE
N2O+H=N2+OH 4.40E+14 0.000 19254
!Tian et al. C&F 156 (2009) 1413-1426
DUPLICATE
!N2O+H=N2+OH 3.30E+10 0.0 4729.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N2O+H=N2+OH 4.40E+14 0.0 19254.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!N2O+H=N2+OH 1.30E+11 0.938 15210.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA01 (Fit#8,
WRA, 3/16/01)
!N2O+H=N2+OH 6.40E+07 1.835 13492
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw
!N2O+H=N2+OH 5.00E+13 0.00 15200
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!N2O+H=N2+OH 3.3E+10 0.000 4729
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MAR/FON87
! DUPLICATE
!N2O+H=N2+OH 4.4E+14 0.000 19254
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
! DUPLICATE
!N2O+H=N2+OH 3.31E+10 0.0 4729.
!Miller personal communication; Original comments: FONTIJN 1987
! DUPLICATE
!N2O+H=N2+OH 4.40E+14 0.0 19254
!Miller personal communication; Original comments: FONTIJN 1987
! DUPLICATE

!H+N2O=NH+NO 8.50E+20 -1.62 35349.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
! DUPLICATE
!NH+NO=N2O+H 3.00E+18 -1.65 1430.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
! DUPLICATE
!NH+NO=N2O+H 3.650E+14 -0.450 0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NH+NO=N2O+H 2.90E+14 -0.400 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MIL/MEL92 [EDIT TEST]
! DUPLICATE
!NH+NO=N2O+H -2.20E+13 -0.230 0
!Tian et al. C&F 156 (2009) 1413-1426 [EDIT TEST]
! DUPLICATE
!NH+NO=N2O+H 2.90E+14 -0.4 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+NO=N2O+H -2.2E+13 -0.2 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NH+NO=N2O+H 3.50E+14 -0.46 16.1
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; B.Williams fit
of MM calc
!NH+NO=N2O+H 1.80E+14 -0.351 -244
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST] [EDIT TEST
2]
!NH+NO=N2O+H 5.00E+14 -0.40 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

```



NH+NO=N2O+H 2.9E+14 -0.400 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MIL/MEL92  
 [EDIT TEST]  
 DUPLICATE  
 NH+NO=N2O+H -2.2E+13 -0.230 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: [EDIT TEST]  
 DUPLICATE  
 !NH+NO=N2O+H 2.94E+14 -0.4 0.0  
 !Miller personal communication; Original comments: MILL&MEL 24TH  
 ! DUPLICATE  
 !NH+NO=N2O+H -2.16E+13 -0.23 0.0  
 !Miller personal communication; Original comments: MILL&MEL 24TH  
 ! DUPLICATE  
  
 !H+N2O=NNH+O 2.40E+19 -1.26 47065.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NNH+O=N2O+H 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
 !NNH+O=N2O+H 1.00E+14 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 [EDIT TEST]  
 !NNH+O=N2O+H 1.40E+14 -0.40 477.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 B&D95,QRRK,preprint on O+NNH  
 !NNH+O=N2O+H 1.90E+14 -0.274 -22  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: pw [EDIT TEST]  
 NNH+O=N2O+H 1.0E+14 0.000 0  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est [EDIT  
 TEST]  
 !NNH+O=N2O+H 0.100E+15 0.000 0.000  
 !Miller personal communication; Original comments:  
  
 !NH2+NO=N2O+H2 5.00E+13 0.0 24481.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: LIND94  
 !NH2+NO=N2O+H2 7.00E+13 0.0 2780.  
 !Roose et al. Int. Symp. on Combust. 18 (1981) 853-862.  
 NH2+NO=H2+N2O 1.00E+13 0.00 33700  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
  
 !NO+NO=N2O+O 3.61E+12 0.0 65335.  
 !2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! DUPLICATE  
 !N2O+O=NO+NO 6.62E+13 0.0 26611.  
 !Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 ! DUPLICATE  
 !N2O+O=NO+NO 2.90E+13 0.0 23135.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !N2O+O=2NO 2.900E+13 0.000 23150.00  
 !GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)  
 !N2O+O=NO+NO 9.20E+13 0.000 27679  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEA/AND00  
 !N2O+O=NO+NO 9.20E+13 0.0 27679.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !N2O+O=NO+NO 9.155E+13 0.0 27680.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&A00  
 !N2O+O=NO+NO 9.20E+13 0.000 27679  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEA/AND00  
 !N2O+O=NO+NO 6.92E+13 0.00 26600  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 !N2O+O=NO+NO 9.2E+13 0.000 27679  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEA/AND00  
 !N2O+O=NO+NO 9.16E+13 0.0 27679.  
 !Miller personal communication; Original comments: Meagher&Anderson JPC A 2000  
  
 !N2O+O=O2+N2 1.02E+14 0.0 28001.  
 !2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 !N2O+O=N2+O2 1.40E+12 0.0 10803.

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+O=N2+O2 1.400E+12 0.000 10810.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!N2O+O=N2+O2 3.70E+12 0.000 15936  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEA/AND00  
!N2O+O=N2+O2 3.70E+12 0.0 15936.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!N2O+O=N2+O2 3.692E+12 0.0 15940.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; M&A00  
!N2O+O=N2+O2 3.70E+12 0.000 15936  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEA/AND00  
!N2O+O=N2+O2 1.00E+14 0.00 28200  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!N2O+O=N2+O2 3.7E+12 0.000 15936  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEA/AND00  
!N2O+O=N2+O2 3.69E+12 0.0 15936.  
!Miller personal communication; Original comments:

!HNO+NO=N2O+OH 8.50E+12 0.0 29570.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+OH=HNO+NO 1.20E-04 4.330 25080  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
N2O+OH=HNO+NO 1.20E-04 4.3 25080.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+NO=N2O+OH 1.70E+13 0.0 29590.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; comment follows  
!N2O+OH=HNO+NO 1.20E-04 4.330 25080  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96  
!N2O+OH=HNO+NO 1.2E-4 4.330 25080  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
!N2O+OH=HNO+NO 1.18E-4 4.33 25081  
!Miller personal communication; Original comments:

!N2O+OH=N2+HO2 1.30E-02 4.72 36540.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+OH=N2+HO2 2.000E+12 0.000 21060.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!N2O+OH=N2+HO2 1.30E-02 4.720 36560  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
!N2O+OH=N2+HO2 1.30E-02 4.7 36560.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!N2O+OH=N2+HO2 1.29E-02 4.72 36561  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Mebel et al 96, per DB00  
!N2O+OH=N2+HO2 1.30E-02 4.720 36560  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96  
N2O+OH=N2+HO2 1.00E+14 0.00 30000  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!N2O+OH=N2+HO2 1.3E-2 4.720 36560  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
!N2O+OH=N2+HO2 1.29E-2 4.72 36561  
!Miller personal communication; Original comments: Mebel, Lin IJCK 1996

!NNH+O2=N2O+OH 2.90E+11 -0.34 149.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NNH+O2=N2O+OH 2.90E+11 -0.34 150  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

!HNO+HNO=H2O+N2O 8.43E+08 0.0 3100.  
!2-10 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
!HNO+HNO=N2O+H2O 8.50E+08 0.0 3078.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO+HNO=N2O+H2O 9.00E+08 0.000 3100  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91  
!HNO+HNO=N2O+H2O 9.00E+08 0.0 3100.0

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+HNO=N2O+H2O 3.63E-03 3.98 1190.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; LHM92  
!HNO+HNO=N2O+H2O 9.00E+08 0.000 3100  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 NBS91  
!HNO+HNO=N2O+H2O 9.0E+08 0.000 3100  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 NBS91  
!HNO+HNO=N2O+H2O 9.0E+8 0.0 3100  
!Miller personal communication; Original comments: NH2-NO2 paper

!NH+N2O=N2+HNO 2.00E+12 0.00 6000  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011

!N2H2+NO=N2O+NH2 4.00E+12 0.000 11922  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!N2H2+NO=NH2+H2O 4.00E+12 0.0 11922.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ 2000  
!N2H2+NO=N2O+NH2 4.00E+12 0.0 11915.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000) [EDIT TEST]  
!N2H2+NO=N2O+NH2 4.00E+12 0.000 11922  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
N2H2+NO=N2O+NH2 3.00E+10 0.00 0.0  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011 [EDIT TEST]  
!N2H2+NO=N2O+NH2 4.0E+12 0.000 11922  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00  
!N2H2+NO=N2O+NH2 0.300E+13 0.000 0.000  
!Miller personal communication; Original comments: NH3 CST

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! !!  
!! HNNO Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!HNNO+M=H+N2O+M 2.20E+15 0.0 21600.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+M=H+N2O+M 2.2E+15 0.0 21600.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,  
IJCK 27,867(1995)  
!N2O+H=HNNO 1.20E+24 -4.46 10694.  
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+H=HNNO 1.30E+25 -4.48 10763.  
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+H=HNNO 3.20E+26 -4.58 11220.  
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+H(+M)=HNNO(+M) 1.10E+27 -3.48 10763.  
!10 atm & T>1000K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!N2O+H(+M)=HNNO(+M) 1.10E+27 -3.48 10763.  
!1 atm & T>300K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNNO+M=N2+OH+M 1.00E+15 0.0 25600.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+M=N2+OH+M 1.0E+15 0.0 25600.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,  
IJCK 27,867(1995)

!HNNO+H=H2+N2O 2.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+H=H2+N2O 2.0E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra est

!NH2+NO=HNNO+H 8.000E+13 0.00 28000  
!Miller, Smooke, Green, Kee Combust. Sci. Technol., Vol. 34 (1983), pp 149-176

```

!HNNO+OH=H2O+N2O                2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid
!HNNO+OH=H2O+N2O                2.0E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra est
!NNH+HO2=HNNO+OH                2.40E+13    0.0    1698.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNNO+NO=N2O+HNO                1.00E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  NH2NO Chemistry            !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!NH2+NO=NH2NO                    1.90E+30   -6.67   3495.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NO=NH2NO                    3.50E+31   -6.75   3724.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2+NO=NH2NO                    1.70E+33   -6.92   4607.
!10 atm                           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO=N2+H2O                   4.10E+33   -7.18   35150.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2NO=N2+H2O                   3.10E+34   -7.11   36262.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2NO=N2+H2O                   2.90E+31   -5.91   36153.
!10 atm                           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO+H=HNNO+H2                4.80E+08    1.50    7407.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!N2H3+O=NH2NO+H                 3.00E+13    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!H2NN+OH=NH2NO+H                2.00E+12    0.0     0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO+O=HNNO+OH                3.30E+08    1.50    4697.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO+OH=HNNO+H2O              2.40E+06    2.00    -70.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!H2NN+HO2=NH2NO+OH              6.60E+05    1.94    7050.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO+HO2=HNNO+H2O2            2.90E+04    2.69    12620.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NO+NH2=HNNO+NH3             1.80E+06    1.94    4538.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !! ***** MUST INCLUDE HNNHO
!!  NH2NHO Chemistry            !! ***** rename to H2NNHO
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!NH2NHO=NH2+HNO                 2.70E+39   -8.74   41594.

```

```

!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2NHO=NH2+HNO          2.40E+40   -8.73   41584.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH2NHO=NH2+HNO          1.20E+41   -8.64   41554.
!10 atm           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+H=NHNHO+H2          4.80E+08   1.50   -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+O=NHNHO+OH          3.30E+08   1.50   -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+OH=NHNHO+H2O          2.40E+06   2.00   -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!N2H3+HO2=NH2NHO+OH          3.00E+13   0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+HO2=NHNHO+H2O2          2.90E+04   2.69   -1599.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+NH2=NHNHO+NH3          1.80E+06   1.94   -1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  NO2 Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NO2(+M)=NO+O(+M)          7.60E+18   -1.27   73245.
!3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      LOW/          2.47E+28   -3.37   74756. /
!2      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      TROE/ 0.100 295.1 972.7 4981.6 /
!NO2(+M)=NO+O(+M)          5.70E+15   0.0    59954.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO2(+M)=NO+O(+M)          7.60E+18   -1.27   73290.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Original
comments: Tsang & Herron
!      LOW/          2.47E+28   -3.37   74800. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; keyed to
N2=1.0
!      T&H/ 0.95 -1.0E-04 /
      N2O/1.5/ H2O/4.4/ N2/1.0/ CO2/2.3/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; EFFICIENCIES
FROM Baulch et al,
      DUPLICATE
NO+O(+M)=NO2(+M)          1.30E+15   -0.75   0.
!3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      LOW/          4.71E+24   -2.87   1551. /
!1.3-3      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
      TROE/ 0.100 295.1 972.7 4681.6 /
      DUPLICATE
!NO+O+M=NO2+M          1.060E+20   -1.410   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri\_mech/)
!      H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!      CO2/2.00/ C2H6/3.00/ AR/ .70/
!NO+O(+M)=NO2(+M)          1.30E+15   -0.750   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 ALL/DRY97,NBS91
!      LOW/          4.72E+24   -2.87   1550 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 ALL/DRY97 (Fc=0.95-1E-
04*T)
!      TROE/ 0.880 1E03 1E04 1E30 /

```

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a ( 1bar)
! AR/0/
!NO+O(+M)=NO2(+M) 1.30E+15 -0.8 0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
! LOW/ 0.75E+20 -1.41 0.0 /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
! N2/1.7/ O2/1.5/ H2O/10.0/
!NO+O(+M)=NO2(+M) 1.30E+15 -0.750 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 ALL/DRY97,NBS91
! LOW/ 4.72E+24 -2.87 1550 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 ALL/DRY97
(Fc=0.95-1E-04*T)
! TROE/ 0.880 1E03 1E04 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
! AR/0/
!NO+O(+AR)=NO2(+AR) 1.30E+15 -0.750 0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08aLL/DRY97,NBS91
! LOW/ 7.56E+19 -1.41 0 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 YAR/SUT91 (Fc=0.95-1E-
04*T)
! TROE/ 0.750 1E03 1E05 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a ( 1bar)
!NO+O(+AR)=NO2(+AR) 1.30E+15 -0.750 0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08aLL/DRY97,NBS91
! LOW/ 7.56E+19 -1.41 0 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 YAR/SUT91
(Fc=0.95-1E-04*T)
! TROE/ 0.750 1E03 1E05 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!NO+O(+M)=NO2(+M) 1.30E+15 -0.75 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
! LOW/ 4.72E+24 -2.87 1550 /
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
! TROE/ 9.62E-01 1.00E+01 7.96E+03 /
! O2/0.8/ N2O/4.4/ H2O/10/ AR/0.6/
! NO2/6.2/ NO/1.8/
!NO+O=NO2 1.30E+15 -0.75 0.0
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011
!NO+O(+M)=NO2(+M) 1.3E+15 -0.750 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08
ALL/DRY97,NBS91
! LOW/ 4.72E+24 -2.87 1550 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 ALL/DRY97
(Fc=0.95-1E-04*T)
! TROE/ 0.880 1E+03 1E+04 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a ( 1bar) Ć!
AR/0/
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
!NO+O(+AR)=NO2(+AR) 1.3E+15 -0.750 0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
RAS/GLA08aLL/DRY97,NBS91
! LOW/ 7.56E+19 -1.41 0 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 YAR/SUT91
(Fc=0.95-1E-04*T)
! TROE/ 0.750 1E+03 1E+05 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a ( 1bar)
Ć!NO+O+M=NO2+M 7.5E+19 -1.41 0.0
!Miller personal communication; Original comments: PG
! N2/1.7/ O2/1.5/ H2O/10/

!NO2+H=NO+OH 8.43E+13 0.0 0.
!1.3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
NO2+H=NO+OH 1.30E+14 0.0 357.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO2+H=NO+OH 1.320E+14 0.000 360.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

```

!NO2+H=NO+OH	1.30E+14	0.000	362
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 KO/FON91			
!NO2+H=NO+OH	1.30E+14	0.0	362.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NO2+H=NO+OH	1.30E+14	0.0	361.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; KF91			
!NO2+H=NO+OH	1.30E+14	0.000	362
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 KO/FON91			
!NO2+H=NO+OH	1.32E+14	0.00	362
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NO2+H=NO+OH	1.3E+14	0.000	362
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 KO/FON91			
!NO2+H=NO+OH	8.4E+13	0.0	0.0
!Miller personal communication; Original comments: TSANG&HERRON (PG)			
!NH+O2=H+NO2	2.30E+10	0.0	2482.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NO2+O=O2+NO	3.91E+12	0.0	-238.
!1.2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!NO2+O=NO+O2	3.90E+12	0.0	-238.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NO2+O=NO+O2	3.900E+12	0.000	-240.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NO2+O=NO+O2	1.10E+14	-0.520	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BEM/CLY74			
!NO2+O=NO+O2	3.90E+12	0.0	-238.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NO2+O=NO+O2	3.90E+12	0.0	-238.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 89			
!NO2+O=NO+O2	1.10E+14	-0.520	0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BEM/CLY74			
!NO2+O=NO+O2	3.91E+12	0.00	-238
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NO2+O=NO+O2	1.1E+14	-0.520	0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BEM/CLY74			
!NO2+O=NO+O2	3.9E+12	0.0	-238.
!Miller personal communication; Original comments: TSANG&HERRON (PG)			
NO2+OH=HO2+NO	1.81E+13	0.0	6673.
!1.2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663			
!NO+HO2=NO2+OH	2.10E+12	0.000	-497
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 CEC05			
!NO+HO2=NO2+OH	2.10E+12	0.0	-480.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NO+HO2=NO2+OH	2.11E+12	0.0	-479.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HS84 (from CJ Howard)			
!HO2+NO=NO2+OH	2.20E+12	0.0	-476
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HO2+NO=NO2+OH	2.110E+12	0.000	-480.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NO+HO2=NO2+OH	2.10E+12	0.000	-497
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 CEC05			
!NO2+OH=HO2+NO	1.81E+13	0.00	6680
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011			
!NO+HO2=NO2+OH	2.1E+12	0.000	-497
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 CEC05			
!HO2+NO=NO2+OH	0.211E+13	0.000	-479.000
!Miller personal communication; Original comments: HOWARD			
!HON+O2=NO2+OH	1.00E+12	0.0	4968.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NO2+N=N2O+O	3.49E+12	0.0	-437.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid			

!NO2+N=N2O+O 3.49E+12 0.0 -437.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97

!NH+NO2=N2O+OH 1.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HAR/PHI86  
!NH+NO2=N2O+OH 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH+NO2=N2O+OH 4.00E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; branching per QH95

NH+NO2=N2O+OH 4.10E+12 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: HAR/PHI86  
!NH+NO2=N2O+OH 1.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HAR/PHI86  
!NO2+NH=N2O+OH 1.0E+13 0.0 0.0  
!Miller personal communication; Original comments: PHILLIPS

!NH+NO2=NO+HNO 5.70E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; branching per QH95

NH+NO2=HNO+NO 5.90E+12 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: HAR/PHI86

!NO2+NH2=N2O+H2O 1.50E+16 -1.44 268.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+NO2=N2O+H2O 1.60E+16 -1.440 268  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 PAR/LIN97  
NH2+NO2=N2O+H2O 3.00E+14 -0.770 242  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SONG  
!NH2+NO2=N2O+H2O 1.60E+16 -1.4 268.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+NO2=N2O+H2O 1.62E+16 -1.44 270  
!Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
!NH2+NO2=N2O+H2O 1.6E+16 -1.440 268  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 PAR/LIN97  
!NO2+NH2=N2O+H2O 1.62E+16 -1.44 268  
!Miller personal communication; Original comments: Park&Lin JPC 1997

!NO2+NH2=NH2O+NO 6.60E+16 -1.44 268.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+NO2=NH2O+NO 1.30E+15 -0.770 242  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SONG  
!NH2+NO2=NH2O+NO 6.50E+16 -1.440 268  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 PAR/LIN97  
!NH2+NO2=NH2O+NO 6.50E+16 -1.4 268.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2+NO2=NH2O+NO 6.5E+16 -1.440 268  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 PAR/LIN97  
!NH2+NO2=NH2O+NO 6.48E+16 -1.44 268  
!Miller personal communication; Original comments:

!H2NN+O2=NH2+NO2 1.50E+12 0.000 5961  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 DEA/BOZ00  
!H2NN+O2=NH2+NO2 1.50E+12 0.0 5958.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!H2NN+O2=NH2+NO2 1.50E+12 0.000 5961  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 DEA/BOZ00  
!H2NN+O2=NH2+NO2 1.5E+12 0.000 5961  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 DEA/BOZ00

!HNNO+NO=NNH+NO2 3.20E+12 0.0 270.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+NO=NNH+NO2 3.2E+12 0.00 270.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al, IJCK 27,867(1995)



N2O+NO=NO2+N2 5.30E+05 2.230 46280  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
 !N2O+NO=NO2+N2 5.30E+05 2.2 46280.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !N2O+NO=NO2+N2 5.30E+05 2.230 46280  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 MEB/LIN96!  
 !N2O+NO=N2+NO2 4.29E+13 0.00 47130.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA, 11/95;  
 fit to reanalyzed  
 !N2O+NO=N2+NO2 2.75E+14 0.00 50000  
 !Duynslaegher et al. Proceedings of the European Combustion Meeting 2011  
 !N2O+NO=NO2+N2 5.3E+05 2.230 46280  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
 !N2O+NO=NO2+N2 5.26E+5 2.23 46281  
 !Miller personal communication; Original comments:  
  
 !NO+NO+NO=N2O+NO2 1.07E+10 0.0 26800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GVO 79  
  
 !HNO+NO+NO=HNNO+NO2 1.70E+11 0.0 2100.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
 !HNO+NO+NO=HNNO+NO2 1.70E+11 0.00 2100.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,  
 IJCK 27,867(1995)  
  
 !NO2+NO2=NO+NO+O2 1.63E+12 0.0 26108.  
 !1.5-2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 !NO2+NO2=NO+NO+O2 4.50E+12 0.000 27599  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98  
 !NO2+NO2=NO+NO+O2 1.60E+12 0.0 26123.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NO2+NO2=NO+NO+O2 4.51E+12 0.0 27600.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; PGML00  
 !NO2+NO2=NO+NO+O2 4.50E+12 0.000 27599  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98  
 !NO2+NO2=NO+NO+O2 4.5E+12 0.000 27599  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98  
 !NO2+NO2=NO+NO+O2 1.63E+12 0.0 26123.  
 !Miller personal communication; Original comments: TSANG&HERRON  
  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !! !!  
 !! HONO Chemistry !!  
 !! !!  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
  
 HONO (+M)=OH+NO (+M) 1.20E+19 -1.23 49667.  
 !1.4-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 LOW/ 3.01E+30 -3.8 50322. /  
 !Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 TROE/ 0.370 11.98 100000 /  
 DUPLICATE  
 !HONO (+M)=OH+NO (+M) 2.00E+31 -4.56 51146.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 NO+OH (+M)=HONO (+M) 1.99E+12 -0.05 -721.  
 !1.4-3 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 LOW/ 5.08E+23 -2.51 -68. /  
 !1.5-4 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 TROE/ 0.370 11.98 100000 /  
 DUPLICATE  
 !NO+OH (+M)=HONO (+M) 1.10E+14 -0.300 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 FUL/TRO98  
 ! LOW/ 3.392E+23 -2.5 0 /  
 ! TROE/ 0.75 1E-30 1E30 1E30 /  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 FUL/TRO98 [M=He,T=400K]

```

!NO+OH(+M)=HONO(+M)                2.00E+12   -0.1   -721.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   LOW/                               0.50E+24   -2.51   -68.0   /
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   N2/1.0/ O2/1.0/ H2O/6.7/ AR/0.67/
!NO+OH(+M)=HONO(+M)                1.988E+12  -0.05   -721.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang & Herron
!   LOW/                               5.08E+23   -2.51   -67.6   /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; keyed to
N2=1.0.
!   T&H/ 0.62 /
!   N2O/5.0/ H2O/8.3/ N2/1.0/ CO2/1.5/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 from
TH91;
!NO+OH(+M)=HONO(+M)                1.10E+14   -0.300   0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 FUL/TRO98
!   LOW/                               3.392E+23   -2.5   0   /!
!   TROE/ 0.75 1E-30 1E30 1E30 /
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 FUL/TRO98
[M=He,T=400K]
!NO+OH(+M)=HONO(+M)                1.1E+14   -0.300   0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 FUL/TRO98
!   LOW/                               3.392E+23   -2.5   0   /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:
!   TROE/ 0.75 1E-30 1E+30 1E+30 /
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 FUL/TRO98
[M=He,T=400K]
!OH+NO+M=HONO+M                    5.08E+23   -2.51   -67.6
!Miller personal communication; Original comments: TSANG&HERRON
!   CO2/0.0/ H2O/5/

!HONO+H=H2+NO2                      1.20E+13   0.0   7348.
!20   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
!HONO+H=H2+NO2                      2.00E+08   1.55   6613.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NO2+H2=HONO+H                      2.41E+13   0.0   28795.
!5   Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663
NO2+H2=HONO+H                      1.30E+04   2.760   29770
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98
!NO2+H2=HONO+H                      4.50E+12   0.0   27600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!H2+NO2=HONO+H                      1.30E+04   2.76   29770.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; PGML98; see
also MGYD00
!NO2+H2=HONO+H                      1.30E+04   2.760   29770
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98
!NO2+H2=HONO+H                      1.3E+04   2.760   29770
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98
!HONO+H=H2+NO2                      1.2E+13   0.0   7352
!Miller personal communication; Original comments: TSANG&HERRON

HONO+H=H2O+NO                      8.10E+06   1.89   3843.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HONO+H=NO+H2O                      8.10E+06   1.890   3850
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HSU/MEL97
!HONO+H=NO+H2O                      8.10E+06   1.9   3850.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HONO+H=H2O+NO                      8.13E+06   1.89   3847.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLMM97
!HONO+H=NO+H2O                      8.10E+06   1.890   3850
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HSU/MEL97
!HONO+H=NO+H2O                      8.1E+06   1.890   3850
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HSU/MEL97

HONO+H=OH+HNO                      5.60E+10   0.86   4965.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!HONO+H=HNO+OH 5.60E+10 0.860 5000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 HSU/MEL97  
 !HONO+H=HNO+OH 5.60E+10 0.9 5000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HONO+H=HNO+OH 5.63E+10 0.86 4969.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLMM97  
 !HONO+H=HNO+OH 5.60E+10 0.860 5000  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 HSU/MEL97  
 !HONO+H=HNO+OH 5.6E+10 0.860 5000  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 HSU/MEL97  
  
 !HON+OH=HONO+H 4.00E+13 0.0 0.0  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !HON+OH=HONO+H 4.00E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
  
 !HONO+O=OH+NO2 1.20E+13 0.0 5958.  
 !10 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 !HONO+O=OH+NO2 1.70E+08 1.50 3028.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !HONO+O=NO2+OH 1.20E+13 0.000 5960  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91  
 !HONO+O=NO2+OH 1.20E+13 0.0 6000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HONO+O=OH+NO2 1.2E+13 0.0 5961.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91  
 !HONO+O=NO2+OH 1.20E+13 0.000 5960  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 NBS91  
 !HONO+O=NO2+OH 1.2E+13 0.000 5960  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 NBS91  
 !HONO+O=OH+NO2 1.2E+13 0.0 5961.  
 !Miller personal communication; Original comments: TSANG&HERRON  
  
 !HON+O2=HONO+O 1.00E+12 0.0 4965.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
  
 HONO+OH=H2O+NO2 1.26E+10 1.0 135.  
 !2-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
 !HONO+OH=H2O+NO2 1.20E+06 2.00 -596.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !HONO+OH=NO2+H2O 4.00E+12 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HONO+OH=NO2+H2O 1.70E+12 0.000 -520  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BUR/RAV92  
 !HONO+OH=H2O+NO2 1.27E+10 1.0 135.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91  
 !HONO+OH=NO2+H2O 1.70E+12 0.000 -520  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BUR/RAV92  
 !HONO+OH=NO2+H2O 1.7E+12 0.000 -520  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BUR/RAV92  
 !HONO+OH=H2O+NO2 4.0E+12 0.0 0.0  
 !Miller personal communication; Original comments: RAVI IJCK 1992  
  
 !NO2+HO2=HONO+O2 1.90E+00 3.320 3044  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a  
 !NO2+HO2=HONO+O2 6.30E+08 1.2 5000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NO2+HO2=HONO+O2 1.00E+12 0.0 5000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler  
 !NO2+HO2=HONO+O2 1.90E+00 3.320 3044  
 !Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a  
 !NO2+HO2=HONO+O2 1.9E+00 3.320 3044  
 !Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a  
  
 !NH+HONO=NH2+NO2 1.00E+13 0.000 0

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
NH+HONO=NH2+NO2 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH+HONO=NH2+NO2 1.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH+HONO=NH2+NO2 1.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

!HONO+NH2=NO2+NH3 9.20E+05 1.94 1916.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NH2+HONO=NH3+NO2 7.10E+01 3.020 -4940  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 MEB/MOR96  
NH2+HONO=NH3+NO2 7.10E+01 3.0 -4940.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HONO+NH2=NO2+NH3 1.0E+10 1.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; wra, est,  
better analysis than B&T72  
!NH2+HONO=NH3+NO2 7.10E+01 3.020 -4940  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 LIN96  
!NH2+HONO=NH3+NO2 7.1E+01 3.020 -4940  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 MEB/MOR96  
!HONO+NH2=NO2+NH3 71.1 3.02 -4941  
!Miller personal communication; Original comments: Lin,Morokuma JPC 1996

!HNNO+NO=N2+HONO 2.60E+11 0.0 810.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNNO+NO=N2+HONO 2.6E+11 0.0 810.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Diau et al,  
IJCK 27,867(1995)

HNO+NO2=HONO+NO 4.40E+04 2.640 4040  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 MEB/MOR98  
!HNO+NO2=HONO+NO 6.00E+11 0.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNO+NO2=HONO+NO 4.42E+04 2.64 4042.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MLM98  
!HNO+NO2=HONO+NO 4.40E+04 2.640 4040  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 MEB/LIN98  
!HNO+NO2=HONO+NO 4.4E+04 2.640 4040  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 MEB/MOR98  
!NO2+HNO=HONO+NO 6.0E+11 0.0 2000.  
!Miller personal communication; Original comments: TSANG&HERRON

!NH2O+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!NH2O+NO2=HONO+HNO 6.00E+11 0.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NH2O+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!NH2O+NO2=HONO+HNO 6.0E+11 0.000 2000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est  
!NH2O+NO2=HNO+HONO 6.0E+11 0.0 2000.  
!Miller personal communication; Original comments: HNO+NO2

!HNOH+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 JAM est  
!HNOH+NO2=HONO+HNO 6.00E+11 0.0 2000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNOH+NO2=HONO+HNO 6.00E+11 0.0 2000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MG99, est.  
!HNOH+NO2=HONO+HNO 6.00E+11 0.000 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: SKR/GLA04 JAM est  
!HNOH+NO2=HONO+HNO 6.0E+11 0.000 2000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: SKR/GLA04 JAM est

!HNNO+NO2=N2O+HONO 1.00E+12 0.0 0.0

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

HONO+HONO=NO+NO2+H2O 3.50E-01 3.640 12140  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 MEB/MEL98  
!HONO+HONO=NO+NO2+H2O 3.50E-01 3.6 12100.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!2HONO=NO+NO2+H2O 0.349 3.64 12140.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MLM98  
!HONO+HONO=NO+NO2+H2O 3.50E-01 3.640 12140  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 MEB/MEL98  
!HONO+HONO=NO+NO2+H2O 3.5E-01 3.640 12140  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 MEB/MEL98

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! !!  
!! HNO2 Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!HNO2=HONO 7.10E+27 -5.40 52507.  
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO2=HONO 1.30E+29 -5.47 52785.  
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO2=HONO 2.00E+30 -5.50 53658.  
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO2 (+M)=HONO (+M) 2.50E+14 0.000 32300  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a  
! LOW/ 3.10E+18 0.0 31500 /  
! TROE/ 1.149 1E-30 3125 1E30 /  
!HNO2 (+M)=HONO (+M) 2.50E+14 0.000 32300  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a  
! LOW/ 3.10E+18 0.0 31500 /!  
! TROE/ 1.149 1E-30 3125 1E30 /  
!HNO2 (+M)=HONO (+M) 2.5E+14 0.000 32300  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a  
! LOW/ 3.1E+18 0.0 31500 /  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
! TROE/ 1.149 1E-30 3125 1E+30 /  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
  
!HNO2+H=H2+NO2 2.40E+08 1.50 4160.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO2+H=H2+NO2 2.40E+08 1.50 4163  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.  
12/22/95  
!NO2+H2=HNO2+H 2.40E+00 3.730 32400  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a  
!NO2+H2=HNO2+H 2.40E+00 3.730 32400  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a  
!NO2+H2=HNO2+H 2.4E+00 3.730 32400  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a  
  
!HNO2+O=OH+NO2 1.70E+08 1.50 2363.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNO2+O=NO2+OH 1.70E+08 1.500 2000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 DEA/BOZ00  
!HNO2+O=OH+NO2 1.70E+08 1.50 2365  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.  
12/22/95  
!HNO2+O=NO2+OH 1.70E+08 1.500 2000  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 DEA/BOZ00  
!HNO2+O=NO2+OH 1.7E+08 1.500 2000  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 DEA/BOZ00

```

!HNO2+OH=H2O+NO2          1.20E+06    2.00    -794.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+OH=NO2+H2O          4.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a
!HNO2+OH=H2O+NO2          1.20E+06    2.00    -795
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95
!HNO2+OH=NO2+H2O          4.00E+13    0.000    0
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!HNO2+OH=NO2+H2O          4.0E+13    0.000    0
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

!NO2+HO2=HNO2+O2          1.90E+01    3.260    4983
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08a
!NO2+HO2=HNO2+O2          1.90E+01    3.260    4983
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08a
!NO2+HO2=HNO2+O2          1.9E+01    3.260    4983
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08a

!HNO2+NH2=NO2+NH3          9.20E+05    1.94    874.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO2+NH2=NO2+NH3          9.20E+05    1.94    874
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST.
12/22/95

!HNO+NO2=HNO2+NO          6.02E+11    0.0    1986.
!5      Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!      !!
!!  HNOO Chemistry  !!
!!      !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!NH+O2=HNOO          3.50E+23    -5.00    2274.
!0.1 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O2=HNOO          3.70E+24    -5.00    2294.
!1.0 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O2=HNOO          5.40E+25    -5.05    2453.
!10 atm      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NH+O2+M=HNOO+M          3.00E+26    -4.00    2274.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNOO+M=OH+NO+M          1.50E+36    -6.18    31119.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!      !!
!!  HONHO Chemistry  !!
!!      !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!HNOH+HO2=HONHO+OH          4.00E+13    0.0    0.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!      !!
!!  NH2NO2 Chemistry  !!
!!      !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

!NH2+NO2=NH2NO2 3.50E+31 -6.8 3726.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DEA/BOZ  
2000

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! !!  
!! NO3 Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NO2+O(+M)=NO3(+M) 1.32E+13 0.0 0.  
!2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
! LOW/ 1.49E+28 -4.08 2466. /  
!1.3-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
! TROE/ 0.326 500.0 6204.9 2606.0 /  
!NO2+O(+M)=NO3(+M) 3.50E+12 0.240 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 HAH/TRO00  
! LOW/ 2.50E+20 -1.50 0 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 (M=N2)  
! TROE/ 0.71 1E-30 1700 1E30 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.71\*exp(-T/1700)  
!NO2+O(+M)=NO3(+M) 1.30E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! LOW/ 0.10E+29 -4.08 2470.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! N2/1.50/ O2/1.50/ H2O/10.0/  
!NO2+O=NO3 1.32E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
TSA/HER86  
!O+NO2(+M)=NO3(+M) 1.33E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 keyed to  
N2  
! LOW/ 1.49E+28 -4.08 2470. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
! T&H/ 0.79 -1.8E-04 /  
! N2O/5.0/ H2O/9./ N2/1.0/ HNO3/5.0/  
! NH3/5.0/ NO3/5.0/  
!NO2+O(+M)=NO3(+M) 3.50E+12 0.240 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 HAH/TRO00  
! LOW/ 2.50E+20 -1.50 0 /  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 (M=N2)  
! TROE/ 0.71 1E-30 1700 1E30 /  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.71\*exp(-  
T/1700)  
!NO2+O(+M)=NO3(+M) 3.5E+12 0.240 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 HAH/TRO00  
! LOW/ 2.5E+20 -1.50 0 /  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 (M=N2)  
! TROE/ 0.71 1E-30 1700 1E+30 /  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.71\*exp(-  
T/1700)  
!NO2+O(+M)=NO3(+M) 1.3E+13 0.0 0.0  
!Miller personal communication; Original comments: TSANG&HERRON  
! LOW/ 1.0E+28 -4.08 2470. /  
! N2/1.5/ O2/1.5/ H2O/18.6/  
  
!NO3+H=NO2+OH 6.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+H=NO2+OH 6.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO3+H=NO2+OH 6.00E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; from refs in  
NIST database

!NO3+H=NO2+OH 6.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+H=NO2+OH 6.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+H=NO2+OH 6.0E+13 0.0 0.0  
!Miller personal communication; Original comments: BECKER ET AL 92/N (PG)

!NO3+O=NO2+O2 1.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+O=NO2+O2 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO3+O=NO2+O2 1.00E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 92/99  
!NO3+O=NO2+O2 1.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+O=NO2+O2 1.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+O=NO2+O2 1.0E+13 0.0 0.0  
!Miller personal communication; Original comments: ATKINSON ET AL 92 (PG)

!NO3+OH=NO2+HO2 1.40E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+OH=NO2+HO2 1.40E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO3+OH=HO2+NO2 1.20E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ATK/BAU 99  
!NO3+OH=NO2+HO2 1.40E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+OH=NO2+HO2 1.4E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 ATK/TRO92  
!NO3+OH=NO2+HO2 1.4E+13 0.0 0.0  
!Miller personal communication; Original comments: ATKINSON ET AL 92 (PG)

!NO3+HO2=NO2+O2+OH 1.50E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+HO2=NO2+O2+OH 1.50E+12 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO3+HO2=NO2+O2+OH 2.50E+12 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; controversial reaction  
!NO3+HO2=NO2+O2+OH 1.50E+12 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+HO2=NO2+O2+OH 1.5E+12 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 BEC/SCH92  
!NO3+HO2=NO2+O2+OH 1.5E+12 0.0 0.0  
!Miller personal communication; Original comments: BECKER ET AL 92 (PG)

!NO3+NH=HNO+NO2 1.50E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP Laidler

!NO3+NH2=NH2O+NO2 9.00E+05 0.0 100.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP DB00

!HNNO+NO2=NNH+NO3 1.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: HE93

!NO2+NO2=NO3+NO 9.64E+09 -0.73 20911.  
!2-5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
!NO2+NO2=NO3+NO 9.60E+09 0.730 20900  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 NBS91  
!NO2+NO2=NO3+NO 9.60E+09 0.7 20900.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO2+NO2=NO+NO3 9.64E+09 0.73 20920.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; T&H91



!NO2+NO2=NO3+NO 9.60E+09 0.730 20900  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 NBS91  
!NO2+NO2=NO3+NO 9.6E+09 0.730 20900  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 NBS91  
!NO2+NO2=NO3+NO 9.6E+9 0.73 20900.  
!Miller personal communication; Original comments: TSANG&HERRON

!NO3+NO2=NO+NO2+O2 5.00E+10 0.000 2940  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DEM/RAV90  
!NO3+NO2=NO+NO2+O2 5.00E+10 0.0 2940.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NO2+NO3=NO+NO2+O2 2.71E+10 0.0 2500.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97  
!NO3+NO2=NO+NO2+O2 5.00E+10 0.000 2940  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: GLA/MIL98 DEM/RAV90  
!NO3+NO2=NO+NO2+O2 5.0E+10 0.000 2940  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: GLA/MIL98 DEM/RAV90  
!NO3+NO2=NO+NO2+O2 5.0E+10 0.0 2940.  
!Miller personal communication; Original comments: DEMORE ET AL 90 (PG)

!NO3+NO3=NO2+NO2+O2 5.12E+11 0.0 4870.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: DeMore97  
!NO3+NO3=2NO2+O2 5.12E+11 0.0 4870.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!! \*\*\* change HONO2 to HNO3  
!! HNO3 Chemistry !!  
!! !!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NO2+OH(+M)=HNO3(+M) 2.41E+13 0.0 0.  
!1.2 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
LOW/ 6.42E+32 -5.49 2349. /  
!2.5 Tsang & Herron J Phys Chem Ref Data 20 (1991) 609-663  
TROE/ 0.400 450.7 1584.0 /  
!NO2+OH(+M)=HNO3(+M) 3.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 TRO01  
! LOW/ 2.938E+25 -3.0 0 /  
! TROE/ 0.4 1E-30 1E30 1E30 /  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 Fc=0.4  
!NO2+OH(+M)=HNO3(+M) 2.40E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! LOW/ 0.64E+33 -5.49 2351.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! N2/1.00/ AR/0.70/ H2O/6.00/  
!OH+NO2(+M)=HNO3(+M) 2.41E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 keyed to N2  
! LOW/ 6.42E+32 -5.49 2350. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
! T&H/ 0.725 -2.5E-04 /  
N2O/5.0/ H2O/9./ N2/1.0/ HNO3/5.0/  
NH3/5.0/ !NO3/5.0/  
!NO2+OH(+M)=HNO3(+M) 3.00E+13 0.000 0  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 TRO01  
! LOW/ 2.938E+25 -3.0 0 /  
!Klippenstein et al. C&F 158 (2011) 774-789.  
! TROE/ 0.4 1E-30 1E30 1E30 /  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 Fc=0.4  
!NO2+OH(+M)=HNO3(+M) 3.0E+13 0.000 0  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 TRO01  
! LOW/ 2.938E+25 -3.0 0 /

!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments:  
! TROE/ 0.4 1E-30 1E+30 1E+30 /  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 Fc=0.4

!HNO3+H=H2+NO3 5.60E+08 1.500 16400  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=NO3+H2 5.60E+08 1.5 16400.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
BOUGHT97  
!HNO3+H=NO3+H2 2.40E+08 1.5 11600.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following DB00 EP  
!HNO3+H=H2+NO3 5.60E+08 1.500 16400  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=H2+NO3 5.6E+08 1.500 16400  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97

!HNO3+H=H2O+NO2 6.10E+01 3.300 6285  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=NO2+H2O 6.00E+13 0.0 9800.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNO3+H=NO2+H2O 6.00E+13 0.0 9800.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following Laidler EP  
!HNO3+H=H2O+NO2 6.10E+01 3.300 6285  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=H2O+NO2 6.1E+01 3.300 6285  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97

!HNO3+H=OH+HONO 3.80E+05 2.300 6976  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=HONO+OH 2.00E+13 0.0 8000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HNO3+H=HONO+OH 2.00E+13 0.0 8000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; JWB est  
!HNO3+H=OH+HONO 3.80E+05 2.300 6976  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 BOU/LIN97  
!HNO3+H=OH+HONO 3.8E+05 2.300 6976  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 BOU/LIN97

!HNO3+H=HNO2+OH 6.00E+13 0.0 7000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following Laidler EP

!HNO3+O=OH+NO3 1.80E+07 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
DeMore97  
!HNO3+O=NO3+OH 2.00E+13 0.0 12000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following Laidler EP

!HNO3+OH=H2O+NO3 1.00E+10 0.000 -1240  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 LAM/BEN84  
!HNO3+OH=H2O+NO3 9.00E+10 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: ATK2004  
!HNO3+OH(+M)=H2O+NO3(+M) 2.47E+08 0.0 -2860.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! LOW/ 6.89E+14 0.0 -1440.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! N2O/5.00/ H2O/9.00/ HNO3/5.00/ NO3/5.00/  
! NH3/5.00/  
!HNO3+OH=H2O+NO3 4.34E+09 0.0 -1560.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97  
!HNO3+OH(+M)=H2O+NO3(+M) 2.47E+08 0.0 -2860.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; DEM/SAN 97  
! LOW/ 6.89E+14 0.0 -1440.0 /

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
! N2O/5.0/ H2O/9./ N2/1.0/ HNO3/5.0/  
! NH3/5.0/ NO3/5.0/  
!HNO3+OH=H2O+NO3 1.00E+10 0.000 -1240  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 LAM/BEN84  
!HNO3+OH=H2O+NO3 1.0E+10 0.000 -1240  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 LAM/BEN84

!NO3+H2O2=HNO3+HO2 1.00E+12 0.0 8500.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!NO3+H2O2=HNO3+HO2 1.00E+12 0.0 8500.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following Laidler EP

!NO3+NH=HNO3+N 1.00E+12 0.0 5000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!NO3+NH2=HNO3+NH 1.00E+12 0.0 10000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!HNO3+NH=HNOH+NO2 1.50E+13 0.0 6000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!HNO3+NH2=NO3+NH3 9.00E+05 2.0 7300.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est  
following DB00 EP

!HNO3+NH2=NH2O+HNO2 3.00E+12 0.0 9000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!HNO3+NH3=NH2O+H2O+NO 23.2 3.5 44930.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML98 + Liau et  
al 1999 JANNAF

!NH3+HNO3=H2O+NH2NO2 8.00E-01 3.5 43100.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: MUSIN98

!HNO3+NO=HONO+NO2 8.00E+06 2.0 11000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; est Ea from  
Laidler EP, set  
!HONO+NO2=HNO3+NO 2.00E+11 0.000 32700  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08 PAR/LIN98  
!NO2+HONO=NO+HNO3 6.03E+01 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
STREIT79  
!HONO+NO2=HNO3+NO 2.00E+11 0.000 32700  
!Klippenstein et al. C&F 158 (2011) 774-789. ; Original comments: RAS/GLA08 PAR/LIN98  
!HONO+NO2=HNO3+NO 2.0E+11 0.000 32700  
!Lucassen et al. C&F (2012) 159 (2012) 2254-2279 ; Original comments: RAS/GLA08 PAR/LIN98

!HONO+NO3=HNO3+NO2 1.00E+12 0.0 6000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: McQuaid  
!HONO+NO3=HNO3+NO2 1.00E+12 0.0 6000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!HNO2+NO3=HNO3+NO2 1.00E+12 0.0 5000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est, EP  
Laidler

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! N2O4 Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

N2O4 (+M)=NO2+NO2 (+M) 4.05E+18 -1.1 12840.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments:  
BORRELL88  
LOW/ 1.96E+28 -3.80 12840.0 /  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!N2O4 (+M)=NO2+NO2 (+M) 4.05E+18 -1.1 12840.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
! LOW/ 1.96E+28 -3.8 12800. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010)  
  
!N2O4+H2O=HONO+HNO3 2.52E+14 0.0 11586.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007 ; Original comments: FIT  
NIST

!-----  
!=====  
!= H/C/N/O Reactions Subset =  
!=====

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!!  
!! No CN Chemistry !!  
!!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NH+CH3=CH4+N 8.20E+05 1.87 5848.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3+NH=N+CH4 8.20E+05 1.870 5852  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!NH+CH3=N+CH4 8.20E+05 1.9 5852.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
!CH3+NH=N+CH4 8.2E05 1.870 5852  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
!C2H5+N=C2H4+NH 4.30E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: STI95  
!C2H5+N=C2H4+NH 4.3E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: STI95  
  
CH3+NH2=CH4+NH 2.80E+06 1.94 9205.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3+NH2=CH4+NH 2.80E+06 1.940 9210  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3+NH2=CH4+NH 2.80E+06 1.9 9210.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
!CH3+NH2=CH4+NH 2.8E06 1.940 9210  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
!CH4+NH=CH3+NH2 9.0E13 0.000 20000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ROH/WAG94 C  
CH3+NH2=CH2+NH3 1.60E+06 1.87 7566.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3+NH2=CH2+NH3 1.6E06 1.870 7570  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
!CH3+NH2=CH2+NH3 1.60E+06 1.870 7570  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CH3+NH2=CH2+NH3 1.60E+06 1.9 7570.0  
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH2SING+NH3=CH3+NH2 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: v9 (change products) \*

CH4+NH2=CH3+NH3 1.50E+03 3.010 9940  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SON/FRI03  
 !CH4+NH2=CH3+NH3 1.5E03 3.010 9940  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SON/FRI03

!C2H+NH3=C2H2+NH2 7.20E+12 0.000 -735  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: CAR/PEE04 (i  
 !C2H+NH3=C2H2+NH2 7.2E12 0.000 -735  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/PEE04 (i

!C2H4+NH2=C2H3+NH3 5.30E+12 0.000 10274  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: HEN/WAG95(p)  
 !C2H4+NH2=C2H3+NH3 5.3E12 0.000 10274  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HEN/WAG95(p)

!C2H6+NH2=C2H5+NH3 4.50E+01 3.460 5600  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: MEB/LIN99  
 !C2H6+NH2=C2H5+NH3 4.5E01 3.460 5600  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: MEB/LIN99

!NNH+CH3<=>CH4+N2 2.50E+13 0.000 0.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

!N2H2+CH3=NNH+CH4 1.60E+06 1.87 2969.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H2=NNH+CH4 1.60E+06 1.870 2971  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H2=NNH+CH4 1.6E06 1.870 2971  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!H2NN+CH3=CH4+NNH 1.60E+06 1.87 129.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NN=CH4+NNH 1.60E+06 1.870 129  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NN=CH4+NNH 1.6E06 1.870 129  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!N2H3+CH3=N2H2+CH4 8.20E+05 1.87 1817.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H3=N2H2+CH4 8.20E+05 1.870 1818  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H3=N2H2+CH4 8.2E05 1.870 1818  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!N2H3+CH3=H2NN+CH4 3.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H3=H2NN+CH4 3.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H3=H2NN+CH4 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!N2H4+CH3=N2H3+CH4 3.30E+06 1.87 5322.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+N2H4=N2H3+CH4 3.30E+06 1.870 5325  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+N2H4=N2H3+CH4 3.3E06 1.870 5325  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2SING+NO=CH2+NO 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94  
 !CH2SING+NO=CH2+NO 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

```

!NO+C=CO+N                1.70E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!C+NO<=>CO+N                2.90E+13    0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!NO+C=CO+N                1.70E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!C+NO=CO+N                2.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94
!C+NO<=>CO+N                2.90E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!C+NO=CO+N                2.8E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

!CH+NO=N+HCO                2.90E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO<=>N+HCO                2.46E+13    0.000    0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH+NO=HCO+N                6.80E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO<=>N+HCO                2.46E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH+NO=HCO+N                6.8E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

!CH+NO=NH+CO                5.50E+12    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO=CO+NH                9.10E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO=CO+NH                9.1E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

CH2+NO=NH2+CO                2.30E+16    -1.43    1331.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!C2+NO=C2O+N                2.30E+13    0.000    8640
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: KRU/ROT99
!C2+NO=C2O+N                2.3E13    0.000    8640
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KRU/ROT99

N+CO2<=>NO+CO                3.00E+12    0.000    11300.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

NH+CO2<=>HNO+CO                1.00E+13    0.000    14350.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

HNO+CH3=NO+CH4                8.20E+05    1.87    480.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNO+CH3=NO+CH4                8.20E+05    1.9    953.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH3+HNO=NO+CH4                2.30E+14    0.000    8400
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d (Ea from [XIA/ZHA06],A
scaled to match room-T data)
!CH3+HNO=NO+CH4                2.3E14    0.000    8400
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d (Ea from [XIA/ZHA06],A
scaled to match room-T data)

!C2H3+NO=C2H2+HNO                1.00E+12    0.000    1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: JAM est
!C2H3+NO=C2H2+HNO                1.0E12    0.000    1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est

HCO+NO=HNO+CO                7.23E+12    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91; test
!HCO+NO=HNO+CO                7.00E+13    -0.4    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```

!HCO+NO=HNO+CO 6.9E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07  
 !HCO+NO=HNO+CO 6.90E+12 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07  
  
 !HCO+HNO=CH2O+NO 6.00E+11 0.0 2000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91 -  
 estimated  
 !HCO+HNO=NO+CH2O 6.00E+11 0.0 2000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HCO+HNO=NO+CH2O 5.80E-01 3.840 115  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN04  
 !HCO+HNO=NO+CH2O 5.8E-01 3.840 115  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN04  
  
 !CH3O+NO=CH2O+HNO 8.40E+12 0.0 2050.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; HE88  
 !CH3O+NO=CH2O+HNO 1.30E+14 -0.70 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
 CH3O+NO=HNO+CH2O 7.50E+12 0.000 2017  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d CAR/DEV98  
 DUPLICATE  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
 CH3O+NO=HNO+CH2O 2.50E+18 -2.560 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
 DUPLICATE  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
 !CH3O+NO=HNO+CH2O 7.5E12 0.000 2017  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d CAR/DEV98  
 !  
 DUPLICATE  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 !CH3O+NO=HNO+CH2O 2.5E18 -2.560 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
 !  
 DUPLICATE  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
  
 !CH2OH+NO=CH2O+HNO 1.30E+12 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NES/STI89/p  
 !CH2OH+NO=CH2O+HNO 1.3E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NES/STI89/p  
  
 !CH3O+HNO=NO+CH3OH 3.20E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d HE/LIN88  
 !CH3O+HNO=NO+CH3OH 3.2E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d HE/LIN88  
  
 !CH2OH+HNO=NO+CH3OH 3.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
 !CH2OH+HNO=NO+CH3OH 3.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
  
 !CH2CHO+NO=HNO+CH2CO 1.00E+12 0.0 8600.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est. E/P  
  
 !NH2O+CH3=CH3O+NH2 2.00E+13 0.0 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NO=CH3O+NH2 2.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NO=CH3O+NH2 2.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !NH2O+CH3=CH4+HNO 1.60E+06 1.87 2959.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+H2NO=CH4+HNO 1.60E+06 1.870 2961  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3+H2NO=CH4+HNO 1.6E06 1.870 2961

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!HNOH+CH3=CH4+HNO 1.60E+06 1.87 2095.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2OH+CH3=HNOH+CH4 1.60E+06 1.87 6345.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2OH+CH3=NH2O+CH4 8.20E+05 1.87 5491.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH+NO2=HCO+NO 1.01E+14 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WCFS82  
!CH+NO2=HCO+NO 1.00E+14 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 WAG/SAD82,RIM/HER98  
!CH+NO2=HCO+NO 1.0E14 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 WAG/SAD82,RIM/HER98

CH2+NO2=CH2O+NO 5.00E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ave STWW89 & DM95  
!CH2+NO2=CH2O+NO 5.90E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SEI/WAG89  
!CH2+NO2=CH2O+NO 5.9E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SEI/WAG89

NO2+CH3=NO+CH3O 1.40E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3+NO2=CH3O+NO 1.40E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ave GT74, YSG81,  
!CH3+NO2=CH3O+NO 1.30E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; GLA74  
!CH3+NO2=CH3O+NO 1.10E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/BEN98,WOL/CRO00  
!CH3+NO2=CH3O+NO 1.1E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/BEN98,WOL/CRO00

!C2H3+NO2=NO+CH2CHO 7.70E+14 -0.600 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GEP/HAL04 (i  
!C2H3+NO2=NO+CH2CHO 7.7E14 -0.600 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GEP/HAL04 (i

!C2H5+NO2=NO+C2H5O 4.00E+13 -0.200 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NO2+CH3=NO+CH3O  
!C2H5+NO2=NO+C2H5O 4.0E13 -0.200 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NO2+CH3=NO+CH3O

CO+NO2=NO+CO2 9.04E+13 0.0 33780.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91  
!CO+NO2=CO2+NO 9.00E+13 0.0 33800.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CO+NO2=NO+CO2 9.00E+13 0.000 33800  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 NBS91  
!CO+NO2=NO+CO2 9.0E13 0.000 33800  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 NBS91

HCO+NO2=CO+NO+OH 1.20E+23 -3.3 2355.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCO+NO2=NO+CO+OH 5.00E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (15%)  
!HCO+NO2=NO+CO+OH 5.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (15%)

HCO+NO2=H+CO2+NO 8.39E+15 -0.75 1930.



!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al;  
TH91

!HCO+NO2=H+CO2+NO	8.40E+15	-0.8	1930.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCO+NO2=NO+CO2+H	2.30E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (70%)			
!HCO+NO2=NO+CO2+H	2.3E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (70%)			

!CH2CHO+NO2=CHOCH2O+NO	8.0E12	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DOU/HAY96 (i			

!CH3CO+NO2=>CH3+CO2+NO	1.50E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: (CH3CO2+NO) (i			
!CH3CO+NO2=>CH3+CO2+NO	1.5E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: (CH3CO2+NO) (i			

!HONO+CH3=NO2+CH4	8.10E+05	1.87	5501.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!CH4+NO2=CH3+HONO	1.20E+13	0.0	30000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; SG81			
CH4+NO2=HONO+CH3	6.50E+14	0.000	45800
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d YAM/SUZ99			
!CH4+NO2=HONO+CH3	6.5E14	0.000	45800
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d YAM/SUZ99			

!C2H4+NO2=HONO+C2H3	6.50E+14	0.000	41400
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d			
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol			
!C2H4+NO2=HONO+C2H3	6.5E14	0.000	41400
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d			
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol			

!C2H6+NO2=HONO+C2H5	6.50E+14	0.000	41400
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d			
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol			
!C2H6+NO2=HONO+C2H5	6.5E14	0.000	41400
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d			
NO2+CH4=HONO+CH3[YAM/SUZ99],A,Ea-4400cal/mol			

!HOCO+NO=CO+HONO	1.50E+12	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: PET/MOO93,OLK/SMI01			
!HOCO+NO=CO+HONO	1.5E12	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: PET/MOO93,OLK/SMI01			

HCO+NO2=CO+HONO	1.24E+23	-3.29	2355.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al; TH91			
!HCO+NO2=HONO+CO	5.00E+12	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAM/FRI07 (15%)			
!HCO+NO2=HONO+CO	5.0E12	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAM/FRI07 (15%)			

CH2O+NO2=HCO+HONO	8.02E+02	2.77	13730.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Lin et al; TH91			
!CH2O+NO2=HONO+HCO	1.40E-07	5.640	9220
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN03			
!CH2O+NO2=HONO+HCO	1.4E-07	5.640	9220
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN03			

CH3O+NO2=CH2O+HONO	6.00E+12	0.00	2285.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99			

!CH2OH+NO2=HONO+CH2O	5.00E+12	0.000	0
----------------------	----------	-------	---

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d NES/STI89  
 !CH2OH+NO2=HONO+CH2O 5.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d NES/STI89  
  
 !CH3OH+NO2=HONO+CH2OH 1.50E+02 3.320 20035  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XIA/ZHA06  
 !CH3OH+NO2=HONO+CH2OH 1.5E02 3.320 20035  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XIA/ZHA06  
  
 !CH2CHO+NO2=HONO+CH2CO 8.90E+12 0.0 -160.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2CHO+NO2=CH2CO+HONO 8.90E+12 0.000 -159  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: BAR/WEI91 (i  
 !CH2CHO+NO2=CH2CO+HONO 8.9E12 0.000 -159  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: BAR/WEI91 (i  
 !CH2CHO+NO2=CH2CO+HONO 2.0E15 -0.680 1430  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DOU/HAY96 (i  
  
 !CH3CHO+NO2=HONO+CH2CHO 1.30E+12 0.0 3700.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
  
 !HNO2+CH3=NO2+CH4 8.10E+05 1.87 4836.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH4+NO2=HNO2+CH3 6.00E+14 0.000 37600  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d YAM/SUZ99  
 !CH4+NO2=HNO2+CH3 6.0E14 0.000 37600  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d YAM/SUZ99  
  
 !C2H4+NO2=HNO2+C2H3 6.00E+14 0.000 33200  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
 NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
 !C2H4+NO2=HNO2+C2H3 6.0E14 0.000 33200  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
 NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
  
 !C2H6+NO2=HNO2+C2H5 6.00E+14 0.000 33200  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d  
 NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
 !C2H6+NO2=HNO2+C2H5 6.0E14 0.000 33200  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d  
 NO2+CH4=HNO2+CH3[YAM/SUZ99],A,Ea-4400cal/mol  
  
 !CH2O+NO2=HNO2+HCO 1.10E-01 4.220 19850  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XU/LIN03  
 !CH2O+NO2=HNO2+HCO 1.1E-01 4.220 19850  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XU/LIN03  
  
 !CH3OH+NO2=HNO2+CH2OH 2.40E+03 2.900 27470  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d XIA/ZHA06  
 !CH3OH+NO2=HNO2+CH2OH 2.4E03 2.900 27470  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d XIA/ZHA06  
  
 ! OCHCHO+NO2=>p 7.9E11 0.000 1980  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: (i  
  
 !CH2SING+N2O=CH2O+N2 3.80E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: KOC/WAG90(p)  
 !CH2SING+N2O=CH2O+N2 3.8E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KOC/WAG90(p)  
  
 CO+N2O=N2+CO2 2.70E+11 0.0 20237.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CO+N2O=N2+CO2 2.70E+11 0.000 20237  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: SKR/GLA04 NBS91  
 !CO+N2O=N2+CO2 2.7E11 0.000 20237  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SKR/GLA04 NBS91

```

!NH2NO+CH3=HNNO+CH4          1.60E+06   1.87   7179.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NH2NHO+CH3=NHNHO+CH4        1.60E+06   1.87   377.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   CN Chemistry               !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CN+M=C+N+M                    2.50E+14   0.0    141100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92,
keyed to Ar=1.0
!   N2/1.5/ CO2/2.4/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92

!CH+N=CN+H                    1.70E+14  -0.09   0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N=CN+H                    1.30E+13   0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!CH+N=CN+H                    1.70E+14  -0.1    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH+N=CN+H                    1.30E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MES/CAR81
!CH+N=CN+H                    1.30E+13   0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH+N=CN+H                    1.3E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MES/CAR81

!CN+O=CO+N                    7.70E+13   0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+O=CO+N                    2.05E+13   0.0    417.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992.
!CN+O=CO+N                    1.90E+12   0.5    723.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
CN+O=CO+N                    1.90E+12   0.460   723
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 COB96
!CN+O<=>CO+N                  7.70E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+O=CO+N                    1.9E12   0.460   723
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 COB96

!NO+C=CN+O                    1.10E+13   0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!C+NO=CN+O                    6.60E+13   0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!NO+C=CN+O                    1.10E+13   0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!C+NO=CN+O                    2.00E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 CEC94
!C+NO<=>CN+O                  1.90E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!C+NO=CN+O                    2.0E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 CEC94

!CH+NO=OH+CN                  3.30E+12   0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO=CN+OH                  1.10E+12   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO=CN+OH                  1.1E12   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

```

```

!CN+O2=NO+CO                2.80E+17   -2.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+O2=NO+CO                2.80E+17   -2.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05, RIM/HER99
!CN+O2=NO+CO                2.8E17   -2.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05, RIM/HER99

!CN+N=C+N2                   2.40E+13    0.0    -556.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+N=C+N2                   1.04E+15   -0.5    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!CN+N=C+N2                   2.40E+13    0.0    -556.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CN+N=C+N2                   5.90E+14   -0.400   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!C+N2<=>CN+N                 6.30E+13    0.000  46020.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+N=C+N2                   1.80E+14    0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!C+N2=CN+N                   6.3E13    0.000  46000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98
!CN+N=C+N2                   5.9E14   -0.400   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CEC05

!CN+NO=N2+CO                 3.90E+11    0.0    27820.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95, tst
calc

!C+N2O=CN+NO                 4.80E+12    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DOR/MAR91
!C+N2O=CN+NO                 4.8E12    0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 DOR/MAR91

!CN+NO2=CO+N2O               4.90E+14   -0.8    344.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+NO2=CO+N2O               4.90E+14   -0.752  344
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05
!CN+NO2=CO+N2O               4.9E14   -0.752  344
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

!CN+NO2=N2+CO2               3.70E+14   -0.8    344.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+NO2=N2+CO2               3.70E+14   -0.752  344
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05
!CN+NO2=N2+CO2               3.7E14   -0.752  344
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

!C2+N2=CN+CN                 1.50E+13    0.000  41730
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: Sommer+97
!C2+N2=CN+CN                 1.5E13    0.000  41730
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: Sommer+97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   HCN Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!HCN(+M)=H+CN(+M)            8.30E+17   -0.93   123800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; T&H91 [13,0]
!   LOW/                       3.57E+26   -2.6    124900. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!   TSA/ 0.95  -1.0E-04 /
!   TROE/0.7342 1120.08 1.0E5/
!   N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/

```

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed
per Tsang;
!HCN+M=H+CN+M                      3.40E+35   -5.1      133000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   N2/0.0/ O2/1.5/ H2O/10.0/
!HCN+M=H+CN+M                      3.40E+35   -5.130   133000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS91
!   N2/0.0/ O2/1.5/ H2O/10/
!HCN+M<=>H+CN+M                    1.04E+29   -3.300   126600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   H2/2.00/ CH4/2.00/ CO/1.50/ !H2O/6.00/
!   C2H6/3.00/ AR/0.70/ !CO2/2.00/
!HCN+M = H+CN+M                    3.4E35    -5.130   133000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS91
!   N2/0.0/ O2/1.5/ H2O/10/

!CH2+N=HCN+H                       5.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+N=HCN+H                       5.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!CH2+N=HCN+H                       5.00E+13    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89
!CH2+N=HCN+H                       5.00E+13    0.0      0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2+N=HCN+H                       5.0E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

CN+H2=HCN+H                       3.60E+08    1.55     2999.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+H2=HCN+H                       3.61E+08    1.55     3000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992.;
whb95 is similar
!CN+H2=HCN+H                       1.10E+05    2.6      1908.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+H2=HCN+H                       1.10E+05    2.600    1908
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!CN+H2<=>HCN+H                     2.95E+05    2.450    2240.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+H2=HCN+H                       3.60E+08    1.6      3000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CN+H2 = HCN+H                     1.1E05     2.600    1908
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

!CH+NH=HCN+H                       3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est
!CH+NH=HCN+H                       3.0E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est

!CH3+N=HCN+H2                     3.70E+12    0.15     -89.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+N<=>HCN+H2                     3.70E+12    0.150    -90.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH3+N<=>HCN+H2                     3.70E+12    0.150    -90.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH3+N<=>HCN+H2                     3.70E+12    0.1      -90.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!C2H3+N=HCN+CH2                   2.00E+13    0.0      0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89
!C2H3+N=HCN+CH2                   2.00E+13    0.0      0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CN+CH4=HCN+CH3                   1.20E+05    2.64     -159.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
CH4+CN=CH3+HCN                     8.60E+05    2.300    -32
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 HER/SPE92

```

!CH4+CN=CH3+HCN 8.6E05 2.300 -32  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 HER/SPE92

!C3H3+N=HCN+C2H2 1.00E+13 0.0 0.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!H2CCCH+N=HCN+C2H2 1.0E14 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est

!C2H6+CN=C2H5+HCN 1.20E+08 1.800 -994  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 HER/SPE92  
 !C2H6+CN=C2H5+HCN 1.2E08 1.800 -994  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 HER/SPE92

!CH+N2=HCN+N 4.40E+12 0.0 21964.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH+N2=HCN+N 4.40E+12 0.0 21976.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH+N2<=>HCN+N 3.12E+09 0.880 20130.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH+N2=HCN+N 4.40E+12 0.0 21976.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH2+N2=HCN+NH 1.00E+13 0.0 73954.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2+N2<=>HCN+NH 1.00E+13 0.000 74000.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2+N2=HCN+NH 1.00E+13 0.0 74000.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89  
 !CH2+N2=HCN+NH 1.00E+13 0.000 74000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !CH2+N2<=>HCN+NH 1.00E+13 0.000 74000.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !CH2+N2=HCN+NH 1.00E+13 0.0 74000.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH2+N2=HCN+NH 1.0E13 0.000 74000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

!CH2SING+N2<=>NH+HCN 1.00E+11 0.000 65000.00  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 !CH2SING+N2<=>NH+HCN 1.00E+11 0.000 65000.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

!CN+NH3=HCN+NH2 9.20E+12 0.0 -357.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCN+N2=H+CN+N2 3.60E+26 -2.6 124890.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HCN+N2=H+CN+N2 3.60E+26 -2.600 124890  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS91  
 !HCN+N2 = H+CN+N2 3.6E26 -2.600 124890  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS91

!HCN+O=NH+CO 5.40E+08 1.21 7487.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !HCN+O=NH+CO 3.45E+03 2.64 4980.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
 MB89;Perry&Melius 85 similar  
 HCN+O=NH+CO 3.50E+03 2.6 4980.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !HCN+O=NH+CO 3.50E+03 2.640 4980  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89  
 !HCN+O<=>NH+CO 5.07E+03 2.640 4980.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !HCN+O=NH+CO 3.5E03 2.640 4980  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

!HCN+O=CN+OH	4.20E+10	0.40	20663.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HCN+O=CN+OH	2.70E+09	1.58	26600.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89; from Perry&Melius 85			
!HCN+O=CN+OH	4.20E+10	0.4	20665.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCN+O=CN+OH	4.20E+10	0.400	20665
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HCN+O<=>CN+OH	3.91E+09	1.580	26600.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HCN+O=CN+OH	4.2E10	0.400	20665
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
HCN+OH=CN+H2O	3.90E+06	1.83	10287.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!CN+H2O=HCN+OH	7.80E+12	0.0	7447.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HCN+OH=CN+H2O	3.90E+06	1.83	10290.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WHB95			
!HCN+OH=CN+H2O	3.90E+06	1.8	10300.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCN+OH=CN+H2O	3.90E+06	1.830	10300
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO/BOW95			
!CN+H2O<=>HCN+OH	8.00E+12	0.000	7460.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HCN+OH=CN+H2O	3.9E06	1.830	10300
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO/BOW95			
!OH+HCN=NH2+CO	1.60E+02	2.56	8996.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
OH+HCN=NH2+CO	7.83E-04	4.0	4000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!HCN+OH=NH2+CO	7.80E-04	4.0	4000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCN+OH=NH2+CO	7.80E-04	4.000	4000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89			
!HCN+OH<=>NH2+CO	1.60E+02	2.560	9000.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HCN+OH=NH2+CO	7.8E-04	4.000	4000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89			
!HCN+O2=CN+HO2	3.00E+13	0.0	75100.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCN+O2=CN+HO2	3.00E+13	0.000	75100
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 est			
!HCN+O2 = CN+HO2	3.0E13	0.000	75100
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 est			
!HCCO+N=HCN+CO	5.00E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89			
!HCCO+N=HCN+CO	5.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est			
!HCCO+N=HCN+CO	5.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est			
!CN+CH2O=HCN+HCO	4.20E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!CH2O+CN=HCO+HCN	1.70E+03	2.720	-1427
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: FEN/PAN97			
!CH2O+CN=HCO+HCN	1.7E03	2.720	-1427
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: FEN/PAN97			
!CH+NO=HCN+O	5.30E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			

```

!CH+NO=HCN+O                1.10E+14    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!CH+NO=HCN+O                7.90E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: CEC05
!CH+NO<=>HCN+O              4.10E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH+NO=HCN+O                7.9E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          CEC05

CH2+NO=HCN+OH                2.90E+14   -0.69    755.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+NO<=>OH+HCN            2.90E+14   -0.690    760.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2+NO=HCN+OH              3.90E+11    0.000   -378
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: ATA/WOL92,FIC/TEM01
!CH2+NO<=>OH+HCN            2.90E+14   -0.690    760.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH2+NO=HCN+OH              3.9E11    0.000   -378
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          ATA/WOL92,FIC/TEM01

!CH2SING+NO<=>OH+HCN        2.90E+14   -0.690    760.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2SING+NO=HCN+OH          2.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!CH2SING+NO<=>OH+HCN        2.90E+14   -0.690    760.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH2SING+NO=HCN+OH          2.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est

CH3+NO=HCN+H2O              4.90E+08    0.46    12392.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NO<=>HCN+H2O           9.60E+13    0.000   28800.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH3+NO=HCN+H2O             1.50E-01    3.520   3950
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MIL98
!CH3+NO<=>HCN+H2O           9.60E+13    0.000   28800.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH3+NO=HCN+H2O             1.5E-1    3.520   3950
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MIL98

!C2H+NO=HCN+CO              6.00E+13    0.000    570
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: PEE/CEU96
!C2H+NO=HCN+CO              6.0E13    0.000    570
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          PEE/CEU96

!C2H3+NO=HCN+CH2O           7.00E+21   -3.382   1025
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: STR/TAA04 (i
!C2H3+NO=HCN+CH2O           7.0E21   -3.382   1025
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          STR/TAA04 (i

!NO+HCCO=HCN+CO2            1.40E+13    0.0    695.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCCO+NO=HCN+CO2            3.70E+14   -0.750   -90
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/GLA03
!HCCO+NO=HCN+CO2            3.7E14   -0.750   -90
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          MIL/GLA03

!CN+HNO=HCN+NO              1.80E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+HNO=HCN+NO              1.80E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!CN+HNO=HCN+NO              1.8E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

!CN+HONO=HCN+NO2            1.20E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

```



```

!CN+HONO=HCN+NO2          1.20E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!CN+HONO=HCN+NO2          1.2E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

!CH+N2O=HCN+NO            1.90E+13    0.000    -511
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/WIE93
!CH+N2O=HCN+NO            1.9E13    0.000    -511
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 BEC/WIE93

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                          !!
!!   HNC Chemistry         !!
!!                          !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
HCN=HNC                    1.50E+23    -4.20    49428.
!0.1 atm                   Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN=HNC                   1.90E+24    -4.23    49548.
!1.0 atm                   Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN=HNC                   5.30E+25    -4.34    50163.
!10 atm                    Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN(+M)=HNC(+M)          1.60E+26    -3.23    49548.
!T>1000K                  Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HCN+M=HNC+M               1.60E+26    -3.2    54600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
H2O/7.0/ CO2/2.0/ !AR/0.7/
!HCN+M=HNC+M              4.36E+26    -3.34    50194.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; 2nd order
form, easiest to use
!HCN+M=HNC+M              1.60E+26    -3.230    54600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00, mod Ea
! AR/0.7/ H2O/7.0/ CO2/2.0/
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!HCN+M = HNC+M            1.6E26    -3.230    54600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00, mod Ea
! AR/0.7/ H2O/7.0/ CO2/2.0/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

HNC+H=HCN+H               7.80E+13    0.0    3600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+H=HCN+H             7.80E+13    0.000    3600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 SUM/NGU98
!HNC+H = HCN+H           7.8E13    0.000    3600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 SUM/NGU98

O+HNC=NH+CO               4.60E+12    0.0    2184.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNC+O=NH+CO              5.44E+12    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TDLLM (Lin),
1994, preprint
!HNC+O=NH+CO              4.60E+12    0.0    2200.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+O=NH+CO              4.60E+12    0.000    2200
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!HNC+O = NH+CO            4.6E12    0.000    2200
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!HNC+OH=CN+H2O            1.50E+12    0.00    7680.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TST result
from TDLLM, 1994

!HNC+O2=NH+CO2            1.60E+19    -2.25    1777.0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  CH2N Chemistry              !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!NCH2=HCN+H                      1.30E+29   -6.03   29878.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2=HCN+H                      6.00E+31   -6.46   32092.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2=HCN+H                      3.50E+29   -5.46   32529.
!10 atm                           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000) ratioed
per Tsang;
!NCH2=HCN+H                      4.00E+28   -6.0    29897.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+M=HCN+H+M                  3.00E+14   0.0    22000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89
!NCH2=HCN+H                      1.30E+29   -6.030  29894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 atm
!H+HCN(+M)<=>NCH2(+M)            3.30E+13   0.000  0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!  LOW/                          1.40E+26   -3.400  1900.00 /
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!  H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!  CO2/2.00/ AR/0.70/ !C2H6/3.00/
!HCN+H(+M)=NCH2(+M)              3.31E+13   0.0    4844.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TH91
!  LOW/                          1.60E+24   -2.73   7660. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!  TSA/ 0.95  -1.0E-04 /
!  N2O/5.0/ N2/1.0/ !H2O/5.0/ CO2/2.0/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2
!H+HCN(+M)<=>NCH2(+M)            3.30E+13   0.0    0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!  LOW/                          1.40E+26   -3.40   1900. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NCH2=HCN+H                      1.3E29    -6.030  29894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 atm

!CH+NH3=NCH2+H+H                 4.40E+13   0.000  -630
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 BEC/WIE93

!NCH2+H=HCN+H2                   2.40E+08   1.50   -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+H=HCN+H2                   4.00E+13   0.00   0.0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; lower limit
!NCH2+H=HCN+H2                   2.40E+08   1.5    -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCH2+H=HCN+H2                   2.40E+08   1.500  -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCH2+H=HCN+H2                   2.40E+08   1.5    -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!NCH2+H=HCN+H2                   2.4E08    1.500  -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!CH3+N=NCH2+H                    6.10E+14   -0.31   288.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+N<=>NCH2+H                   6.10E+14   -0.310  290.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH3+N=NCH2+H                    6.10E+14   -0.3    288.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH3+N=NCH2+H                    7.10E+13   0.000  0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 DAV/HAN91B
!CH3+N<=>NCH2+H                   6.10E+14   -0.310  290.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH3+N<=>NCH2+H                   6.10E+14   -0.3    290.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

```

!CH3+N=NCH2+H	7.1E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 DAV/HAN91B			
!CH+NH2=NCH2+H	3.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est			
!CH+NH2=NCH2+H	3.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est			
!CH3+NH=NCH2+H2	3.50E+13	0.0	290.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WF97			
!NCH2+CH3=HCN+CH4	8.10E+05	1.87	-1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+CH3=HCN+CH4	8.10E+05	1.9	-1113.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!C2H5+N=CH3+NCH2	2.30E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: STI95			
!C2H5+N=CH3+NCH2	2.3E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: STI95			
!NCH2+N=HCN+NH	7.20E+13	0.00	400.0
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!NCH2+N=N2+CH2	6.00E+13	0.0	397.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+N<=>N2+CH2	6.00E+13	0.000	400.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!NCH2+N=N2+CH2	2.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; MB89			
!NCH2+N=CH2+N2	2.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est			
!NCH2+N<=>N2+CH2	6.00E+13	0.000	400.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!NCH2+N=N2+CH2	6.00E+13	0.0	397.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NCH2+N=CH2+N2	2.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est			
!NCH2+NH=HCN+NH2	1.70E+08	1.500	-894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est NCH2+O			
!NCH2+NH=HCN+NH2	1.7E08	1.500	-894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est NCH2+O			
!NCH2+NH2=HCN+NH3	9.20E+05	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NCH2+NH2=HCN+NH3	9.20E+05	1.940	-1152
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!NCH2+NH2=HCN+NH3	9.20E+05	1.9	-1152.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!NCH2+NH2=HCN+NH3	9.2E05	1.940	-1152
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!CH2+NO=NCH2+O	8.10E+07	1.42	4111.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+O=HCN+OH	1.70E+08	1.50	-894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCH2+O=HCN+OH	1.00E+07	2.0	6100.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
!NCH2+O=HCN+OH	1.70E+08	1.5	-894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NCH2+O=HCN+OH	1.70E+08	1.500	-894

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!NCH2+O=HCN+OH 1.7E08 1.500 -894  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!CH3+NO=NCH2+OH 2.20E+09 0.75 11717.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH3+NO<=>NCH2+OH 1.00E+12 0.000 21750.00  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
!CH3+NO=NCH2+OH 1.50E-01 3.520 3950  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 MIL98  
!CH3+NO<=>NCH2+OH 1.00E+12 0.000 21750.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!CH3+NO=NCH2+OH 1.5E-1 3.520 3950  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 MIL98

!NCH2+OH=HCN+H2O 2.10E+17 -1.68 318.  
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCH2+OH=HCN+H2O 1.50E+19 -2.18 2165.  
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCH2+OH=HCN+H2O 9.50E+21 -2.91 5630.  
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCH2+OH=HCN+H2O 1.20E+06 2.00 -1192.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCH2+OH=HCN+H2O 1.00E+07 2.0 3700.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
98  
!NCH2+OH=HCN+H2O 1.50E+19 -2.2 2166.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! DUPLICATE  
!NCH2+OH=HCN+H2O 1.20E+06 2.0 -1192.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! DUPLICATE  
!NCH2+OH=HCN+H2O 2.10E+17 -1.680 318  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2  
! DUPLICATE  
!NCH2+OH=HCN+H2O 1.20E+06 2.000 -1192  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:  
! DUPLICATE  
!NCH2+OH=HCN+H2O 2.1E17 -1.680 318  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2  
! DUPLICATE  
!NCH2+OH=HCN+H2O 1.2E06 2.000 -1192  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:  
! DUPLICATE

!NCH2+O2=CH2O+NO 3.00E+12 0.0 5958.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCH2+O2=CH2O+NO 3.00E+12 0.0 5961.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NCH2+O2=CH2O+NO 3.00E+12 0.000 5961  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!NCH2+O2=CH2O+NO 3.0E12 0.000 5961  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!NCH2+O2=HCN+HO2 2.70E+04 2.0 17300.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
98  
!NCH2+O2=HCN+HO2 2.70E+04 2.0 17300.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!NCH2+HO2=HCN+H2O2 1.40E+04 2.69 -1609.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!NCH2+NO=HCN+HNO 1.00E+07 2.0 4400.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
98

```

!NCH2+NO=HCN+HNO                                1.00E+07    2.0    4400.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                !!
!!  CHNH Chemistry  !!
!!                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CHNH=HCN+H                                7.70E+25    -5.20    21974.
!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH=HCN+H                                6.10E+28    -5.69    24257.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH=HCN+H                                6.20E+26    -4.77    24804.
!10 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH=HCN+H                                6.10E+28    -5.7     24271.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH=HCN+H                                7.70E+25    -5.200   21986
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
!CHNH=HCN+H                                6.10E+28    -5.7     24271.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH=HCN+H                                7.7E25     -5.200   21986
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

!CH3+N=CHNH+H                                1.20E+11    0.52    -367.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CHNH+H=NCH2+H                                2.00E+13    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+H=NCH2+H                                2.00E+13    0.0     0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+H=NCH2+H                                2.00E+13    0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+H=NCH2+H                                2.00E+13    0.0     0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+H=NCH2+H                                2.0E13     0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CHNH+H=HCN+H2                                2.40E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+H=HCN+H2                                2.40E+08    1.5     -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+H=HCN+H2                                2.40E+08    1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+H=HCN+H2                                2.40E+08    1.5     -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+H=HCN+H2                                2.4E08     1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CHNH+O=HCN+OH                                1.70E+08    1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+O=HCN+OH                                1.70E+08    1.5     -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+O=HCN+OH                                1.70E+08    1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+O=HCN+OH                                1.7E08     1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CHNH+OH=HCN+H2O                                1.20E+06    2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+OH=HCN+H2O                                1.20E+06    2.0     -1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CHNH+OH=HCN+H2O                                1.20E+06    2.000   -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+OH=HCN+H2O                                1.2E06     2.000   -1192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

```

```

!CHNH+CH3=HCN+CH4          8.20E+05    1.87    -1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CHNH+CH3=HCN+CH4          8.20E+05    1.870    -1113
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CHNH+CH3=HCN+CH4          8.20E+05    1.9      -1113.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CHNH+CH3=HCN+CH4          8.2E05    1.870    -1113
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!  CH2NH Chemistry            !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH2NH+M=HCN+H2+M          1.00E+14    0.0      10000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH2NH+M=HCN+H2+M          1.00E+14    0.0      10000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; CAT96
!CH2NH=HCN+H2              1.00E+14    0.0      9060.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+M=HCN+H2+M          1.00E+14    0.0      10000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!NH+CH3=CH2NH+H           4.00E+13    0.0      0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH=CH2NH+H           4.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!NH+CH3=CH2NH+H           4.00E+13    0.0      0.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH=CH2NH+H           4.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH+H=NCH2+H2          2.40E+08    1.50     7318.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+H=NCH2+H2          2.40E+08    1.500    7322
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+H=NCH2+H2          2.40E+08    1.5      7322.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+H=NCH2+H2          2.4E08    1.500    7322
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH+H=CHNH+H2          3.00E+08    1.50     6126.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+H=CHNH+H2          3.00E+08    1.500    6130
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+H=CHNH+H2          3.00E+08    1.5      6130.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+H=CHNH+H2          3.0E08    1.500    6130
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH+NH3=CH2NH+H           4.4E13    0.000    -630
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 BEC/WIE93, prod est (v12)

!CH2SING+NH2=CH2NH+H      3.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est
!CH2SING+NH2=CH2NH+H      3.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 est

!CH2SING+NH3=CH2NH+H+H    1.00E+14    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 est

!CH3+NH2=CH2NH+H2        2.10E+11    -0.10    19084.
!0.1 atm                  Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

```

!CH3+NH2=CH2NH+H2 4.80E+11 -0.20 19392.  
 !1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2NH+H2 2.90E+12 -0.40 20494.  
 !10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3+NH2=CH2NH+H2 2.10E+11 -0.100 19095  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2  
 !CH3+NH2<=>CH2NH+H2 2.40E+06 1.2 17369.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3+NH2=CH2NH+H2 2.1E11 -0.100 19095  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2  
  
 !CH2NH+O=NCH2+OH 1.70E+08 1.50 4627.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=NCH2+OH 3.16E+08 2.0 6100.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+O=NCH2+OH 1.70E+08 1.5 4630.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+O=NCH2+OH 1.70E+08 1.500 4630  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=NCH2+OH 1.7E08 1.500 4630  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !CH2NH+O=CHNH+OH 2.20E+08 1.50 5402.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=CHNH+OH 2.20E+08 1.500 5404  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=CHNH+OH 2.2E08 1.500 5404  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !CH2NH+O=CH2O+NH 1.70E+06 2.08 0.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+O=CH2O+NH 1.00E+07 2.0 2800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+O=CH2O+NH 1.70E+06 2.1 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+O=CH2O+NH 1.70E+06 2.080 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+O=CH2O+NH 1.7E06 2.080 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !CH2NH+OH=NCH2+H2O 1.20E+06 2.00 -89.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+OH=NCH2+H2O 1.00E+07 2.0 4000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+OH=NCH2+H2O 1.20E+06 2.0 -89.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
 !CH2NH+OH=NCH2+H2O 1.20E+06 2.000 -89  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+OH=NCH2+H2O 1.2E06 2.000 -89  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !CH2NH+OH=CHNH+H2O 2.40E+06 2.00 457.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH2NH+OH=CHNH+H2O 2.40E+06 2.000 457  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH2NH+OH=CHNH+H2O 2.4E06 2.000 457  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00  
  
 !CH2NH+OH=CH2O+NH2 1.80E+05 2.0 14800.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98  
 !CH2NH+OH=CH2O+NH2 1.80E+05 2.0 14800.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

```

!NCH2+HO2=CH2NH+O2          1.40E+04    2.69    -1609.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCH2+HO2=CH2NH+O2          7.87E+04    2.0      21700.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!NCH2+HO2=CH2NH+O2          1.40E+04    2.7      -1609.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000

!CH2NH+CH3=NCH2+CH4          8.20E+05    1.87    7119.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+CH3=NCH2+CH4          8.20E+05    1.870    7123
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+CH3=NCH2+CH4          8.20E+05    1.9      7123.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+CH3=NCH2+CH4          8.2E05    1.870    7123
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH+CH3=CHNH+CH4          5.30E+05    1.87    9681
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000).
!CH2NH+CH3=CHNH+CH4          5.30E+05    1.870    9687
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+CH3=CHNH+CH4          5.30E+05    1.9      9687.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+CH3=CHNH+CH4          5.3E05    1.870    9687
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH+NH2=NCH2+NH3          9.20E+05    1.94    4438.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+NH2=NCH2+NH3          9.20E+05    1.940    4441
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+NH2=NCH2+NH3          9.20E+05    1.9      4441.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+NH2=NCH2+NH3          9.2E05    1.940    4441
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH+NH2=CHNH+NH3          1.80E+06    1.94    6087.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH+NH2=CHNH+NH3          1.80E+06    1.940    6090
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH+NH2=CHNH+NH3          1.80E+06    1.9      6090.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH+NH2=CHNH+NH3          1.8E06    1.940    6090
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!!   CH3N Chemistry           !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!CH3N(+M)<=>CH2NH(+M)          1.83E+13    0.2      43980.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   LOW/                        2.23E+28    -4.45    46000. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   TROE/ 1.0 911000 10.0 0.260E+09 /
!CH3N(+M)<=>NCH2+H(+M)          7.40E+11    0.9      35470.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   LOW/                        1.87E+30    -4.52    37950. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   TROE/ 0.749 218 10.0 0.260E+09 /

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!

```



```

!! CH3NH Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH3NH=CH2NH+H 1.60E+36 -7.92 36322.
!0.1 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH=CH2NH+H 1.30E+42 -9.24 41316.
!1.0 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH=CH2NH+H 2.30E+44 -9.51 45218.
!10 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+M=CH2NH+H+M 1.00E+16 0.0 23800.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NH=CH2NH+H 1.60E+36 -7.920 36342
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
(600-2500K)
!DUPLICATE
!CH3NH(+M)<=>CH2NH+H(+M) 7.91E+11 0.3 36260.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! LOW/ 1.64E+39 -7.02 40100. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!DUPLICATE
!CH3NH=CH2NH+H 1.6E36 -7.920 36342
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2
(600-2500K)

!CH3NH+M=CH3+NH+M 1.00E+14 0.0 18000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96

!CH3+NH2=CH3NH+H 1.20E+13 -0.15 16135.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH+H 4.40E+13 -0.31 16632.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH+H 1.40E+14 -0.42 17853.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+H=CH3+NH2 6.00E+13 0.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3+NH2=CH3NH+H 1.20E+13 -0.150 16144
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
!CH3+NH2<=>CH3NH+H 9.08E+13 -0.4 15714.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH2=CH3NH+H 1.2E13 -0.150 16144
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

!CH3NH+H=CH2NH+H2 7.20E+08 1.50 -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+H=CH2NH+H2 1.00E+08 2.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NH+H=CH2NH+H2 7.20E+08 1.500 -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH+H=CH2NH+H2 7.20E+08 1.5 -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH+H=CH2NH+H2 7.2E08 1.500 -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH+O=CH2NH+OH 5.00E+08 1.50 -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+O=CH2NH+OH 1.00E+08 2.0 0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+O=CH2NH+OH 5.00E+08 1.5 -894.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH3NH+O=CH2NH+OH 5.00E+08 1.500 -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00

```

```

!CH3NH+O=CH2NH+OH          5.0E08  1.500  -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH+O=CH3O+NH          6.00E+13  0.0  0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+O=CH3O+NH          6.00E+13  0.0  0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!CH3NH+OH=CH2NH+H2O      3.60E+06  2.00  -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+OH=CH2NH+H2O      1.00E+08  2.0  0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+OH=CH2NH+H2O      3.60E+06  2.0  -1192.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!CH3NH+OH=CH2NH+H2O      3.60E+06  2.000  -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH+OH=CH2NH+H2O      3.6E06  2.000  -1192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH+OH=CH4+HNO        6.00E+12  0.0  0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+OH=CH4+HNO        6.00E+12  0.0  0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!HNOH+CH3=CH3NH+OH       2.00E+13  0.0  0
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NH+O2=CH2NH+HO2      1.00E+07  2.0  6300.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+O2=CH2NH+HO2      1.00E+07  2.0  6300.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!CH3NH+O2=CH3O+HNO       6.00E+12  0.0  4000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
98
!CH3NH+O2=CH3O+HNO       6.00E+12  0.0  4000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; KANT97

!CH3NH+CH3=CH2NH+CH4     2.40E+06  1.87  -1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3NH+CH3=CH2NH+CH4     2.40E+06  1.870  -1113
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH3NH+CH3=CH2NH+CH4     2.40E+06  1.9  -1113.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3NH+CH3=CH2NH+CH4     2.4E06  1.870  -1113
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! !!
!! CH2NH2 Chemistry !!
!! !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH2NH2=CH2NH+H          1.10E+45  -10.24  47790.
!0.1 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2=CH2NH+H          2.40E+48  -10.82  52010.
!1.0 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2=CH2NH+H          3.20E+46  -9.95  53500.
!10 atm 600-2500K      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2=CH2NH+H          1.10E+45  -10.240  47817
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
(600-2500K)

```

```

!DUPLICATE
!CH2NH2(+M)<=>CH2NH+H(+M)          7.91E+11    0.3      36260.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   LOW/          1.64E+39    -7.02    40100. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!   TROE/ 1.0 911000 10.0 0.260E+09 /
!DUPLICATE
!CH2NH2=CH2NH+H          1.1E45 -10.240  47817
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2
(600-2500K)

!CH3+NH2=CH2NH2+H          1.10E+13    -0.13    9900.
!0.1 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H          1.40E+14    -0.43    11101.
!1.0 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H          7.40E+12     0.0     12064.
!10 atm          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH2NH2+H          1.10E+13    -0.130   9905
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
!CH3+NH2<=>CH2NH2+H          5.15E+14    -0.6     10155.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH2=CH2NH2+H          1.1E13    -0.130   9905
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2

!CH2NH2+H=CH2NH+H2          4.00E+08     1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+H=CH2NH+H2          4.80E+08     1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+H=CH2NH+H2          4.80E+08     1.5     -894.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH2+H=CH2NH+H2          4.8E08     1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+O=CH2O+NH2          7.00E+13     0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+O=CH2O+NH2          7.00E+13     0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+O=CH2O+NH2          7.0E13     0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+O=CH2NH+OH          3.30E+08     1.50    -894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+O=CH2NH+OH          3.30E+08     1.500   -894
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+O=CH2NH+OH          3.3E08     1.500   -894
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+OH=CH2OH+NH2          4.00E+13     0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+OH=CH2OH+NH2          4.00E+13     0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+OH=CH2OH+NH2          4.0E13     0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+OH=CH2NH+H2O          2.40E+06     2.00    -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+OH=CH2NH+H2O          2.40E+06     2.000   -1192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+OH=CH2NH+H2O          2.4E06     2.000   -1192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+O2=CH2NH+HO2          1.00E+22     -3.09    6752.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+O2=CH2NH+HO2          1.00E+22     -3.090   6756
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+O2=CH2NH+HO2          1.0E22     -3.090   6756

```

```

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+O2=NH2+CH2O+O          6.00E+18   -1.59   30175.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH2NH2+CH3=C2H5+NH2          2.00E+13    0.0    2701.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+CH3=C2H5+NH2          2.00E+13    0.000   2702
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+CH3=C2H5+NH2          2.00E+13    0.0    2702.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH2+CH3=C2H5+NH2          2.0E13     0.000   2702
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH2NH2+CH3=CH2NH+CH4          1.60E+06    1.87   -626.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2NH2+CH3=CH2NH+CH4          1.60E+06    1.870  -626
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00
!CH2NH2+CH3=CH2NH+CH4          1.60E+06    1.9    -626.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH2NH2+CH3=CH2NH+CH4          1.6E06     1.870  -626
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

! CH2NH2+O2=PROD                4.7E13     0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JANSIL99
addition?

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                               !!
!! CH3NH2 Chemistry             !!
!!                               !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH3+NH2=CH3NH2                1.30E+54   -12.72  15599.
!0.1 atm 600-2500K   Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH2                5.10E+52   -11.99  16781.
!1.0 atm 600-2500K   Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH2                1.60E+47   -10.15  15679.
!10 atm 600-2500K   Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NH2=CH3NH2                1.30E+54   -12.72  15608
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00 0.1 ATM N2
(600-2500K)
!CH3+NH2<=>CH3NH2              1.03E+33   -6.3    5750.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
!CH3+NH2(+M)=CH3NH2(+M)        7.2E12     0.420    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JODGRO95
! LOW /2.2E30 -3.85 0/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!CH3+NH2=CH3NH2                1.3E54   -12.720  15608
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00 0.1 ATM N2
(600-2500K)

!CH3NH2+M=CH2NH+H2+M           2.40E+13    0.000   107260
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 ZHA/LEE00
!CH3NH2(+M)<=>CH2NH+H2(+M)      9.99E+08    1.2    102880.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! LOW/                          2.46E+30   -4.75   107000. /
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.
! TROE/ 0.82 154.59 1.0 401000 /
!DUP
!CH3NH2+M=CH2NH+H2+M           2.4E13     0.000   107260
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00
!DUP

!CH3NH2(+M)<=>CH2NH2+H(+M)       3.93E+15   -0.1    93820.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

```

! LOW/ 6.82E+40 -7.01 98400 /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 231.01 1.0 401000 /

!CH3NH2(+M)<=>CH3NH+H(+M) 1.44E+16 -0.3 100940.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.14E+38 -6.35 105000. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.67 169.67 1.0 401000 /

!CH3NH2+M=CHNH2+H2+M 1.3E14 0.000 82560  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00

!CH3NH2+M=CH3N+H2+M 9.8E14 0.000 117550  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 ZHA/LEE00

!CH3NH2+H=CH2NH2+H2 5.60E+08 1.50 5461.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+H=CH2NH2+H2 5.60E+08 1.500 5464  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH2+H=CH2NH2+H2 5.60E+08 1.5 5464.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3NH2+H=CH2NH2+H2 5.6E08 1.500 5464  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH2+H=CH3NH+H2 4.80E+08 1.50 9701.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+H=CH3NH+H2 4.80E+08 1.500 9706  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH2+H=CH3NH+H2 4.80E+08 1.5 9706.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 !CH3NH2+H=CH3NH+H2 4.8E08 1.500 9706  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH2+O=CH2NH2+OH 4.00E+08 1.50 5193.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+O=CH2NH2+OH 4.00E+08 1.500 5196  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH2+O=CH2NH2+OH 4.0E08 1.500 5196  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH2+O=CH3NH+OH 3.30E+08 1.50 6345.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+O=CH3NH+OH 3.30E+08 1.500 6348  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH2+O=CH3NH+OH 3.3E08 1.500 6348  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!CH3NH2+OH=CH2NH2+H2O 3.60E+06 2.00 238.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+OH=CH2NH2+H2O 1.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 CAR/CRO98  
 !CH3NH2+OH=CH2NH2+H2O 8.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/CRO98,GALALV08

!CH3NH2+OH=CH3NH+H2O 2.40E+06 2.00 447.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+OH=CH3NH+H2O 2.40E+06 2.000 447  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
 !CH3NH2+OH=CH3NH+H2O 2.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: CAR/CRO98,GALALV08

!CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.87 9163.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !CH3NH2+CH3=CH2NH2+CH4 1.50E+06 1.870 9170  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00

!CH3NH2+CH3=CH2NH2+CH4	1.50E+06	1.9	9170.0	
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.				
!CH3NH2+CH3=CH2NH2+CH4	1.5E06	1.870	9170	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00				
!CH3NH2+CH3=CH3NH+CH4	1.60E+06	1.87	8837.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH3NH2+CH3=CH3NH+CH4	1.60E+06	1.870	8842	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00				
!CH3NH2+CH3=CH3NH+CH4	1.60E+06	1.9	8842.0	
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.				
!CH3NH2+CH3=CH3NH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00				
!CH3NH2+NH2=CH2NH2+NH3	2.80E+06	1.94	5491.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH3NH2+NH2=CH2NH2+NH3	2.80E+06	1.940	5494	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00				
!CH3NH2+NH2=CH2NH2+NH3	2.80E+06	1.9	5494.0	
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.				
!CH3NH2+NH2=CH2NH2+NH3	2.8E06	1.940	5494	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00				
!CH3NH2+NH2=CH3NH+NH3	1.80E+06	1.94	7139.	
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH3NH2+NH2=CH3NH+NH3	1.80E+06	1.940	7143	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00				
!CH3NH2+NH2=CH3NH+NH3	1.80E+06	1.9	7143.0	
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.				
!CH3NH2+NH2=CH3NH+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00				
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!!		!!		
!! C2N1 Chemistry		!!		
!!		!!		
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!CH3NCH=CH3+HCN	8.1E15	-2.375	14942	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
!CH3NCH+H=CH2NCH2+H	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+h
!CH2NCH2=CH3NCH	1.3E45	-10.068	66111	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar, 700-3000 K
!CH2NCH2+H=CH3+NCH2	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2NCH2+O=CH2O+NCH2	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2NCH2+OH=CH2OH+NCH2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2NCH2+H=CH3NCH2	5.8E13	0.180	-125	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2chch2+h
!** CH3NCH2+H=CH3+CH2NH	7.0E10	0.840	-238	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3no+h
!CH3NCH2+H=CH2NCH2+H2	5.6E08	1.500	5464	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CH3NCH2+H=CH3NCH+H2	3.0E08	1.500	6130	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+h
!CH3NCH2+O=CH2NCH2+OH	4.0E08	1.500	5196	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
!CH3NCH2+O=CH3NCH+OH	2.2E08	1.500	5404	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+o
!CH3NCH2+OH=CH2NCH2+H2O	8.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh
!CH3NCH2+OH=CH3NCH+H2O	2.4E06	2.000	457	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+oh
!CH3NCH2+CH3=CH2NCH2+CH4	1.5E06	1.870	9170	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
!CH3NCH2+CH3=CH3NCH+CH4	5.3E05	1.870	9687	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+ch3
!CH3NCH2+NH2=CH2NCH2+NH3	2.8E06	1.940	5494	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
!CH3NCH2+NH2=CH3NCH+NH3	1.8E06	1.940	6090	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+nh2
!CH3NCH3=CH3NCH2+H	1.6E15	-7.544	38425	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
!CH3NCH3+H=CH3NCH2+H2	3.2E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Curran
!CH3NCH3+OH=CH3NCH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Curran
!CH3NCH3+CH3=CH3NCH2+CH4	6.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				SEEKOS88
!CH3NHCH2=CH3+CH2NH	9.8E43	-10.302	37459	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
!CH3NHCH2=CH3NCH2+H	5.9E44	-10.314	46803	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar
!CH3NHCH2+H=CH3NCH2+H2	4.8E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+h
!CH3NHCH2+O=CH2O+CH3NH	7.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+o
!CH3NHCH2+O=CH3NCH2+OH	3.3E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+o
!CH3NHCH2+OH=CH2OH+CH3NH	4.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+oh
!CH3NHCH2+OH=CH3NCH2+H2O	2.4E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+oh
!CH3NHCH2+CH3=C2H5+CH3NH	2.0E13	0.000	2702	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+ch3
!CH3NHCH2+CH3=CH3NCH2+CH4	1.6E06	1.870	-626	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2+ch3
!** CH3NHCH2+O2=CH2O+CH3+HNO	2.5E11	0.000	-1700	

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3och2+o2
!CH3NHCH2+H(+M)=CH3NHCH3(+M)	5.2E17	-0.990	1580	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h5+h(+m)
! LOW /1.99E41 -7.08 6685/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! TROE /0.8422 125 2219 6882/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH3NCH3+H=CH3NHCH3	1.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH3NHCH3+H=CH3NHCH2+H2	5.6E08	1.500	5464	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CH3NHCH3+H=CH3NCH3+H2	4.8E08	1.500	9706	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CH3NHCH3+O=CH3NHCH2+OH	6.1E12	0.000	556	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78, est br ratio
!CH3NHCH3+O=CH3NCH3+OH	3.0E12	0.000	556	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78, est br ratio
!CH3NHCH3+OH=CH3NHCH2+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 (ktot), GALALV08 (br)
!CH3NHCH3+OH=CH3NCH3+H2O	1.9E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 (ktot), GALALV08 (br)
!CH3NHCH3+CH3=CH3NHCH2+CH4	1.5E06	1.870	9170	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
!CH3NHCH3+CH3=CH3NCH3+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
!CH3NHCH3+NH2=CH3NHCH2+NH3	2.8E06	1.940	5494	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
!CH3NHCH3+NH2=CH3NCH3+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
!CHCNH+H=CH2+HNC	1.5E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+h
!CHCNH+O=H+CO+HNC	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+o
!CHCNH+OH=HCO+CHNH	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+oh
!CHCNH+O2=HNC+CO+OH	1.6E11	-0.020	1020	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+o2
!CHCNH+O2=HNC+HCO+O	2.2E02	2.690	3540	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcco+o2
!CH2SING+HCN=CH2CN+H	1.8E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				KOC/WAG90
!CH2SING+HCN=CH2CN+H	1.80E+14	0.000	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: KOC/WAG90				
!CH3+CN=CH2CN+H	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				GLA/MIL98 JAM est



!CH3+CN=CH2CN+H 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 !CH2CN+O=CH2O+CN 1.00E+14 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
 !CH2CN+O=CH2O+CN 1.3E12 0.640 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: HOYSEE95  
  
 !CH2OH+CN=CH2CN+OH 5.00E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: JAM est  
 !CH2OH+CN=CH2CN+OH 5.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: JAM est  
  
 !CH3CN=CH2CN+H 7.9E14 0.000 94940  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 !CH3CN(+M)=CH3NC(+M) 3.2E13 0.000 62000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SAIMUR84  
 ! LOW / 2.5E13 0.00 38000/  
  
 !CH3CN+H=HCN+CH3 4.4E10 0.800 6800  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
 !CH3CN+H=HCN+CH3 4.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 !CH3CN+H=HNC+CH3 2.8E15 -0.320 20030  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
  
 !CH3CN+H=CH2CN+H2 6.0E04 3.010 8522  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: WANGU01  
 !CH3CN+H=CH2CN+H2 3.00E+07 2.000 1000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 !CH3CN+O=CH2CN+OH 4.7E08 1.180 14360  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SUNWAN10  
  
 !CH3CN+OH=CH2CN+H2O 2.0E07 2.000 2000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM est  
 !CH3CN+OH=CH2CN+H2O 2.00E+07 2.000 2000  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est  
  
 !CH3CN+CH3=CH2CN+CH4 5.0E12 0.000 7000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 !CH3CN+CN=CH2CN+HCN 5.0E13 0.000 2000  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SENMAC99  
  
 !c-C2H3N=CH3CN 4.7E13 0.000 41500  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw  
  
 !c-C2H3N+H=CH2NCH2 9.8E09 1.212 1969  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw  
  
 !c-C2H3N+H=CH2CHNH 1.1E10 1.229 2422  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw  
  
 !c-C2H3N+O=>NCH2+HCO 1.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est  
  
 !c-C2H3N+O=>C2H3+NO 1.0E13 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est  
  
 !c-C2H3N+OH=>NCH2+CH2O 5.0E12 0.000 0  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est  
  
 !CH2CHN(S)+M=CH2CHN+M 1.0E13 0.000 0

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
! H/0/				
!CH2CHN(S)+H=CH2CHN+H	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN(S)+H=CH3+HCN	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN(S)=c-C2H3N	3.0E13	0.000	4000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN(S)=CH3CN	3.0E13	0.000	8000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN(S)+O=>HCO+HCN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN(S)+OH=>CH2O+HCN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CNH=CH3CN	2.5E13	0.000	70300	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				DOUMAC94
!CH2CNH+H=CH3CN+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CNH+H=CH3+HNC	3.3E10	0.851	2840	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+h
!CH2CNH+H=CHCNH+H2	3.0E07	2.000	10000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+h
!CH2CNH+H=CH2CN+H2	2.4E08	1.500	7322	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+h
!CH2CNH+O=CH2+HNCO	1.8E12	0.000	1350	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+o
!CH2CNH+O=CHCNH+OH	2.0E07	2.000	10000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+o
!CH2CNH+O=CH2CN+OH	1.7E08	1.500	4630	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+o
!CH2CNH+OH=CH2OH+HNC	1.0E12	0.000	-1013	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+oh
!CH2CNH+OH=CHCNH+H2O	1.0E07	2.000	3000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2co+oh
!CH2CNH+OH=CH2CN+H2O	1.2E06	2.000	-89	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+oh
!CH2CNH+CH3=CH2CN+CH4	8.2E05	1.870	7123	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+ch3
!CH2CNH+NH2=CH2CN+NH3	9.2E05	1.940	4441	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh+nh2
!CH2CHN+H=CH3+HCN	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est
!CH2CHN+O=CH2O+HCN	5.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				est

!CHCNH2+H=CHCNH+H2	4.8E08	1.500	9706	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CHCNH2+O=CHCNH+OH	3.3E08	1.500	6348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
!CHCNH2+O=HCCO+NH2	1.4E07	2.000	1900	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+o
!CHCNH2+OH=CHCNH+H2O	2.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh
!CHCNH2+CH3=CHCNH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
!CHCNH2+NH2=CHCNH+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
!CH3+HCN=CH3CHN	1.0E12	0.000	9900	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				Wang01, est
!CH3CHN+H=CH3CN+H2	2.4E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+h
!CH3CHN+H=CH2CHN+H2O	9.0E13	0.000	15100	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+h
!CH2CHN(S)+H2=CH3CHN+H	7.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CH2SING+h2
!CH3CHN+O=CH3CN+OH	1.7E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+O
!CH3CHN+OH=CH3CN+H2O	1.2E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+Oh
!CH3CHN+OH=CH2CHN+H2O	1.1E03	3.000	2780	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+oh
!CH3CHN+OH=CH2CHN(S)+H2O	4.4E13	-0.3485	-727	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+oh
!CH3CHN+NH2=CH3CN+NH3	9.2E05	1.940	-1152	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				h2cn+nh2
!CH3CNH=CH3+HNC	6.5E18	-2.520	33000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co; Ea+17 (1 atm)
!CH3CNH=CH3CN+H	7.7E25	-5.200	24000	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh; Ea+2 0.1 atm
!CH3CNH+H=CH3+CHNH	2.1E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+h
!CH3CNH+H=CH2CNH+H2	1.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+h
!CH3CNH+H=CH3CN+H2	2.4E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+h
!CH3CNH+O=CH2CNH+OH	5.3E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+o
!CH3CNH+O=CH3CN+OH	1.7E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+o

!CH3CNH+OH=CH2CNH+H2O	1.2E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+oh
!CH3CNH+OH=CH3CN+H2O	1.2E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+oh
!CH3CNH+O2=CH2O+CO+NH2	1.9E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+o2
!CH3CNH+CH3=CH2CNH+CH4	5.3E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3co+ch3
!CH3CNH+CH3=CH3CN+CH4	8.2E05	1.870	-1113	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				hcnh+ch3
!CH2CHNH+H=CH3+CHNH	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
!CH2CHNH+H=CH3CNH+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
!CH2CHNH+H=CH2CNH+H2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+h
!CH2CHNH+O=CH2CNH+OH	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+o
!CH2CHNH+OH=CH2CNH+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+oh
!CH2CHNH+OH=CH2OH+CHNH	1.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+oh
!CH2CHNH+O2=CH2O+CO+NH2	5.7E17	-1.757	11067	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2cho+o2 (1 atm)
!CHCNH2+H (+M)=CH2CNH2 (+M)	1.7E10	1.266	2709	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+h (+m)
! LOW /6.3E31 -4.664 3780 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! TROE /0.7878 -10212 1.E30 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! H2/2/ CO/2/ CO2/3/ H2O/5/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH2CNH2+H=CHCNH2+H2	4.5E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+h
!CH2CNH2+O=CH2CO+NH2	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+o
!CH2CNH2+OH=CHCNH2+H2O	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+oh
!CH2CNH2+O2=OCHCHO+NH2	4.0E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				chchoh+o2
!CH2CNH2+CH3=CHCNH2+CH4	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h3+ch3
!NH2+C2H2=CHCHNH2	7.8E-18	8.310	7430	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				LINMOS98 ktot (350mbar)
!CHCNH2+H (+M)=CHCHNH2 (+M)	1.7E10	1.266	2709	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h2+h (+m)
! LOW /6.3E31 -4.664 3780 /				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				

```

!      TROE /0.7878 -10212 1.E30 /
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!      H2/2/ CO/2/ CO2/3/ H2O/5/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

!CHCHNH2+H=CHCNH2+H2          4.5E13  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      c2h3+h

!CHCHNH2+O=OCCHNH2+H          3.0E13  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      c2h3+o

!CHCHNH2+OH=CHCNH2+H2O        2.0E13  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      c2h3+oh

!CHCHNH2+O2=OCHCHO+NH2         4.0E12  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      chchoh+o2

!CHCHNH2+CH3=CHCNH2+CH4        2.0E13  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      c2h3+ch3

!CH2CHNH+H=CH3CHNH            5.8E13  0.180  -125
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2chch2+h Klippenstein
v7

!CH3+CHNH=CH3CHNH              1.8E13  0.000  0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3+hco

!CH3CHNH+H=CH3CNH+H2          4.7E13  -0.350  3000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+h

!CH3CHNH+H=CH2CHNH+H2         1.9E12  0.400  5359
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+h

!CH3CHNH+H=CH3CHN+H2          2.4E08  1.500  7322
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2nh+h

!CH3CHNH+O=CH3CNH+OH          1.8E18  -1.900  2975
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+o

!CH3CHNH+O=CH2CHNH+OH         3.7E13  -0.200  3556
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+o

!CH3CHNH+O=CH3CHN+OH           1.7E08  1.500  4630
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2nh+o

!CH3CHNH+OH=CH3CNH+H2O        2.4E11  0.300  -1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+oh

!CH3CHNH+OH=CH2CHNH+H2O        3.0E13  -0.600  800
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+oh

!CH3CHNH+OH=CH3CHN+H2O        1.2E06  2.000  -89
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2nh+oh

!CH3CHNH+CH3=CH3CNH+CH4        3.9E-07  5.800  2200
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+ch3

!CH3CHNH+CH3=CH2CHNH+CH4       2.5E01  3.150  5727
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch3hco+ch3

!CH3CHNH+CH3=CH3CHN+CH4        8.2E05  1.870  7123
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2nh+ch3

!CH3CHNH+NH2=CH3CHN+NH3        9.2E05  1.940  4441
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:      ch2nh+nh2

```

!CHCHNH2+H(+M)=CH2CHNH2(+M)	3.9E13	0.200	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h3+h(+m)				
! LOW /2.10E24 -1.3 0/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! TROE /0.5 1E-30 1E30 1E30/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH2CNH2+H(+M)=CH2CHNH2(+M)	3.9E13	0.200	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h3+h(+m)				
! LOW /2.10E24 -1.3 0/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! TROE /0.5 1E-30 1E30 1E30/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH3CHNH=CH2CHNH2	5.0E18	-2.4965	67995	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: pw (0.04 bar, 1300-3000 K)				
!CH2CHNH2+H=CHCHNH2+H2	2.4E02	3.630	11266	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+h				
!CH2CHNH2+H=CH2CNH2+H2	2.4E02	3.630	11266	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+h				
!CH2CHNH2+H=CH2CHNH+H2	4.8E08	1.500	9700	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+h				
!CH3CHNH+H=CH2CHNH2+H	3.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est				
!CH2CHNH2+O=CH2CHNH+OH	3.3E08	1.500	6348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+o				
!CH2CHNH2+OH=CHCHNH2+H2O	1.3E-1	4.200	-860	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+oh				
!CH2CHNH2+OH=CH2CNH2+H2O	1.3E-1	4.200	-860	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+oh				
!CH2CHNH2+OH=CH2CHNH+H2O	2.4E06	2.000	447	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+oh				
!CH2CHNH2+O2=>p	*			
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH2CHNH2+CH3=CHCHNH2+CH4	6.0E07	1.560	16630	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+ch3				
!CH2CHNH2+CH3=CH2CNH2+CH4	6.0E07	1.560	16630	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+ch3				
!CH2CHNH2+CH3=CH2CHNH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+ch3				
!CH2CHNH2+NH2=CHCHNH2+NH3	5.3E12	0.000	10274	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+nh2				
!CH2CHNH2+NH2=CH2CNH2+NH3	5.3E12	0.000	10274	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: c2h4+nh2				
!CH2CHNH2+NH2=CH2CHNH+NH3	1.8E06	1.940	7143	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+nh2				
!CH3CH2NH=CH2NH+CH3	1.9E10	0.000	23500	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: C2H5O, 0.04 bar, Ea+8				
MATDIX07				

!CH3CH2NH=CH3CHNH+H	1.6E36	-7.920	36342	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh
!CH3CH2NH+H=CH3+CH2NH2	1.4E12	0.701	346	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				C2H5O+h XULIN11
!CH3CH2NH+H=CH3CHNH+H2	7.2E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+h
!CH3CH2NH+O=CH3CHNH+OH	5.0E08	1.500	-894	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+o
!CH3CH2NH+OH=CH3CHNH+H2O	3.6E06	2.000	-1192	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+oh
!CH3CH2NH+CH3=CH3CHNH+CH4	2.4E06	1.870	-1113	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh+ch3
!CH2CHNH2+H(+M)=CH3CHNH2(+M)	1.4E09	1.463	1355	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h4+h(+m)
! LOW /2.0E39 -6.642 5769/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
! TROE /-0.569 299 9147 152.4/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH3CHNH2=CH3CHNH+H	1.1E45	-10.240	47817	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch2nh2
!CH3CHNH2+H=CH2CHNH2+H2	4.9E08	1.700	588	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
!CH3CHNH2+H=CH3+CH2NH2	8.4E16	-0.891	2903	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
!CH3CHNH2+H=C2H4+NH3	4.7E21	-3.020	2845	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3choh XULIN11
!CH3CHNH2+H=C2H5+NH2	2.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
!CH3CHNH2+O=CH2CHNH2+OH	2.5E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 Hoyerermann
!CH3CHNH2+OH=CH2CHNH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
!CH3CHNH2+O2=CH2CHNH2+HO2	6.7E20	-3.020	2504	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 NIST
!CH3CHNH2+CH3=CH2CHNH2+CH4	1.8E13	0.000	-769	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 NIST
!C2H4+NH2=CH2CH2NH2	1.2E11	0.000	3955	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				KHELES79 (addition, close to hpl)
!CH2CH2NH2+H=CH2CHNH2+H2	1.8E12	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
!CH2CH2NH2+O=CH2O+CH2NH2	9.6E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
!CH2CH2NH2+OH=CH2CHNH2+H2O	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88

!CH2CH2NH2+HO2=>CH2O+OH+CH2NH2	2.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
!CH2CH2NH2+O2=CH2CHNH2+HO2	3.7E16	-1.630	3418	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 NIST
!CH2CH2NH2+CH3=CH2CHNH2+CH4	1.2E13	-0.320	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
!CH3CH2NH2=C2H4+NH3	6.2E67	-15.944	99348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				pw 0.04 bar, 1000-2500 K
!C2H5+NH2 (+M)=CH3CH2NH2 (+M)	7.2E12	0.420	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3+nh2, DEMLES82 (298K 400 Pa), est
! LOW /2.2E30 -3.85 0/				
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				
!CH3CHNH2+H=CH3CH2NH2	1.7E13	0.220	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7+h Klippenstein
!CH2CH2NH2+H=CH3CH2NH2	5.4E13	0.160	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				c2h5+h Klippenstein
!CH3CH2NH2+H=CH2CH2NH2+H2	1.2E07	1.800	5100	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+h Marinov
!CH3CH2NH2+H=CH3CHNH2+H2	2.6E07	1.650	2830	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+h Marinov
!CH3CH2NH2+H=CH3CH2NH+H2	4.8E08	1.500	9700	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+h
!CH3CH2NH2+H=C2H5+NH3	*			
!CH3CH2NH2+H=C2H6+NH2	*			
!CH3CH2NH2+O=CH2CH2NH2+OH	9.4E07	1.700	5460	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+o Marinov
!CH3CH2NH2+O=CH3CHNH2+OH	6.8E12	0.000	1275	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ATKPIT78 (ktot)
!CH3CH2NH2+O=CH3CH2NH+OH	3.3E08	1.500	6348	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+o
!CH3CH2NH2+OH=CH2CH2NH2+H2O	1.6E12	0.000	1300	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+oh CARSEAl1
!CH3CH2NH2+OH=CH3CHNH2+H2O	1.4E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				CARCRO98 - ass dom ch as for ch3ch2oh+oh Marinov
!CH3CH2NH2+OH=CH3CH2NH+H2O	2.4E06	2.000	447	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+oh - minor ch in agr with GALALV08 theo
!CH3CH2NH2+HO2=CH2CH2NH2+H2O2	1.2E04	2.550	15750	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ho2 Marinov
!CH3CH2NH2+HO2=CH3CHNH2+H2O2	8.2E03	2.550	10750	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ho2 Marinov
!CH3CH2NH2+CH3=CH2CH2NH2+CH4	2.2E02	3.180	9620	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3 Marinov



!CH3CH2NH2+CH3=CH3CHNH2+CH4	7.3E02	2.990	7950	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3 Marinov
!CH3CH2NH2+CH3=CH3CH2NH+CH4	1.6E06	1.870	8842	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+ch3
!CH3CH2NH2+NH2=CH2CH2NH2+NH3	2.2E02	3.180	9620	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3
!CH3CH2NH2+NH2=CH3CHNH2+NH3	7.3E02	2.990	7950	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3ch2oh+ch3
!CH3CH2NH2+NH2=CH3CH2NH+NH3	1.8E06	1.940	7140	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				ch3nh2+nh2
!CH2CH2NH2+HCO=CH3CH2NH2+CO	6.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				n-c3h7 TSA88
!CH3CHNH2+HCO=CH3CH2NH2+CO	1.2E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				i-c3h7 TSA88
!C2H2+NH2=NH2C2H2	4.6E06	8.310	7430	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				MOS/LIN98 (0.46 bar)
!C2+NO=CCN+O	5.2E13	0.000	8640	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				KRU/ROT99
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!!				!!
!! C1N2 Chemistry				!!
!!				!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
!CH+N2=NCN+H	2.22E+07	1.48	23367.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML00				
!CH+N2=NCN+H	2.22E+07	1.5	23367.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid				
!CH+N2=NCN+H	3.70E+07	1.420	20723	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/WAL97,MOS/LIN00				
!CH+N2=NCN+H	3.7E07	1.420	20723	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				MIL/WAL97,MOS/LIN00
!H+NCN=HCN+N	1.89E+14	0.0	8425.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ML00				
!H+NCN=HCN+N	1.89E+14	0.0	8425.0	
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid				
!NCN+H=HCN+N	1.00E+14	0.000	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est				
!NCN+H=HCN+N	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				GLA/MIL98 JAM est
!CN+NO=NCN+O	1.80E+13	0.0	38190.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95, tst calc				
!NCN+O=CN+NO	1.00E+14	0.000	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est				
!NCN+O=CN+NO	1.0E14	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				GLA/MIL98 JAM est
!NCN+OH=HCN+NO	5.00E+13	0.000	0	
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est				
!NCN+OH=HCN+NO	5.0E13	0.000	0	
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				GLA/MIL98 JAM est
!NCN+N=CN+N2	2.00E+13	0.0	0.	
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est.				

```

!NCN+N=CN+N2                2.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid

!CN+N2O=NCN+NO              4.20E+11    0.0    7169.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+N2O=NCN+NO              2.40E+13    0.0    13330.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Williams
etal1995, upp limb
!CN+N2O=NCN+NO              3.80E+03    2.6    3700.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+N2O=NCN+NO              3.80E+03    2.600  3700
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92, WIL/NEL95
!CN+N2O=NCN+NO              3.8E03    2.600  3700
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92, WIL/NEL95

!CH+N2=HCNN                  2.30E+27   -5.78   2443.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N2=HCNN                  3.60E+28   -5.84   2621.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N2=HCNN                  1.80E+30   -6.02   3445.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+N2(+M)<=>HCNN(+M)        3.10E+12    0.150   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   LOW/                      1.30E+25   -3.160   740.00 /
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!   TROE/ 0.6670 235.00 2117.00 4536.00 /
!   H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
!   CO2/2.00/ C2H6/3.00/ AR/1.0/
!CH+N2=HCNN                  3.60E+28   -5.8    2623.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!HCNN+H<=>CH2+N2            1.00E+14    0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HCNN+O<=>CO+H+N2           2.20E+13    0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HCNN+O<=>HCN+NO            2.00E+12    0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HCNN+OH<=>H+HCO+N2         1.20E+13    0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HCNN+O2=H+CO2+N2           4.00E+12    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCNN+O2=HCO+N2O            4.00E+12    0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCNN+O2<=>O+HCO+N2         1.20E+13    0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!CH2+N2=CH2NN               9.30E+30   -7.01   19730.
!0.1 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+N2=CH2NN               1.60E+32   -7.07   19958.
!1.0 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+N2=CH2NN               4.30E+33   -7.18   20852.
!10 atm                      Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+N2=CH2NN               1.60E+32   -7.1    19969.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NN=CH3+N2               3.00E+06    0.0     0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
CH3NN+M=CH3+N2+M            1.00E+11    0.0     5900.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

```

CH3NNH(+M)<=>CH3+NNH(+M) 3.30E+16 -0.1 55000.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 LOW/ 1.88E+31 -4.55 57500. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 TROE/ 0.97 250.59 1.0 401000 /

!H2NN+CH3=CH3NNH+H 8.30E+05 1.93 6494.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

CH3NNH+O=CH3NN+OH 9.60E+12 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

CH3NNH+OH=CH3NN+H2O 3.92E+13 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH3NN+HO2=CH3NNH+O2 1.00E+06 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH3NNH+HO2=CH3NN+H2O2 1.00E+11 0.0 1987.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH3NNH+CH3=CH4+CH3NN 4.60E+13 0.0 4850.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 CH3NNH+CH3=CH4+CH3NN 7.40E+13 0.0 5210.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NNH+NH2=NH3+CH3NN 4.60E+13 0.0 4850.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 CH3NNH+NH2=NH3+CH3NN 7.40E+13 0.0 5210.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNH+NO2=CH3NN+HONO 2.20E+11 0.0 5900.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 04

!CH2NNH2+H=NCH2+NH3 1.76E+08 1.3 8801.1  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!H2NN+CH3=CH2NNH2+H 8.30E+05 1.93 6494.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NNH2+M=CH3NNH+H+M 1.00E+17 0.0 35770.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 CH3NNH2(+M)<=>CH3NNH+H(+M) 1.35E+08 1.7 47280.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 LOW/ 1.22E+53 -10.75 53560. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NNH2(+M)<=>CH2NNH2+H(+M) 1.15E+09 1.2 50330.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 LOW/ 1.71E+49 -9.94 56000. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 TROE/ 0.0 331 10.0 47800 /

CH3NNH2+O=CH3NNH+OH 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

CH3NNH2+OH=CH3NNH+H2O 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH3NNH2+O2=CH3NNH+HO2 4.00E+12 0.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

!CH3NNH2+HO2=CH3NNH+H2O2 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 98

CH3NNH2+NO2=CH3NNH+HONO 1.00E+08 2.0 0.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 04

!CH2NHNH2 (+M) <=> CH2NH+NH2 (+M) 3.87E+12 0.2 12200.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.62E+27 -3.98 11800. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.866 298 10.0 280000 /

CH2NHNH2 (+M) <=> CH2NNH2+H (+M) 5.92E+11 0.3 36300.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 5.25E+15 -0.72 34800. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 494 10.0 280000 /

CH3NHNH (+M) <=> CH3+N2H2 (+M) 4.64E+09 1.6 35620.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 3.48E+48 -9.70 41200. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 233 10.0 308000 /

CH3NHNH (+M) <=> CH3NNH+H (+M) 1.40E+07 2.0 44660.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.82E+36 -6.56 48600. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 134 10.0 51000 /

CH3NHNH2 (+M) <=> CH3NNH2+H (+M) 4.66E+16 -0.2 77610.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.09E+49 -9.56 83400. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 169 13.7 40000 /

CH3NHNH2 (+M) <=> CH3NHNH+H (+M) 4.69E+16 -0.2 80120.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 4.44E+47 -9.19 85700. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 149 42.8 42400 /

CH3NHNH2 (+M) <=> CH2NHNH2+H (+M) 6.42E+16 -0.2 91800.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.80E+43 -7.98 96700. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.989 107 60.7 60100 /

!CH3NHNH2=CH3NNH+H2 3.16E+13 0.0 57000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Golden et al,  
 72

CH3NHNH2 (+M) <=> CH3NNH+H2 (+M) 9.70E+08 1.3 107500.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.05E+68 -13.84 115000. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 500000 10.0 41700 /

CH3NHNH2 (+M) <=> CH2NNH2+H2 (+M) 2.69E+09 1.2 105430.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 1.05E+68 -13.84 114.0 /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.195 4720 1.0 1.0 /

!CH3NHNH2 (+M) <=> N2H3+CH3 (+M) 3.12E+16 -0.2 65180.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 7.34E+61 -13.01 72900. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 271 10.0 41700 /

!CH3NHNH2 (+M) <=> H2NN+CH4 (+M) 1.36E+09 1.6 67110.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 2.47E+51 -10.4 74300. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 260 10.0 77500 /

CH3NHNH2 (+M) <=> N2H2+CH4 (+M) 1.61E+10 1.1 108880.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 4.382E+63 -12.62 116000. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 978 10.0 41700 /

!CH3NHNH2+M=CH3NH+NH2+M 2.50E+14 0.0 40940.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 !CH3NHNH2 (+M) <=> CH3NH+NH2 (+M) 2.40E+16 -0.1 63790.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 8.92E+64 -13.84 71900. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NHNH2=CH2NH+NH3 1.58E+13 0.0 54000.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Golden et al,  
 72  
 !CH3NHNH2 (+M) <=> CH2NH+NH3 (+M) 3.50E+08 1.4 68330.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 8.05E+48 -10.3 75300. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.0 242 10.0 41700 /

!CH3NHNH2 (+M) <=> CH3N+NH3 (+M) 4.33E+09 1.2 62170.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! LOW/ 7.50E+69 -15.57 71600. /  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.  
 ! TROE/ 0.355 293 10 41300 /

!CH3NHNH2+H=CH3NNH2+H2 1.30E+13 0.0 2500.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 CH3NHNH2+H=CH3NNH2+H2 2.08E+07 1.8 4488.1  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+H=CH3NHNH+H2 1.68E+09 1.1 7289.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+H=CH2NHNH2+H2 7.88E+07 1.7 11162.0  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NHNH2+H=CH3NH+NH3 4.46E+09 0.0 3100.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,  
 96  
 !CH3NHNH2+H=CH3NH+NH3 1.37E+09 1.1 5526.4  
 !Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+O=CH3NNH+H2O	9.60E+12	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
CH3NHNH2+O=CH3NNH2+OH	9.60E+12	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
CH3NHNH2+O=CH3NHNH+OH	2.69E+12	0.0	0.
!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)			
CH3NHNH2+O=CH2NHNH2+OH	1.30E+12	0.0	0.
!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)			
CH3NHNH2+OH=CH3NNH2+H2O	3.92E+13	0.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
CH3NHNH2+OH=CH3NHNH+H2O	1.10E+13	0.0	0.
!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)			
CH3NHNH2+OH=CH2NHNH2+H2O	5.30E+12	0.0	0.
!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)			
!CH3NNH2+HO2=CH3NHNH2+O2	1.00E+06	2.0	0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
!CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 98			
!CH3NHNH2+HO2=CH3NHNH+H2O2	7.56E+10	0.0	1987.
!NJL estimation based on Anderson et al. and divided by 3.57 (ave dif between k's from Sun et al constants)			
!CH3NHNH2+HO2=CH2NHNH2+H2O2	3.65E+10	0.0	1987.
!NJL estimation based on Anderson et al. and divided by 7.39 (ave dif between k's from Sun et al constants)			
!CH3NHNH2+CH3=CH4+CH3NNH2	1.00E+13	0.0	6990.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al, 96			
CH3NHNH2+CH3=CH4+CH3NNH2	4.79E+01	3.4	3578.3
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+CH3=CH3NHNH+CH4	3.21E+02	3.1	5748.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+CH3=CH2NHNH2+CH4	2.27E+01	3.5	7669.4
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH3NNH2+NH2	1.45E+02	3.3	4435.5
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH3NHNH+NH2	6.20E+02	3.1	7062.4
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
CH3NHNH2+NH=CH2NHNH2+NH2	3.93E+01	3.6	10910.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.			
!CH3NHNH2+NH2=NH3+CH3NNH2	1.00E+11	0.5	1990.

```

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
CH3NHNH2+NH2=CH3NNH2+NH3          1.65E+02    3.0      870.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+NH2=CH3NHNH+NH3          5.98E+01    3.1      2110.2
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+NH2=CH2NHNH2+NH3         1.04E+00    3.6      1894.1
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

CH3NHNH2+NO2=CH3NNH2+HONO         2.20E+11    0.0       5900.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
04

CH3NHNH2+NO2=CH3NHNH+HONO          7.87E+10    0.0       8839.
!NJL estimation off LFE relationships

CH3NHNH2+NO2=CH2NHNH2+HONO         1.39E+09    0.0       9803.
!NJL estimation off LFE relationships

CH3NHNH2+NO=CH3NNH2+HNO           1.85E+13    0.0       8524.
!NJL estimation off LFE relationships

CH3NHNH2+NO=CH3NHNH+HNO           1.24E+12    0.0       9605.
!NJL estimation off LFE relationships

CH3NHNH2+NO=CH2NHNH2+HNO          5.05E+12    0.0      11310.
!NJL estimation off LFE relationships

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                !!
!!  C2N2 Chemistry !!
!!                !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!NCCN(+M)=CN+CN(+M)                1.60E+34    -4.32    130005.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+CN(+M)=NCCN(+M)                5.66E+12    0.0      0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992
!   LOW/                             3.43E+25    -2.61    0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!   TSA/ 0.5  0.0 /
!   N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed
per Tsang;
!NCCN+M=CN+CN+M                    1.10E+34    -4.3     130079.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!   N2/1.5/ O2/1.50/ H2/1.5/ H2O/10.0/
!   CO2/3.0/

!CN+HCN=NCCN+H                     1.50E+07    1.71    1529.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCCN+H=HCN+CN                     1.40E+14    0.0     7944.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+HCN=NCCN+H                     1.51E+07    1.71    1530.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92, from
Yang et al 92;
!HCN+CN=NCCN+H                     1.50E+07    1.7     1530.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+HCN=NCCN+H                     1.50E+07    1.7     1530.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!HCN+CN=NCCN+H                     1.50E+07    1.710   1530
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!HCN+CN=NCCN+H                     1.5E07     1.710   1530
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

```

```

!HNC+CN=NCCN+H                1.00E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNC+CN=NCCN+H                1.00E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PET/OSA04 est
!HNC+CN=NCCN+H                1.0E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PET/OSA04 est

!CH3NNCH3=CH3NN+CH3           6.90E+15    0.0    50880.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NNCH3=CH3NN+CH3           6.92E+15    0.0    50875.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!CH3NNCH3=C2H6+N2             2.00E+11    0.0    33000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
96
!CH3NNCH3=C2H6+N2             2.00E+11    0.0    33000.0
!Sun et al. Int. J. Chem. Kinetics 41 (2009) 176-186.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!   all other                !!
!! Non CNO Chemistry         !!
!!                           !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! C2H4+CN=CH2CHCN+H           5.9E14   -0.240    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:                HER/SPE92
! C2H2+CN=C2HCN+H             3.6E15   -0.530    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:                HER/SPE92

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                           !!
!!   HCNO Chemistry          !!
!!                           !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!NCO(+M)=N+CO(+M)             3.30E+14    0.0    54016.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+M=N+CO+M                 1.14E+23   -1.95    59930.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992, N2
! N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.5/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; CO2/N2 per
Tsang, others guessed
!NCO+M=N+CO+M                 2.20E+14    0.0    54050.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
! N2/1.5/
!NCO+M=N+CO+M                 2.20E+14    0.000    54050
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
! N2/1.5/
!NCO+M<=>N+CO+M               3.10E+14    0.000    54050.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
! CO2/2.00/ C2H6/3.00/ AR/0.70/
!NCO+M=N+CO+M                 2.2E14    0.000    54050
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05
! N2/1.5/

CN+OH=NCO+H                   4.00E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+OH=NCO+H                   4.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,92;
WHB95 confirm
!CN+OH=NCO+H                   1.00E+15   -0.4    0.0

```



```

!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!CN+OH=NCO+H          1.00E+15   -0.437   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO96,DEC/MAC03
!CN+OH<=>NCO+H        4.00E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+OH=NCO+H          1.0E15   -0.437   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO96,DEC/MAC03

!CH+NO=H+NCO          2.00E+13   0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH+NO<=>H+NCO        1.62E+13   0.000   0.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH+NO<=>H+NCO        1.62E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH+NO=NCO+H          1.8E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          CEC05

!HCN+O=NCO+H          2.00E+08   1.47    7586.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCN+O=NCO+H          1.38E+04   2.64    4980.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
MB89;Perry&Melius 85 similar
HCN+O=NCO+H           1.40E+04   2.6     4980.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCN+O=NCO+H           1.40E+04   2.640   4980
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89
!HCN+O=NCO+H           1.4E04   2.640   4980
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89
!HCN+O<=>NCO+H        2.03E+04   2.640   4980.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!HNC+O=H+NCO          1.60E+01   3.08    -224.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TDLLM, 1994

NCO+H=NH+CO           5.20E+13   0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+H=NH+CO           5.40E+13   0.0     0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang 92
!NCO+H=CO+NH           7.20E+13   0.0     1000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+H=CO+NH           7.20E+13   0.000   1000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05
!NCO+H=CO+NH           7.2E13   0.000   1000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05
!NCO+H<=>NH+CO         5.40E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!CN+O2=NCO+O           1.00E+13   0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CN+O2=NCO+O           2.60E+14   -0.5    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; S&S88
!CN+O2=NCO+O           7.20E+12   0.0     -417.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!
!   DUPLICATE
!CN+O2=NCO+O           -2.8E17   -2.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!
!   DUPLICATE
!CN+O2=NCO+O           7.20E+12   0.000   -417
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05,RIM99
!
!   DUPLICATE
!CN+O2=NCO+O           -2.80E+17  -2.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!
!   DUPLICATE
!CN+O2<=>NCO+O         6.14E+12   0.000   -440.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CN+O2=NCO+O           7.2E12   0.000   -417

```

```

!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05,RIM99
!   DUP
!CN+O2=NCO+O           -2.8E17  -2.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!   DUP

!NCO+O=NO+CO           4.20E+13   0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+O=NO+CO           4.52E+13   0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992
!NCO+O=NO+CO           2.00E+15   -0.5    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+O=NO+CO           2.00E+15   -0.500   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 GAO/MAC03
!NCO+O<=>NO+CO         2.35E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+O=NO+CO           2.0E15   -0.500    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 GAO/MAC03

!NCO+O=N+CO2           8.00E+12   0.0    2502.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+O=N+CO2           8.00E+12   0.0    2503.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000

!NCO+OH=HON+CO         5.30E+12   -0.07   5124.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+OH=HON+CO         5.30E+12   -0.1    5126.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+OH=HON+CO         5.30E+12   -0.070  5126
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCO+OH=HON+CO         5.3E12   -0.070  5126
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!NCO+OH=H+CO+NO        8.30E+12   -0.05   18032.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+OH=NO+CO+H        2.00E+13   0.0    7500.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est
!NCO+OH=H+CO+NO        8.30E+12   -0.1    18042.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+OH=H+CO+NO        8.30E+12   -0.050  18042
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00
!NCO+OH<=>NO+H+CO      0.25E+13   0.000   0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+OH=H+CO+NO        8.3E12   -0.050  18042
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!NCO+O2=NO+CO2         2.00E+12   0.0    20000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB91
!NCO+O2=NO+CO2         2.00E+12   0.0    20000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+O2=NO+CO2         1.00E+13   0.000  10000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: BEC/WIE00, est Ć!NCO+O2<=>NO+CO2
2.00E+12   0.000  20000.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!NCO+O2=NO+CO2         1.0E13   0.000  10000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: BEC/WIE00, est Ć
!CH3CN+O=NCO+CH3       1.50E+04   2.640  4980
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM est
!CH3CN+O=CH3+NCO       6.0E09   1.800  8130
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SUNWAN10

!CH3NCH+O=>CH3+NCO+H   7.0E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcnh+h

!C2H2+NCO=HCCO+HCN     1.40E+12   0.000  1815
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 BEC/WIE95

```

!C2H2+NCO=HCCO+HCN 1.4E12 0.000 1815  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 BEC/WIE95

CN+CO2=NCO+CO 3.67E+06 2.16 26900.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WYL, IJCK 91  
!CN+CO2=NCO+CO 3.70E+06 2.2 26900.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CO2+CN=NCO+CO 3.70E+06 2.160 26900  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WAN/LIN91  
!CO2+CN=NCO+CO 3.7E06 2.160 26900  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WAN/LIN91

!C2O+NO=CO+NCO 1.0E14 0.000 670  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: THW/HER04(p)  
!C2O+NO=CO+NCO 1.00E+14 0.000 670  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: THW/HER04(p)

!C2O+NO2=CO2+NCO 5.10E+13 0.000 125  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: THW/HER04(p)  
!C2O+NO2=CO2+NCO 5.1E13 0.000 125  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: THW/HER04(p)

!NCO+N=N2+CO 3.30E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCO+N=N2+CO 2.00E+13 0.0 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!NCO+N=N2+CO 2.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NCO+N=N2+CO 2.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM est  
!NCO+N<=>N2+CO 2.00E+13 0.000 0.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!NCO+N=N2+CO 2.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM est

!CN+NO=NCO+N 5.50E+12 0.0 30620.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HWLM95 (Lin); Shock Waves Symp.  
!CN+NO=NCO+N 9.60E+13 0.0 42100.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CN+NO=NCO+N 9.60E+13 0.000 42100  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 TSA92  
!CN+NO=NCO+N 9.6E13 0.000 42100  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 TSA92

!CN+NO2=NCO+NO 6.20E+15 -0.75 348.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CN+NO2=NCO+NO 6.16E+15 -0.752 344.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WMHB 25th ISC, 94  
CN+NO2=NCO+NO 5.30E+15 -0.8 344.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CN+NO2=NCO+NO 5.30E+15 -0.752 344  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR93/CEC05  
!CN+NO2<=>NCO+NO 6.16E+15 -0.752 345.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!CN+NO2=NCO+NO 5.3E15 -0.752 344  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR93/CEC05

!NCO+NO=CO2+N2 7.80E+17 -1.73 765.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCO+NO=CO2+N2 1.46E+21 -2.74 1824.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZL00, JPC A104, 10807, 2000  
NCO+NO=N2+CO2 1.50E+21 -2.7 1824.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007

!NCO+NO=N2+CO2 1.50E+21 -2.740 1824  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 ZHU/LIN04  
 !NCO+NO<=>N2+CO2 3.80E+18 -2.000 800.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !NCO+NO=N2+CO2 1.5E21 -2.740 1824  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 ZHU/LIN04  
  
 !NCO+NO=N2O+CO 6.20E+17 -1.73 765.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+NO=N2O+CO 3.98E+19 -2.19 1743.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; ZL00, JPC  
 A104, 10807, 2000  
 !NCO+NO=N2O+CO 4.00E+19 -2.2 1743.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+NO<=>N2O+CO 1.90E+17 -1.520 740.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !NCO+NO=N2O+CO 4.0E19 -2.190 1743  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 ZHU/LIN04  
 !NCO+NO=N2O+CO 4.00E+19 -2.190 1743  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 ZHU/LIN04  
  
 !NCN+O2=NO+NCO 4.40E+09 0.510 24580  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: ZHU/LIN05  
 !NCN+O2=NO+NCO 4.4E09 0.510 24580  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ZHU/LIN05  
  
 !N2O+NCO=CO+N2+NO 9.00E+13 0.0 27800.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; TSA92  
 !NCO+NO2=CO+NO+NO 2.50E+11 0.000 -707  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR/HER93,WOO/BOW94  
 !NCO+NO2=CO+NO+NO 2.5E11 0.000 -707  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR/HER93,WOO/BOW94  
  
 !NCO+NO2=CO2+N2O 2.30E+12 0.0 -874.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+NO2=CO2+N2O 1.95E+13 -0.258 -620.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; see below  
 !NCO+NO2=CO2+N2O 3.00E+12 0.0 -707.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCO+NO2=CO2+N2O 3.00E+12 0.000 -707  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 PAR/HER93,WOO/BOW94  
 !NCO+NO2<=>N2O+CO2 3.25E+12 0.000 -705.00  
 !GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
 !NCO+NO2=CO2+N2O 3.0E12 0.000 -707  
 !Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 PAR/HER93,WOO/BOW94  
  
 !NCO+NO2=CO+NO+NO 2.10E+11 0.0 -874.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCO+NO2=CO+NO+NO 1.77E+12 -0.258 -620.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; see below  
 !NCO+NO2=CO+NO+NO 2.50E+11 0.0 -707.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
  
 !NCCN+O=NCO+CN 4.60E+12 0.0 8877.  
 !Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
 !NCCN+O=NCO+CN 4.57E+12 0.0 8880.  
 !Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
 !NCCN+O=CN+NCO 4.60E+12 0.0 8880.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !NCCN+O=NCO+CN 4.57E+12 0.0 8880.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; McQuaid  
  
 !CN+NCO=NCN+CO 1.80E+13 0.0 0.0  
 !Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
 !CN+NCO=NCN+CO 1.80E+13 0.000 0  
 !Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92

```

!CN+NCO=NCN+CO                1.8E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

!NCO+NCO=CO+CO+N2              1.80E+13   0.0   0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!NCO+NCO=CO+CO+N2              1.80E+13   0.000   0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92
!NCO+NCO=CO+CO+N2              1.8E13   0.000   0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

! C2H4+NCO=adduct
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          BEC/WIE95

!HCNO=HCN+O                      2.00E+30   -6.03   60698.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO=HCN+O                      4.20E+31   -6.12   61175.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO=HCN+O                      5.90E+31   -5.85   61900.
!10 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO=HCN+O                      4.20E+31   -6.1    61210.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO=HCN+O                      2.00E+30   -6.030   60733
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2
!HCNO=HCN+O                      2.0E30   -6.030   60733
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00 0.1 ATM N2

!CH2+NO=HCNO+H                  3.80E+13   -0.36   576.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH2+NO=HCNO+H                  3.10E+12   0.000   -378
!!CH2+NO<=>H+HCNO                3.80E+13   -0.360   580.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2+NO=HCNO+H                  3.1E12   0.000   -378
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: ATA/WOL92,FIC/TEM01
!CH2+NO<=>H+HCNO                3.80E+13   -0.360   580.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!CH2+NO=HCNO+H                  3.1E12   0.000   -378
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          ATA/WOL92,FIC/TEM01

!CH2SING+NO<=>H+HCNO            3.80E+13   -0.360   580.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!CH2SING+NO<=>H+HCNO            3.80E+13   -0.360   580.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

!NCH2+O=HCNO+H                  2.00E+13   0.0     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCNO+H=HCN+OH                  2.70E+11   0.18    2115.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO+H<=>OH+HCN                2.70E+11   0.180   2120.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HCNO+H=HCN+OH                  7.20E+10   0.8     8612.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+H=HCN+OH                  7.20E+10   0.841   8612
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+H<=>OH+HCN                2.70E+11   0.180   2120.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCNO+H=HCN+OH                  7.2E10   0.841   8612
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+H=NH2+CO                  1.70E+14   -0.75    2889.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO+H<=>NH2+CO                1.70E+14   -0.750   2890.00
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!HCNO+H<=>NH2+CO                1.70E+14   -0.750   2890.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

```

```

!HCNO+O=HCO+NO                7.00E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCNO+O=HCO+NO                6.30E+13    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+O=HCO+NO                6.30E+13    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA98
!HCNO+O=HCO+NO                6.3E13    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA98

!HCNO+O=NCO+OH                7.00E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+O=NCO+OH                7.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+O=NCO+OH                7.0E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+OH=HCO+HNO              4.50E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=HCO+HNO              4.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=HCO+HNO              4.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+OH=HCOH+NO              4.00E+13    0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HCNO+OH=CH2O+NO              1.00E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=CH2O+NO              1.00E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03 (HCOH)
!HCNO+OH=CH2O+NO              1.0E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03 (HCOH)

!HCNO+OH=NO+CO+H2             6.50E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NO+CO+H2             6.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NO+CO+H2             6.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+OH=NCO+H2O              3.50E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NCO+H2O              3.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NCO+H2O              3.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!HCNO+OH=NCO+H+OH             4.50E+12    0.0    0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HCNO+OH=NCO+H+OH             4.50E+12    0.000    0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/GLA03
!HCNO+OH=NCO+H+OH             4.5E12    0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/GLA03

!NO+HCCO=HCNO+CO              4.60E+13    0.0    695.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HCCO+NO=HCNO+CO              2.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89
!HCCO+NO=HCNO+CO              5.90E+12    0.089    -457
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: MIL/GLA03
!HCCO+NO<=>HCNO+CO            0.90E+13    0.000    0.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HCCO+NO=HCNO+CO              5.9E12    0.089    -457
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: MIL/GLA03

!HCCO+NO2=HCNO+CO2            1.60E+13    0.000    0

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 TEM/WAG92/p  
!HCCO+NO2=HCNO+CO2 1.6E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 TEM/WAG92/p

!HCNO+CN=HCN+CO 6.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: FEN/HER06,PAN/TAN08  
!HCNO+CN=HCN+CO 6.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: FEN/HER06,PAN/TAN08

!HNCO(+M)=NH+CO(+M) 1.30E+16 0.0 84320.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
HNCO(+M)=NH+CO(+M) 6.00E+13 0.0 99800.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992  
LOW/ 2.17E+28 -3.1 101900. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
! TSA/ 0.9 -2.0E-04 /  
TROE/0.4665 1000.0 1.0E6/  
N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed  
per Tsang;  
!HNCO+M=CO+NH+M 1.10E+16 0.0 86000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
! N2/1.5/  
!HNCO+M=CO+NH+M 1.10E+16 0.000 86000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MER/HAN89  
! N2/1.5/  
!HNCO+M<=>NH+CO+M 1.18E+16 0.000 84720.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/  
! CO2/2.00/ C2H6/3.00/ AR/0.70/  
!HNCO+M=CO+NH+M 1.1E16 0.000 86000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MER/HAN89  
! N2/1.5/

!HNCO+M=H+NCO+M 1.00E+17 0.0 112000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; WU90

!HCNO+H<=>H+HNCO 2.10E+15 -0.690 2850.00  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
!HCNO+H=HNCO+H 2.10E+15 -0.69 2850.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HCNO+H<=>H+HNCO 2.10E+15 -0.690 2850.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

CH2+NO=HNCO+H 3.10E+17 -1.38 1271.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CH2+NO<=>H+HNCO 3.10E+17 -1.380 1270.00  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
!CH2+NO<=>H+HNCO 3.10E+17 -1.380 1270.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

!CH2SING+NO<=>H+HNCO 3.10E+17 -1.380 1270.00  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
!CH2SING+NO<=>H+HNCO 3.10E+17 -1.380 1270.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))

!OH+HCN=HNCO+H 4.40E+03 2.26 6395.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
OH+HCN=HNCO+H 1.98E-03 4.0 1000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MB89  
!HCN+OH=HNCO+H 2.00E-03 4.0 1000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCN+OH<=>HNCO+H 4.40E+03 2.260 6400.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HCN+OH=HNCO+H 2.00E-03 4.000 1000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89

!HCN+OH=HNCO+H 2.0E-03 4.000 1000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89

OH+HNC=HNCO+H 2.80E+13 0.0 3694.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNC+OH=HNCO+H 2.80E+13 0.0 3696.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLM, IJCK 24, 1103, (1992).  
!HNC+OH=HNCO+H 2.80E+13 0.0 3700.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNC+OH=HNCO+H 2.80E+13 0.000 3700  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00  
!HNC+OH = HNCO+H 2.8E13 0.000 3700  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00

!NCH2+O=HNCO+H 6.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CHNH+O=HNCO+H 7.00E+13 0.0 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!CHNH+O=HNCO+H 7.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CHNH+O=HNCO+H 7.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: TIA/GLA08 DEA/BOZ00  
!CHNH+O=HNCO+H 7.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!NCO+H2=HNCO+H 7.60E+02 3.00 3972.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNCO+H=NCO+H2 1.80E+05 2.40 9910.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!NCO+H2=HNCO+H 2.07E+06 2.0 6020.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang,1992  
HNCO+H=NCO+H2 9.00E+07 1.7 13900.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNCO+H=NCO+H2 9.00E+07 1.660 13900  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05  
!HNCO+H<=>H2+NCO 1.05E+05 2.500 13300.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HNCO+H=NCO+H2 9.0E07 1.660 13900  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

HNCO+H=NH2+CO 3.60E+04 2.49 2343.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNCO+H=NH2+CO 2.25E+07 1.7 3800.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Miller&Melius IJCK92,TST,  
!HNCO+H=NH2+CO 3.60E+04 2.5 2345.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNCO+H=NH2+CO 3.60E+04 2.490 2345  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 CEC05  
!HNCO+H<=>NH2+CO 2.25E+07 1.700 3800.00  
!GRI MECH 3.0 ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/))  
!HNCO+H=NH2+CO 3.6E04 2.490 2345  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 CEC05

!HNC+O2=HNCO+O 1.50E+12 0.01 4111.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HNCO+O=HNO+CO 1.70E+06 2.08 0.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNCO+O=HNO+CO 1.49E+08 1.57 44010.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC, TST  
!HNCO+O=HNO+CO 1.50E+08 1.6 44012.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007



```

!HNCO+O<=>HNO+CO                1.50E+08    1.570    44000.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=HNO+CO                    1.50E+08    1.570    44012
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 HE/LIN92
!HNCO+O=HNO+CO                    1.5E08     1.570    44012
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 HE/LIN92

!HNCO+O=NH+CO2                    1.70E+06     2.08     0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO+O=CO2+NH                     9.80E+07     1.41    8524.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC,
TST (Lin, p711)
!HNCO+O=NH+CO2                    9.60E+07     1.4     8520.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O=NH+CO2                    9.60E+07     1.410   8520
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92,CEC05
!HNCO+O<=>NH+CO2                  9.80E+07     1.410   8500.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=NH+CO2                    9.6E07     1.410   8520
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92,CEC05

!HNCO+O=NCO+OH                    3.10E+06     1.94    6454.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!NCO+OH=HNCO+O                    7.80E+04     2.27    -993.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
HNCO+O=NCO+OH                     2.20E+06     2.11    11430.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLWM, 92 ISC,
TST
!HNCO+O=NCO+OH                    2.20E+06     2.1     11430.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O=NCO+OH                    2.20E+06     2.110   11430
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92,CEC05
!HNCO+O<=>NCO+OH                  2.20E+06     2.110   11400.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+O=NCO+OH                    2.2E06     2.110   11430
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92,CEC05

!HNCO+OH=NH2+CO2                  6.30E+10     -0.06   11637.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=NH2+CO2                  1.60E+05     2.0     2560.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
Tsang,1992/MB91
!HNCO+OH=NH2+CO2                  6.30E+10     -0.1    11643.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000
!HNCO+OH<=>NH2+CO2                3.30E+06     1.500   3600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)

HNCO+OH=NCO+H2O                   3.60E+07     1.50    3594.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=NCO+H2O                   5.20E+10     -0.03   17555.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!HNCO+OH=H2O+NCO                   4.79E+05     2.0     2560.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
Tsang,1992/MB91
!HNCO+OH=NCO+H2O                   3.60E+07     1.5     3600.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+OH=NCO+H2O                   3.60E+07     1.500   3600
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 WOO/BOW95_hnco
!HNCO+OH<=>NCO+H2O                 3.30E+07     1.500   3600.00
!GRI MECH 3.0 (http://www.me.berkeley.edu/gri_mech/)
!HNCO+OH=NCO+H2O                   3.6E07     1.500   3600
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 WOO/BOW95_hnco

!HNCO+O2=HNO+CO2                  1.00E+12     0.0     35000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007
!HNCO+O2=HNO+CO2                  1.00E+12     0.000   35000

```

!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 GLA/KRI94  
!HNCO+O2=HNO+CO2 1.0E12 0.000 35000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 GLA/KRI94

!NCO+HO2=HNCO+O2 2.00E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!NCO+HO2=HNCO+O2 2.00E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 mc lin est  
!NCO+HO2=HNCO+O2 2.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 mc lin est

!HNCO+HO2=NCO+H2O2 3.00E+11 0.0 23700.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;  
!HNCO+HO2=NCO+H2O2 3.00E+11 0.0 22000.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HNCO+HO2=NCO+H2O2 3.00E+11 0.000 22000  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM est  
!HNCO+HO2=NCO+H2O2 3.0E11 0.000 22000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM est

NCO+CH4=HNCO+CH3 9.80E+12 0.0 8122.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNCO+CH3=NCO+CH4 1.00E+12 0.0 9929.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)  
!HNCO+CH3=NCO+CH4 1.00E+12 0.0 9935.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; DEA/BOZ 2000  
!CH4+NCO=CH3+HNCO 9.80E+12 0.000 8120  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SCH/WOL94  
!CH4+NCO=CH3+HNCO 9.8E12 0.000 8120  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SCH/WOL94

!CH3CNH+O=CH3+HNCO 1.6E14 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3co+o

!CH2CNH+OH=CH3+HNCO 6.7E11 0.000 -1013  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch2co+oh

!C2H6+NCO=C2H5+HNCO 1.50E-09 6.890 -2910  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 SCH/WOL94  
!C2H6+NCO=C2H5+HNCO 1.5E-9 6.890 -2910  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 SCH/WOL94

!NCO+HCO=HNCO+CO 3.60E+13 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!HCO+NCO=HNCO+CO 3.60E+13 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92  
!HCO+NCO=HNCO+CO 3.6E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

CH2O+NCO=HNCO+HCO 6.00E+12 0.000 0  
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92  
!CH2O+NCO=HNCO+HCO 6.00E+12 0.0 0.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007  
!CH2O+NCO=HNCO+HCO 6.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92

!CHCNH+O2=HNCO+HCO 4.9E12 -0.142 1150  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: hcco+o2

!CH2CHN+O2=CH2O+HNCO 1.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

HNCO+N=NH+NCO 2.32E+19 0.0 52500.0  
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; XU99

!HNCO+NH=NH2+NCO 2.00E+13 0.0 19300.

!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; WRA est,  
change due to new thermo

!HNCO+NH=NH2+NCO	3.00E+13	0.0	23700.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HNCO+NH=NH2+NCO	3.00E+13	0.000	23700
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 JAM lr			
!HNCO+NH=NH2+NCO	3.0E13	0.000	23700
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 JAM lr			
NCO+NH3=HNCO+NH2	2.80E+04	2.48	983.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HNCO+NH2=NCO+NH3	1.00E+12	0.0	8936.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!NCO+NH3=HNCO+NH2	2.80E+04	2.5	980.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NCO+NH3=HNCO+NH2	2.80E+04	2.480	980
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 BEC/WIE97			
!NCO+NH3=HNCO+NH2	2.8E04	2.480	980
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 BEC/WIE97			
NCO+HNO=HNCO+NO	1.80E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NCO+HNO=HNCO+NO	1.80E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92			
!NCO+HNO=HNCO+NO	1.8E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92			
!HNC+NO2=HNCO+NO	1.00E+12	0.00	32000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; TST result from TDLLM, 1994			
!NCO+HONO=HNCO+NO2	3.60E+12	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!NCO+HONO=HNCO+NO2	3.60E+12	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92			
!NCO+HONO=HNCO+NO2	3.6E12	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92			
!HNCO+NO2=HNNO+CO2	2.50E+12	0.0	26000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HLLM93			
!HNCO+NO2=CO2+HNNO	2.51E+12	0.0	26000.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007; HE93			
CN+HNCO=HCN+NCO	1.00E+13	0.0	0.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!CN+HNCO=HCN+NCO	1.00E+13	0.000	0
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 NBS92/1.5			
!CN+HNCO=HCN+NCO	1.0E13	0.000	0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 NBS92/1.5			
!OH+HCN=HOCN+H	1.10E+06	2.03	13365.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+H=HCN+OH	2.00E+13	-0.04	2135.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!OH+HCN=HOCN+H	1.10E+06	2.03	13373
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; MILLER/MELIUS			
!HCN+OH=HOCN+H	5.90E+04	2.4	12500.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HCN+OH=HOCN+H	5.90E+04	2.400	12500
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 MIL/BOW89			
!HCN+OH<=>HOCN+H	1.10E+06	2.030	13370.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HCN+OH=HOCN+H	5.9E04	2.400	12500
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 MIL/BOW89			
!HCNO+H=HOCN+H	1.40E+11	-0.19	2482.

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!HOCN+H=HNCO+H	3.10E+08	0.84	1916.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+H=HNCO+H	3.10E+08	0.84	1917
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!HOCN+H=HNCO+H	3.10E+08	0.8	1917.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HOCN+H=HNCO+H	3.10E+08	0.840	1917
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HOCN+H<=>H+HNCO	2.00E+07	2.000	2000.00
!GRI MECH 3.0 ( <a href="http://www.me.berkeley.edu/gri_mech/">http://www.me.berkeley.edu/gri_mech/</a> )			
!HOCN+H=HNCO+H	3.1E08	0.840	1917
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!HOCN+H=NH2+CO	1.20E+08	0.61	2075.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+H=NH2+CO	1.20E+08	0.61	2076
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;			
!HOCN+H=NH2+CO	1.20E+08	0.6	2076.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HOCN+H=NH2+CO	1.20E+08	0.610	2076
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HOCN+H=NH2+CO	1.2E08	0.610	2076
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!HOCN+H=H2+NCO	2.40E+08	1.50	6613.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+H=H2+NCO	2.40E+08	1.50	6617
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; HTRAN EST. 12/22/95			
!HOCN+H=H2+NCO	2.40E+08	1.5	6617.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HOCN+H=H2+NCO	2.40E+08	1.500	6617
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HOCN+H=H2+NCO	2.4E08	1.500	6617
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!HOCN+O=OH+NCO	1.70E+08	1.50	4131.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+O=OH+NCO	1.70E+08	1.5	4133.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HOCN+O=OH+NCO	1.70E+08	1.500	4133
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HOCN+O=OH+NCO	1.7E08	1.500	4133
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!HOCN+OH=H2O+NCO	1.20E+06	2.00	-248.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!HOCN+OH=H2O+NCO	1.20E+06	2.0	-248.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007			
!HOCN+OH=H2O+NCO	1.20E+06	2.000	-248
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00			
!HOCN+OH=H2O+NCO	1.2E06	2.000	-248
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00			
!HOCN+CH3=CH4+NCO	8.20E+05	1.87	6613.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			
!CH3+HOCN=CH3CN+OH	5.0E12	0.000	2000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: GLA/MIL98 JAM			
!CH3+HOCN=CH3CN+OH	5.00E+12	0.000	2000
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: GLA/MIL98 JAM			
!HOCN+NH2=NCO+NH3	9.20E+05	1.94	3644.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)			

!HOCN+NH2=NCO+NH3		9.20E+05	1.9	3646.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007				
!HOCN+NH2=NCO+NH3		9.20E+05	1.940	3646
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: DAG/ALZ08 DEA/BOZ00				
!HOCN+NH2=NCO+NH3		9.2E05	1.940	3646
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: DAG/ALZ08 DEA/BOZ00				
!NCCN+OH=HOCN+CN		2.00E+12	0.0	18985.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!NCCN+OH=CN+HOCN		1.90E+11	0.0	2900.0
!Catoire et al. C&F (2012) doi:10.1016/j.combust?ame.2011.12.007				
!CH2NO=HNCO+H		6.90E+41	-9.30	51673.
!0.1 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO=HNCO+H		2.30E+42	-9.11	53807.
!1.0 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO=HNCO+H		1.70E+38	-7.64	53549.
!10 atm 600-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+H=CH3+NO		4.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+H=HCNO+H2		4.80E+08	1.50	-894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+O=CH2O+NO		7.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+O=HCNO+OH		3.30E+08	1.50	-894.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!NCH2+HO2=CH2NO+OH		3.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+OH=CH2OH+NO		4.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+OH=HCNO+H2O		2.40E+06	2.00	-1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+O2=CH2O+NO2		1.20E+15	-1.01	20117.
!1000-2500K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+O2=CH2O+NO2		2.90E+12	-0.31	17694.
!300-1000K Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+CH3=C2H5+NO		3.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+CH3=HCNO+CH4		1.60E+06	1.87	-1112.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+NH2=CH2NH2+NO		3.00E+13	0.0	0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!CH2NO+NH2=HCNO+NH3		1.80E+06	1.94	-1152.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!OH+HCN=NCHOH		1.70E+29	-6.31	5124.
!0.1 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!OH+HCN=NCHOH		2.80E+30	-6.37	5342.
!1.0 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!OH+HCN=NCHOH		1.10E+32	-6.53	6236.
!10 atm Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)				
!H2NCO (+M)=CO+NH2 (+M)		5.9E12	0.000	25000
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:				YOKBAC73

```

!      LOW / 1.0E14 0.00 21700/

!H2NCO+H=HNCO+H2                3.0E13  0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          est

!H2NCO+O=HNCO+OH                 3.0E13  0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          est

!H2NCO+OH=HNCO+H2O               3.0E13  0.000    0
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          est

!CH2CHNH2+O=CH3+H2NCO            3.9E12  0.000   1494
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          c2h4+o
!      DUPLICATE
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!CH2CHNH2+O=CH3+H2NCO            6.2E13  0.000   6855
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!      DUPLICATE
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:

!CH3+NO(+M)=CH3NO(+M)            9.00E+12  0.00   119.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99
!      LOW/                3.20E+23  -1.87  0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99
!CH3+NO(+M)=CH3NO(+M)            9.00E+12  0.000   192
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d DAV/PIL91
!      LOW/                2.50E+16  0.0   -2841  /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments:
!      TROE/ 5.0 1E-30 120 1E30 /
!Tian et al. C&F 156 (2009) 1413-1426; Original comments: RAS/GLA08d Fc=5.0exp(-T/120)
!CH3+NO(+N2)=CH3NO(+N2)          1.00E+13  0.0    0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!      LOW/                1.90E+18  0.0    0.  /
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!      SRI/ 0.03 790 1.0 /
!CH3+NO(+M)=CH3NO(+M)            9.0E12  0.000   192
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d DAV/PIL91
!      LOW /2.5E16 0.0 -2841/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:
!      TROE /5.0 1E-30 120 1E30/
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: RAS/GLA08d Fc=5.0exp(-T/120)

!CH3+NO=CH3NO                    3.60E+35  -8.25  4806.
!0.1 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NO=CH3NO                    1.00E+37  -8.38  5223.
!1.0 atm                          Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)
!CH3+NO=CH3NO                    4.60E+41  -9.39  8261.
!10 atm                           Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+H=CH2NO+H2                4.40E+08  1.50   377.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+H=CH3+HNO                 1.80E+13  0.0   2780.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+O=CH2NO+OH                3.30E+08  1.50  3614.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+O=CH3+NO2                 1.70E+06  2.08   0.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+OH=CH2NO+H2O              3.60E+06  2.00 -1192.
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+OH=CH3+HONO               2.50E+12  0.0   993.

```

!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NO+CH3=CH2NO+CH4 7.90E+05 1.87 5412.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!CH3NCH3+O=CH3NO+CH3 5.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: est

!CH3NCH3+O2=CH3NO+CH3O 1.0E09 1.000 6000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: LINSKA79,est (Ea,pr)

!CH3NO+NH2=CH2NO+NH3 2.80E+06 1.94 1072.  
!Dean & Bozzelli "Gas-Phase Combustion Chemistry" Ch. 2 (2000)

!H2NCHO (+M)=CO+NH3 (+M) 1.0E14 0.000 75514  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KAKIMA85  
! LOW / 8.3E14 0.00 49084/

!H2NCHO+M=HCO+NH2+M 1.4E16 0.000 72900  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KAKIMA85

!H2NCHO+M=H2NCO+H+M 4.6E15 0.000 64200  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: KAKIMA85

!H2NCHO+H=H2NCO+H2 1.3E13 0.000 6955  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SYRTUR01

!H2NCHO+H=HCO+NH3 1.0E13 0.000 19100  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: SYRTUR01,est

!H2NCHO+O=H2NCO+OH 4.0E08 1.500 5196  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+o

!CH3CHNH2+O=CH3+H2NCHO 4.0E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: i-c3h7 Hoyerermann

!H2NCHO+OH=H2NCO+H2O 8.0E12 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: ch3nh2+oh

!CH3CHNH2+HO2=>CH3+OH+H2NCHO 2.4E13 0.000 0  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: i-c3h7 TSA88

!H2NCHO+CH3=H2NCO+CH4 7.0E05 2.000 9000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: BODBAC70,est

!H2NCHO+NH2=H2NCO+NH3 2.0E06 2.000 5000  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: BACYOK73(573K),est

!CH2NH2+O2=NH2CH2O+O 6.0E18 -1.590 30192  
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info: TIA/QI09 DEA/BOZ00

!H2CNO2=CH2O+NO 1.00E+13 0.00 36000.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3O+NO (+M)=CH3ONO (+M) 6.60E+14 -0.60 0.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
! LOW/ 2.70E+27 -3.50 0. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2 (+M)=CH3+NO2 (+M) 1.80E+16 0.00 58500.  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
! LOW/ 1.30E+17 0.00 42000. /  
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99  
! TSA/ 0.183 0.0 /  
! TROE/0.1832 10.0 1.0E6/

```

!CH3NO2+H=CH3+HONO                3.30E+12    0.00    3730.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+H=CH3NO+OH                 1.40E+12    0.00    3730.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+H=H2CNO2+H2                5.40E+02    3.50    5200.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+O=H2CNO2+OH                1.50E+13    0.00    5350.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+OH=H2CNO2+H2O              5.00E+05    2.00    1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+OH=CH3OH+NO2               2.00E+10    0.00    -1000.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+CH2=H2CNO2+CH3             6.50E+12    0.00    7900.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+CH2SING=H2CNO2+CH3         1.20E+14    0.00    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NO2+CH3=H2CNO2+CH4             5.50E-01    4.00    8300.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CN+NO (+M)=NCNO (+M)              3.98E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Tsang, 1992
!   LOW/                               1.56E+36    -6.2    4878. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;
!   TSA/ 0.65 0.0 /
!   TROE/0.6508 10.0 1.0E6/
!   N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; N2/CO2 ratioed
per Tsang;

CH3O+NO2 (+M)=CH3ONO2 (+M)          1.20E+13    0.00    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99
!   LOW/                               1.40E+30    -4.50    0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; GBD99

!CH3NNH2+NO2 (+M)=CH3N(NH2)NO2 (+M) 1.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
04
!   LOW/                               1.00E+17    0.0    0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

!CH3NNH2+NO2 (+M)=CH3N(NH2)ONO (+M) 1.00E+13    0.0    0.
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ; Catoire et al,
04
!   LOW/                               1.00E+17    0.0    0. /
!Anderson et al. Army Research Laboratory Report ARL-TR-5088 (February 2010) ;

! CH2CHO+NO2=CHOCH2NO2              8.0E22    -3.560    1930
!Lucassen et al. C&F 159 (2012) 2254-2279. Add. ref. info:          DOU/HAY96 (i

```

## A.2 ARL MMH/RFNA Sets

Thermochemical parameters in CHEMKIN format



## THERMO

	300.000	1000.000	5000.000								
(CH2O)3	70590C	3H	6O	3	G	0300.00	4000.00	1500.00			1
	0.01913678E+03	0.08578044E-01	-0.08882060E-05	-0.03574819E-08	0.06605143E-12						2
	-0.06560876E+06	-0.08432507E+03	-0.04662286E+02	0.06091547E+00	-0.04710536E-03						3
	0.01968843E-06	-0.03563271E-10	-0.05665404E+06	0.04525265E+03							4
(CH3)2SICH2	61991H	8C	3SI	1	G	0300.00	2500.00	1500.00			1
	0.01547852E+03	0.01065700E+00	-0.01234345E-05	-0.01293352E-07	0.02528715E-11						2
	-0.06693076E+04	-0.05358884E+03	0.02027522E+02	0.04408673E+00	-0.03370024E-03						3
	0.01484466E-06	-0.02830898E-10	0.03931454E+05	0.01815821E+03							4
AL	62987AL	1			G	0300.00	5000.00	0600.00			1
	0.02559589E+02	-0.01063224E-02	0.07202828E-06	-0.02121105E-09	0.02289429E-13						2
	0.03890214E+06	0.05234522E+02	0.02736825E+02	-0.05912374E-02	-0.04033938E-05						3
	0.02322343E-07	-0.01705599E-10	0.03886795E+06	0.04363880E+02							4
AL2H6	62987AL	2H	6		G	0300.00	1500.00	0600.00			1
	0.02634884E+02	0.02135952E+00	0.03154151E-05	-0.07684674E-07	0.02335832E-10						2
	0.08871346E+05	0.09827515E+02	-0.06800681E+02	0.05080744E+00	0.01039747E-03						3
	-0.01119582E-05	0.08459155E-09	0.01060537E+06	0.05554526E+03							4
AL2ME6	62987AL	2C	6H	18	G	0300.00	1500.00	0600.00			1
	0.01773147E+03	0.04935747E+00	0.01196854E-04	-0.01639826E-06	0.04890867E-10						2
	-0.03855560E+06	-0.05053298E+03	-0.07159750E+01	0.01067109E+01	0.02117605E-03						3
	-0.02193212E-05	0.01644144E-08	-0.03515546E+06	0.03890763E+03							4
ALAS	62987AL	1AS	1		G	0300.00	1500.00	0600.00			1
	0.04790027E+02	-0.01908226E-03	-0.01983390E-05	0.02239358E-08	-0.06904706E-12						2
	0.05259290E+06	0.03259703E+02	0.05047764E+02	-0.06419947E-02	-0.01432071E-04						3
	0.04754391E-07	-0.03297621E-10	0.05254264E+06	0.01985206E+02							4
ALH	62987AL	1H	1		G	0300.00	5000.00	1000.00			1
	0.03392644E+02	0.01215399E-01	-0.04676595E-05	0.08691625E-09	-0.06022669E-13						2
	0.03006845E+06	0.02758899E+02	0.03071503E+02	0.02165549E-01	-0.03275638E-04						3
	0.04136984E-07	-0.01877121E-10	0.03021221E+06	0.04548855E+02							4
ALH2	62987AL	1H	2		G	0300.00	1500.00	0600.00			1
	0.04486543E+02	0.03128832E-01	-0.01969438E-05	-0.01016030E-07	0.03497468E-11						2
	0.01960959E+06	0.08167897E+01	0.02442137E+02	0.09915913E-01	0.02471083E-05						3
	-0.02119583E-06	0.01710234E-09	0.01997588E+06	0.01065270E+03							4
ALH3	62987AL	1H	3		G	0300.00	1500.00	0600.00			1
	0.04186838E+02	0.06159249E-01	-0.03877593E-06	-0.02061928E-07	0.06600276E-11						2
	0.07908079E+05	0.05134396E+01	0.01008323E+02	0.01640324E+00	0.01976746E-04						3
	-0.03528558E-06	0.02753378E-09	0.08484656E+05	0.01585838E+03							4
ALME	62987AL	1C	1H	3	G	0300.00	1500.00	0600.00			1
	0.04662737E+02	0.07097939E-01	0.02520013E-05	-0.02114863E-07	0.06097489E-11						2
	0.08203228E+05	0.01769245E+02	0.02664176E+02	0.01324914E+00	0.02525848E-04						3
	-0.02394396E-06	0.01761855E-09	0.08574173E+05	0.01147449E+03							4
ALME2	62987AL	1C	2H	6	G	0300.00	1500.00	0600.00			1
	0.06481282E+02	0.01474605E+00	0.05816529E-05	-0.04621347E-07	0.01396041E-10						2
	0.03745072E+05	-0.02603326E+02	0.09494573E+01	0.03206354E+00	0.06134021E-04						3
	-0.06500042E-06	0.04911485E-09	0.04761408E+05	0.02419465E+03							4
ALME3	62987AL	1C	3H	9	G	0300.00	1500.00	0600.00			1
	0.06654948E+02	0.02455144E+00	0.01176575E-04	-0.07815023E-07	0.02255622E-10						2
	-0.01340952E+06	-0.03454481E+02	-0.07027567E+01	0.04682764E+00	0.01149903E-03						3
	-0.09160441E-06	0.06687294E-09	-0.01203799E+06	0.03232771E+03							4
AR	120186AR	1			G	0300.00	5000.00	1000.00			1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
	-0.07453750E+04	0.04366001E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00						3
	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366001E+02							4
AR+	121286AR	1E	-1		G	0300.00	5000.00	1000.00			1
	0.02864864E+02	-0.01203573E-02	-0.01065199E-06	0.09074839E-10	-0.09623876E-14						2
	0.01827230E+07	0.03543585E+02	0.02301341E+02	0.08035529E-02	-0.01758806E-05						3
	-0.01781093E-08	-0.08937268E-13	0.01829281E+07	0.06659358E+02							4
AS	62987AS	1			G	0300.00	1500.00	0600.00			1
	0.02617011E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
	0.03720455E+06	0.06995524E+02	0.02617011E+02	0.00000000E+00	0.00000000E+00						3
	0.00000000E+00	0.00000000E+00	0.03720455E+06	0.06995524E+02							4
AS2	62987AS	2			G	0300.00	1500.00	0600.00			1
	0.04394201E+02	0.05389968E-02	-0.02379401E-05	-0.06541924E-09	0.05184186E-12						2
	0.02235094E+06	0.04897919E+02	0.03682892E+02	0.03121811E-01	-0.01074052E-04						3
	-0.05629472E-07	0.05178811E-10	0.02247356E+06	0.08283423E+02							4

AS3	62987AS	3			G	0300.00	1500.00	0600.00	1
	0.07404036E+02	0.07818426E-02	-0.03918297E-05	-0.05203629E-09	0.06291907E-12				2
	0.03063825E+06	-0.03417324E+02	0.06403142E+02	0.04477099E-01	-0.01866642E-04				3
	-0.07394750E-07	0.07012753E-10	0.03080965E+06	0.01337136E+02					4
AS4	62987AS	4			G	0300.00	1500.00	0600.00	1
	0.09695766E+02	0.01306258E-01	-0.05519564E-05	-0.02150874E-08	0.01457935E-11				2
	0.01571732E+06	-0.01618870E+03	0.07853761E+02	0.07916509E-01	-0.02329820E-04				3
	-0.01526312E-06	0.01377435E-09	0.01603629E+06	-0.07409755E+02					4
ASALME	62987AS	1AL	1C	1H	3G	0300.00	1500.00	0600.00	1
	0.07127107E+02	0.07357864E-01	0.02300796E-06	-0.02226399E-07	0.06927227E-11				2
	0.03273438E+06	-0.01847179E+02	0.04053423E+02	0.01726125E+00	0.01833498E-04				3
	-0.03386953E-06	0.02626981E-09	0.03329309E+06	0.01299665E+03					4
ASALME2	62987AS	1AL	1C	2H	6G	0300.00	1500.00	0600.00	1
	0.09909938E+02	0.01463850E+00	0.04118731E-05	-0.04444658E-07	0.01329501E-10				2
	0.02815111E+06	-0.01523531E+03	0.04808530E+02	0.03067687E+00	0.05048001E-04				3
	-0.05908099E-06	0.04462290E-09	0.02908817E+06	0.09471621E+02					4
ASGAET	62987AS	1GA	1C	2H	5G	0300.00	1500.00	0600.00	1
	0.09081073E+02	0.01674632E+00	0.01283130E-05	-0.05590436E-07	0.01781315E-10				2
	0.03807443E+06	-0.09142782E+02	0.06364698E+01	0.04382467E+00	0.06144686E-04				3
	-0.09491641E-06	0.07374198E-09	0.03960893E+06	0.03164673E+03					4
ASGAET2	62987AS	1GA	1C	4H	10G	0300.00	1500.00	0600.00	1
	0.01032429E+03	0.03073571E+00	0.01086335E-04	-0.09971949E-07	0.02945979E-10				2
	0.03039490E+06	-0.01316402E+03	-0.03539248E+01	0.06369772E+00	0.01359742E-03				3
	-0.01286142E-05	0.09572181E-09	0.03236903E+06	0.03865086E+03					4
ASGAME	62987AS	1GA	1C	1H	3G	0300.00	1500.00	0600.00	1
	0.07322183E+02	0.06995479E-01	0.01069351E-05	-0.01995283E-07	0.06040446E-11				2
	0.03949449E+06	-0.07416680E+01	0.04877266E+02	0.01482559E+00	0.01652124E-04				3
	-0.02712058E-06	0.02080196E-09	0.03994071E+06	0.01107670E+03					4
ASGAME2	62987AS	1GA	1C	2H	6G	0300.00	1500.00	0600.00	1
	0.09352436E+02	0.01504820E+00	0.05157975E-05	-0.04553518E-07	0.01348763E-10				2
	0.03735856E+06	-0.01218114E+03	0.04382076E+02	0.03056345E+00	0.05477067E-04				3
	-0.05834108E-06	0.04373509E-09	0.03827434E+06	0.01191111E+03					4
ASGAMEH	62987AS	1GA	1C	1H	4G	0300.00	1500.00	0600.00	1
	0.07842794E+02	0.09682097E-01	0.01060306E-05	-0.02991402E-07	0.09382673E-11				2
	0.04435297E+06	-0.05093455E+02	0.03585119E+02	0.02336317E+00	0.02873356E-04				3
	-0.04737895E-06	0.03674461E-09	0.04512703E+06	0.01547160E+03					4
ASH	62987AS	1H	1		G	0300.00	1500.00	0600.00	1
	0.03219848E+02	0.01001250E-01	-0.04874997E-08	-0.01107653E-08	-0.09254321E-13				2
	0.03008176E+06	0.06647311E+02	0.03865843E+02	-0.01157571E-01	-0.03494372E-05				3
	0.07079686E-07	-0.06014028E-10	0.02996829E+06	0.03549869E+02					4
ASH2	62987AS	1H	2		G	0300.00	1500.00	0600.00	1
	0.03428307E+02	0.03181140E-01	0.01460484E-05	-0.07937145E-08	0.01694414E-11				2
	0.02010282E+06	0.02904703E+02	0.03778945E+02	0.01759233E-01	0.08070807E-05				3
	0.02358763E-07	-0.03043521E-10	0.02004862E+06	0.01272974E+02					4
ASH3	62987AS	1H	3		G	0300.00	1500.00	0600.00	1
	0.04172022E+02	0.04371323E-01	0.02177574E-05	-0.01183264E-07	0.04536374E-11				2
	0.06882916E+05	0.02803477E+02	0.09446356E+01	0.01508469E+00	0.01201696E-04				3
	-0.03397465E-06	0.02767656E-09	0.07459168E+05	0.01832268E+03					4
ASME	62987AS	1C	1H	3	G	0300.00	1500.00	0600.00	1
	0.04657260E+02	0.06976298E-01	0.02147557E-05	-0.02101159E-07	0.06082150E-11				2
	0.02806423E+06	0.03409835E+02	0.02625270E+02	0.01325242E+00	0.02441628E-04				3
	-0.02419567E-06	0.01786944E-09	0.02844080E+06	0.01327336E+03					4
ASME2	62987AS	1C	2H	6	G	0300.00	1500.00	0600.00	1
	0.05981395E+02	0.01521284E+00	0.06993355E-05	-0.04721619E-07	0.01369912E-10				2
	0.01467985E+06	0.01192741E+02	0.01390400E+02	0.02923331E+00	0.06598871E-04				3
	-0.05620560E-06	0.04130368E-09	0.01553302E+06	0.02349981E+03					4
ASME3	62987AS	1C	3H	9	G	0300.00	1500.00	0600.00	1
	0.06347764E+02	0.02466454E+00	0.01154629E-04	-0.07877436E-07	0.02202225E-10				2
	-0.01617323E+05	-0.06316786E+01	0.02667388E+01	0.04253171E+00	0.01165106E-03				3
	-0.07914706E-06	0.05603127E-09	-0.04685540E+04	0.02904591E+03					4
B	41894B	1			G	0300.00	5000.00	0800.00	1
	0.02503383E+02	-0.08121395E-04	0.07407213E-07	-0.02834495E-10	0.03869814E-14				2
	0.06659164E+06	0.04181591E+02	0.02492437E+02	0.07173135E-03	-0.02060547E-05				3
	0.02420212E-08	-0.01013891E-11	0.06659287E+06	0.04227817E+02					4
BCL	41894B	1CL	1		G	0300.00	5000.00	0800.00	1
	0.04001821E+02	0.06522714E-02	-0.02820285E-05	0.05743922E-09	-0.04267682E-13				2

0.01573491E+06	0.02513849E+02	0.03005683E+02	0.03288804E-01-0.01800237E-04	3
-0.07234565E-08	0.06265518E-11	0.01598586E+06	0.07617924E+02	4
BCL2	41894B	1CL 2	G 0300.00 5000.00 0800.00	1
0.06248610E+02	0.08992638E-02-0.04383754E-05	0.01043474E-08-0.08688548E-13		2
-0.01157220E+06-0.03348238E+02	0.03985663E+02	0.07054036E-01-0.03405414E-04		3
-0.03649284E-07	0.02823078E-10-0.01102621E+06	0.08154968E+02		4
BCL3	41894B	1CL 3	G 0300.00 5000.00 1000.00	1
0.08482454E+02	0.01749626E-01-0.07838212E-05	0.01549076E-08-0.01124484E-12		2
-0.05130908E+06-0.01450771E+03	0.04676745E+02	0.01206337E+00-0.08194415E-04		3
-0.07423063E-08	0.01788528E-10-0.05032570E+06	0.05021881E+02		4
BE	81392BE	1	G 0300.00 5000.00 1000.00	1
0.02380618E+02	0.02339856E-02-0.01453949E-05	0.03111727E-09-0.01072959E-13		2
0.03868083E+06	0.02787792E+02	0.02403493E+02	0.06166087E-02-0.01321925E-04	3
0.01144806E-07-0.03437304E-11	0.03864894E+06	0.02549853E+02		4
BE(S)	81392BE	1	S 0300.00 3000.00 1000.00	1
0.01898768E+02	0.01629382E-01-0.03547406E-05	0.01247349E-08-0.01578507E-12		2
-0.06527011E+04-0.01020412E+03-0.09092963E+01	0.01585668E+00-0.02624182E-03			3
0.02044924E-06-0.05872448E-10-0.02390556E+04	0.02598871E+02			4
BE2SIO4(S)	81392BE	2O 4SI 1	S 0300.00 3000.00 1000.00	1
0.01695617E+03	0.06266472E-01-0.02841325E-04	0.06379149E-08-0.04780890E-12		2
-0.02614324E+07-0.09398438E+03-0.06380159E+02	0.09333352E+00-0.01415477E-02			3
0.01101948E-05-0.03462902E-09-0.02558671E+07	0.02162977E+03			4
BE3E2O6(S)	81392B	2BE 3O 6	S 0300.00 3000.00 1000.00	1
0.02640267E+03	0.01142674E+00-0.03773479E-04	0.04332047E-08	0.02356543E-12	2
-0.03849576E+07-0.01487137E+04-0.05230657E+02	0.01105769E+01-0.01614054E-02			3
0.01447797E-05-0.05420786E-09-0.03755957E+07	0.01490974E+03			4
BE3N2(A)	81392BE	3N 2	S 0300.00 3000.00 1000.00	1
0.01097008E+03	0.06416846E-01-0.02938928E-04	0.04564651E-08-0.05509703E-13		2
-0.07519767E+06-0.06231286E+03-0.08167547E+02	0.08515091E+00-0.01355569E-02			3
0.01060406E-05-0.03256815E-09-0.07110460E+06	0.03040606E+03			4
BE3N2(L)	81392BE	3N 2	L 0300.00 4000.00 1000.00	1
0.01610468E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.06338252E+06-0.08701469E+03	0.01610468E+03	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00-0.06338252E+06-0.08701468E+03			4
BEAL2O4(S)	81392AL	2BE 1O 4	S 0300.00 2400.00 1000.00	1
0.01118219E+03	0.01677777E+00-0.06692989E-04-0.01497360E-07	0.01203700E-10		2
-0.02810337E+07-0.06116527E+03-0.07257604E+02	0.01074554E+01-0.01713422E-02			3
0.01295274E-05-0.03740965E-09-0.02780832E+07	0.02383770E+03			4
BEB2O4	81392B	2BE 1O 4	G 0300.00 5000.00 1000.00	1
0.01266018E+03	0.06883210E-01-0.02963169E-04	0.05694789E-08-0.04050458E-12		2
-0.01672990E+07-0.03636876E+03	0.04012008E+02	0.03052847E+00-0.02571938E-03		3
0.09738810E-07-0.01450712E-10-0.01648983E+07	0.08399628E+02			4
BEBO2	81392B	1BE 1O 2	G 0300.00 5000.00 1000.00	1
0.06831273E+02	0.03424464E-01-0.01471236E-04	0.02825118E-08-0.02008790E-12		2
-0.06047559E+06-0.08730609E+02	0.02426203E+02	0.01572415E+00-0.01309160E-03		3
0.04244447E-07-0.02562806E-11-0.05929016E+06	0.01394744E+03			4
BEBR	81392BE	1BR 1	G 0300.00 5000.00 1000.00	1
0.04166357E+02	0.04424462E-02-0.01713095E-05	0.03185381E-09-0.01964221E-13		2
0.01313080E+06	0.03473875E+02	0.03178756E+02	0.03144181E-01-0.01989189E-04	3
-0.04871910E-08	0.06208255E-11	0.01337870E+06	0.08520506E+02	4
BEBR2	81392BE	1BR 2	G 0300.00 5000.00 1000.00	1
0.06814040E+02	0.07848450E-02-0.03497501E-05	0.06885841E-09-0.04984129E-13		2
-0.02974764E+06-0.06362110E+02	0.05216331E+02	0.05128972E-01-0.03678726E-04		3
0.08525872E-09	0.05611721E-11-0.02932967E+06	0.01847829E+02		4
BEBR2(S)	81392BE	1BR 2	S 0300.00 1500.00 1000.00	1
0.07680161E+02	0.03193456E-01-0.02439097E-05-0.09487536E-08	0.03902210E-11		2
-0.04528092E+06-0.03282152E+03	0.05659917E+02	0.08805599E-01-0.02790316E-04		3
-0.04611400E-07	0.03007373E-10-0.04482571E+06-0.02263852E+03			4
BECL	81392BE	1CL 1	G 0300.00 5000.00 1000.00	1
0.04072243E+02	0.05328307E-02-0.02146892E-05	0.04097687E-09-0.02774848E-13		2
0.05990792E+05	0.02639872E+02	0.03006275E+02	0.03385550E-01-0.02274674E-04	3
-0.01333438E-08	0.04447782E-11	0.06271131E+05	0.08126810E+02	4
BECL2	81392BE	1CL 2	G 0300.00 5000.00 1000.00	1
0.06656109E+02	0.09583935E-02-0.04248637E-05	0.08333911E-09-0.06016211E-13		2
-0.04547842E+06-0.08159565E+02	0.04835084E+02	0.05899051E-01-0.04307799E-04		3
0.03113267E-08	0.05292957E-11-0.04499748E+06	0.01210616E+02		4

BECL2 (A)	81392BE	1CL	2	S	0300.00	1500.00	1000.00	1	
0.08380054E+02	0.02572312E-01	-0.07554892E-05	-0.02368242E-08	0.01042547E-11				2	
-0.06177281E+06	-0.03886076E+03	0.08074927E+01	0.03830225E+00	-0.06255340E-03				3	
0.04645940E-06	-0.01295143E-09	-0.06052883E+06	-0.03683825E+02					4	
BECL2 (B)	81392BE	1CL	2	S	0300.00	1500.00	1000.00	1	
0.07791771E+02	0.02945389E-01	-0.04237093E-05	-0.05339604E-08	0.01505044E-11				2	
-0.06231958E+06	-0.03656698E+03	0.03004424E+02	0.02353211E+00	-0.03553037E-03				3	
0.02706855E-06	-0.08144728E-10	-0.06136495E+06	-0.01365758E+03					4	
BECLF	81392BE	1CL	1F	1	G	0300.00	5000.00	1000.00	1
0.06393787E+02	0.01234948E-01	-0.05412476E-05	0.01053150E-08	-0.07557553E-13				2	
-0.07104831E+06	-0.07478512E+02	0.04405415E+02	0.06642228E-01	-0.05154354E-04				3	
0.01063175E-07	0.02287810E-11	-0.07051262E+06	0.02777586E+02					4	
BEF	81392BE	1F	1	G	0300.00	5000.00	1000.00	1	
0.03741370E+02	0.08524818E-02	-0.03436428E-05	0.06466099E-09	-0.04475089E-13				2	
-0.02167667E+06	0.02968223E+02	0.02905108E+02	0.02952099E-01	-0.02747617E-04				3	
0.01918800E-07	-0.07179964E-11	-0.02140972E+06	0.07407617E+02					4	
BEF2	81392BE	1F	2	G	0300.00	5000.00	1000.00	1	
0.06008875E+02	0.01636431E-01	-0.07094651E-05	0.01370220E-08	-0.09780462E-13				2	
-0.09777056E+06	-0.07723693E+02	0.03801759E+02	0.07737988E-01	-0.06427724E-04				3	
0.02097328E-07	-0.01462695E-11	-0.09717092E+06	0.03660784E+02					4	
BEF2 (L)	81392BE	1F	2	L	0300.00	2000.00	1000.00	1	
0.05976585E+02	0.04777009E-01	-0.05064131E-05	0.05012404E-09	0.08570416E-13				2	
-0.01251277E+07	-0.02873833E+03	-0.05587355E+01	0.03423905E+00	-0.05210078E-03				3	
0.04099400E-06	-0.01226767E-09	-0.01239060E+07	0.02162308E+02					4	
BEH	81392BE	1H	1	G	0300.00	5000.00	1000.00	1	
0.03103757E+02	0.01443026E-01	-0.05486383E-05	0.09992518E-09	-0.06823073E-13				2	
0.03762032E+06	0.03113887E+02	0.03220220E+02	0.01660638E-01	-0.03759811E-04				3	
0.05403578E-07	-0.02433378E-10	0.03762484E+06	0.02536116E+02					4	
BEH+	81392BE	1H	1E	-1	G	0300.00	5000.00	1000.00	1
0.02935026E+02	0.01642881E-01	-0.06606950E-05	0.01253854E-08	-0.08322438E-13				2	
0.01381605E+07	0.03342443E+02	0.03203174E+02	0.01918095E-01	-0.04743515E-04				3	
0.06392785E-07	-0.02736265E-10	0.01380944E+07	0.01849186E+02					4	
BEH2	81392BE	1H	2	G	0300.00	5000.00	1000.00	1	
0.03274395E+02	0.04312822E-01	-0.01774785E-04	0.03298131E-08	-0.02286391E-12				2	
0.01367913E+06	0.03758700E+01	0.01761472E+02	0.08827701E-01	-0.01241923E-03				3	
0.01412574E-06	-0.06176309E-10	0.01426447E+06	0.08573833E+02					4	
BEH2O2	81392BE	1H	2O	2	G	0300.00	5000.00	1000.00	1
0.07694718E+02	0.04893975E-01	-0.01780895E-04	0.03055611E-08	-0.02009121E-12				2	
-0.08403520E+06	-0.01751820E+03	0.03118833E+02	0.01997183E+00	-0.01673101E-03				3	
0.03275766E-07	0.01457848E-10	-0.08305301E+06	0.05128545E+02					4	
BEH2O2 (A)	81392BE	1H	2O	2	S	0300.00	1000.00	1000.00	1
0.01357669E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2	
-0.01138925E+07	-0.07369071E+03	-0.07121292E+02	0.08378375E+00	-0.01435144E-02				3	
0.01164084E-05	-0.03597983E-09	-0.01091544E+07	0.02745148E+03					4	
BEH2O2 (B)	81392BE	1H	2O	2	S	0300.00	1000.00	1000.00	1
0.01357669E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2	
-0.01142447E+07	-0.07409333E+03	-0.07121292E+02	0.08378375E+00	-0.01435144E-02				3	
0.01164084E-05	-0.03597983E-09	-0.01095066E+07	0.02704887E+03					4	
BEI	81392BE	1I	1	G	0300.00	5000.00	1000.00	1	
0.04226574E+02	0.03948427E-02	-0.01549696E-05	0.03023851E-09	-0.01932301E-13				2	
0.01912832E+06	0.04229493E+02	0.03358791E+02	0.02864276E-01	-0.01889889E-04				3	
-0.04370942E-08	0.05986692E-11	0.01933641E+06	0.08627578E+02					4	
BEI2	81392BE	1I	2	G	0300.00	5000.00	1000.00	1	
0.06974217E+02	0.06094573E-02	-0.02739783E-05	0.05428767E-09	-0.03948833E-13				2	
-0.09890086E+05	-0.05063732E+02	0.05564008E+02	0.04472664E-01	-0.03090745E-04				3	
-0.02609722E-08	0.06750777E-11	-0.09529549E+05	0.02158152E+02					4	
BEI2 (S)	81392BE	1I	2	S	0300.00	1500.00	1000.00	1	
0.08868316E+02	0.02591978E-01	-0.07796846E-05	-0.02236952E-08	0.01016032E-11				2	
-0.02556556E+06	-0.03709859E+03	0.01301872E+02	0.03830115E+00	-0.06255080E-03				3	
0.04645675E-06	-0.01295046E-09	-0.02432303E+06	-0.01952190E+02					4	
BEN	81392BE	1N	1	G	0300.00	5000.00	1000.00	1	
0.03799137E+02	0.08135072E-02	-0.03271826E-05	0.06267597E-09	-0.04443547E-13				2	
0.05006582E+06	0.03013958E+02	0.02880282E+02	0.03157848E-01	-0.02749300E-04				3	
0.01549304E-07	-0.04944407E-11	0.05034622E+06	0.07854857E+02					4	
BE0 (A)	81392BE	1O	1	S	0300.00	3500.00	1000.00	1	
0.04606101E+02	0.01465013E-01	-0.09316989E-06	-0.08839902E-09	0.01840163E-12				2	

-0.07492927E+06-0.02579358E+03-0.01187545E+01	0.01231168E+00-0.02298405E-04	3		
-0.09318502E-07	0.05331928E-10-0.07364786E+06-0.01151163E+02	4		
BEO (B)	81392BE 1O 1 S 0300.00 3500.00 1000.00	1		
0.04606101E+02	0.01465013E-01-0.09316989E-06-0.08839902E-09	0.01840163E-12	2	
-0.07412403E+06-0.02545418E+03-0.01187545E+01	0.01231168E+00-0.02298405E-04	3		
-0.09318502E-07	0.05331928E-10-0.07284262E+06-0.08117651E+01	4		
BEOH	81392BE 1H 1O 1 G 0300.00 5000.00 1000.00	1		
0.04580703E+02	0.02444079E-01-0.08794693E-05	0.01484750E-08-0.09530468E-13	2	
-0.01534682E+06-0.01819725E+02	0.02577868E+02	0.08977628E-01-0.07867956E-04	3	
0.02536139E-07	0.06057864E-12-0.01489220E+06	0.08162645E+02	4	
BES (S)	81392BE 1S 1 S 0300.00 3000.00 1000.00	1		
0.04944107E+02	0.03098929E-01-0.01308985E-04	0.02564670E-08-0.01377673E-12	2	
-0.03004408E+06-0.02521191E+03-0.03045166E+02	0.03934537E+00-0.06572406E-03	3		
0.05230436E-06-0.01590377E-09-0.02854032E+06	0.01256033E+03	4		
BESO4 (A)	81392BE 1O 4S 1 S 0300.00 2300.00 1000.00	1		
0.02081235E+01	0.03035540E+00-0.07769396E-04-0.02942517E-07	0.01112249E-10	2	
-0.01455278E+07	0.02609183E+01-0.08960041E+02	0.01179726E+01-0.02438390E-02	3	
0.02430177E-05-0.08722741E-09-0.01453005E+07	0.03410812E+03	4		
BESO4 (B)	81392BE 1O 4S 1 S 0300.00 2300.00 1000.00	1		
0.02081235E+01	0.03035540E+00-0.07769396E-04-0.02942517E-07	0.01112249E-10	2	
-0.01453939E+07	0.04157230E+01-0.08960041E+02	0.01179726E+01-0.02438390E-02	3	
0.02430177E-05-0.08722741E-09-0.01451667E+07	0.03426292E+03	4		
BESO4 (GAM)	81392BE 1O 4S 1 S 0300.00 2300.00 1000.00	1		
0.02081235E+01	0.03035540E+00-0.07769396E-04-0.02942517E-07	0.01112249E-10	2	
-0.01430422E+07	0.03005051E+02-0.08960041E+02	0.01179726E+01-0.02438390E-02	3	
0.02430177E-05-0.08722741E-09-0.01428148E+07	0.03685225E+03	4		
C	121086C 1 G 0300.00 5000.00 1000.00	1		
0.02602087E+02-0.01787081E-02	0.09087041E-06-0.01149933E-09	0.03310844E-14	2	
0.08542154E+06	0.04195177E+02	0.02498585E+02	0.08085777E-03-0.02697697E-05	3
0.03040729E-08-0.01106652E-11	0.08545878E+06	0.04753459E+02	4	
C(S)	121286C 1 S 0300.00 5000.00 1000.00	1		
0.01490166E+02	0.01662126E-01-0.06687204E-05	0.01290880E-08-0.09205334E-13	2	
-0.07074019E+04-0.08717785E+02-0.06705661E+01	0.07181500E-01-0.05632921E-04	3		
0.02142299E-07-0.04168562E-11-0.07339498E+03	0.02601596E+02	4		
C+	120186C 1E -1 G 0300.00 5000.00 1000.00	1		
0.02511827E+02-0.01735978E-03	0.09504268E-07-0.02218852E-10	0.01862189E-14	2	
0.02166772E+07	0.04286130E+02	0.02595384E+02-0.04068665E-02	0.06892367E-05	3
-0.05266488E-08	0.01508338E-11	0.02166628E+07	0.03895730E+02	4
C-	121686C 1E 1 G 0300.00 5000.00 1000.00	1		
0.02990221E+02-0.09184596E-02	0.05055560E-05-0.07703410E-09	0.03163271E-13	2	
0.06983931E+06	0.01259453E+02	0.02783903E+02-0.01774288E-01	0.03696761E-04	3
-0.03066693E-07	0.08637622E-11	0.06998511E+06	0.02726281E+02	4
C2	121286C 2 G 0300.00 5000.00 1000.00	1		
0.04135979E+02	0.06531618E-03	0.01837099E-05-0.05295085E-09	0.04712137E-13	2
0.09967272E+06	0.07472923E+01	0.06996045E+02-0.07400602E-01	0.03234704E-04	3
0.04802535E-07-0.03295918E-10	0.09897487E+06-0.01386227E+03	4		
C2-	121286C 2E 1 G 0300.00 5000.00 1000.00	1		
0.03796891E+02	0.02530050E-02	0.09709118E-06-0.01614804E-09-0.03212893E-15	2	
0.05207981E+06	0.01658147E+02	0.03468012E+02-0.02352875E-02	0.01243912E-04	3
0.04705961E-08-0.08164274E-11	0.05231215E+06	0.03886699E+02	4	
C2CL3	40992C 2CL 3 G 0300.00 4000.00 1500.00	1		
0.01183853E+03	0.09460851E-02-0.02920870E-05	0.03847024E-09-0.01539560E-13	2	
0.02313143E+06-0.02891445E+03	0.04808647E+02	0.02212948E+00-0.02548847E-03	3	
0.01372083E-06-0.02812663E-10	0.02514353E+06	0.07232629E+02	4	
C2CL5	40992C 2CL 5 G 0300.00 4000.00 1500.00	1		
0.01775107E+03	0.09220800E-02-0.04852694E-05	0.01190373E-08-0.01100446E-12	2	
-0.02402768E+05-0.05545676E+03	0.06414346E+02	0.03867367E+00-0.04857935E-03	3	
0.02734513E-06-0.05732891E-10	0.04697039E+04	0.01542036E+02	4	
C2CL6	40992C 2CL 6 G 0300.00 4000.00 1500.00	1		
0.02021422E+03	0.01757648E-01-0.05881040E-05	0.08029739E-09-0.03958238E-13	2	
-0.02340156E+06-0.07096011E+03	0.07492710E+02	0.04318468E+00-0.05275048E-03	3	
0.02947143E-06-0.06176554E-10-0.02006555E+06	0.06635582E+02	4		
C2F6	82489C 2F 6 G 0300.00 5000.00 1000.00	1		
0.01602057E+03	0.06273007E-01-0.02797778E-04	0.05517547E-08-0.04004651E-12	2	
-0.01675654E+07-0.05519459E+03	0.03577448E+02	0.03913670E+00-0.02714862E-03	3	
0.04348459E-08	0.04007135E-10-0.01642174E+07	0.09098384E+02	4	

C2H	81193C	2H	1	G	0300.00	4000.00	1000.00	1	
	0.03986367E+02	0.03143123E-01	-0.01267243E-04	0.02924363E-08	-0.02716320E-12			2	
	0.06655884E+06	0.01191063E+02	0.02737704E+02	0.08048446E-01	-0.09244310E-04			3	
	0.06525259E-07	-0.01939580E-10	0.06683813E+06	0.07300220E+02				4	
C2H2	121386C	2H	2	G	0300.00	5000.00	1000.00	1	
	0.04436770E+02	0.05376039E-01	-0.01912817E-04	0.03286379E-08	-0.02156710E-12			2	
	0.02566766E+06	-0.02800338E+02	0.02013562E+02	0.01519045E+00	-0.01616319E-03			3	
	0.09078992E-07	-0.01912746E-10	0.02612444E+06	0.08805378E+02				4	
C2H3	12787C	2H	3	G	0300.00	5000.00	1000.00	1	
	0.05933468E+02	0.04017746E-01	-0.03966740E-05	-0.01441267E-08	0.02378644E-12			2	
	0.03185435E+06	-0.08530313E+02	0.02459276E+02	0.07371476E-01	0.02109873E-04			3	
	-0.01321642E-07	-0.01184784E-10	0.03335225E+06	0.01155620E+03				4	
C2H4	121286C	2H	4	G	0300.00	5000.00	1000.00	1	
	0.03528419E+02	0.01148518E+00	-0.04418385E-04	0.07844601E-08	-0.05266848E-12			2	
	0.04428289E+05	0.02230389E+02	-0.08614880E+01	0.02796163E+00	-0.03388677E-03			3	
	0.02785152E-06	-0.09737879E-10	0.05573046E+05	0.02421149E+03				4	
C2H5	12387C	2H	5	G	0300.00	5000.00	1000.00	1	
	0.07190480E+02	0.06484077E-01	-0.06428065E-05	-0.02347879E-08	0.03880877E-12			2	
	0.01067455E+06	-0.01478089E+03	0.02690702E+02	0.08719133E-01	0.04419839E-04			3	
	0.09338703E-08	-0.03927773E-10	0.01287040E+06	0.01213820E+03				4	
C2H6	121686C	2H	6	G	0300.00	4000.00	1000.00	1	
	0.04825938E+02	0.01384043E+00	-0.04557259E-04	0.06724967E-08	-0.03598161E-12			2	
	-0.01271779E+06	-0.05239507E+02	0.01462539E+02	0.01549467E+00	0.05780507E-04			3	
	-0.01257832E-06	0.04586267E-10	-0.01123918E+06	0.01443229E+03				4	
C2HCL	112989C	2H	1CL	1	G	0300.00	5000.00	1000.00	1
	0.06295372E+02	0.03883113E-01	-0.01506049E-04	0.02700003E-08	-0.01830213E-12			2	
	0.02357279E+06	-0.08137063E+02	0.03618443E+02	0.01331979E+00	-0.01321822E-03			3	
	0.06092024E-07	-0.08879026E-11	0.02415385E+06	0.05050645E+02				4	
C2HCL5	40992H	1C	2CL	5	G	0300.00	4000.00	1500.00	1
	0.01897802E+03	0.02244275E-01	-0.05864788E-05	0.02733950E-09	0.04934135E-13			2	
	-0.02494887E+06	-0.06578714E+03	0.05356044E+02	0.04176390E+00	-0.04710787E-03			3	
	0.02550758E-06	-0.05324478E-10	-0.02079330E+06	0.04970258E+02				4	
C2N	121286C	2N	1	G	0300.00	5000.00	1000.00	1	
	0.06151561E+02	0.01511650E-01	-0.06629362E-05	0.01286148E-08	-0.09160830E-13			2	
	0.06484318E+06	-0.08177850E+02	0.03498544E+02	0.08554433E-01	-0.06288697E-04			3	
	0.08638478E-08	0.04915996E-11	0.06556611E+06	0.05548374E+02				4	
C2N2	121286C	2N	2	G	0300.00	5000.00	1000.00	1	
	0.06548003E+02	0.03984707E-01	-0.01634216E-04	0.03038597E-08	-0.02111069E-12			2	
	0.03490716E+06	-0.09735790E+02	0.04265459E+02	0.01192257E+00	-0.01342014E-03			3	
	0.09192297E-07	-0.02778942E-10	0.03547888E+06	0.01713212E+02				4	
C2O	121286C	2O	1	G	0300.00	5000.00	1000.00	1	
	0.04849809E+02	0.02947585E-01	-0.01090729E-04	0.01792562E-08	-0.01115758E-12			2	
	0.03282055E+06	-0.06453226E+01	0.03368851E+02	0.08241803E-01	-0.08765145E-04			3	
	0.05569262E-07	-0.01540009E-10	0.03317081E+06	0.06713314E+02				4	
C3	121286C	3	G	0300.00	5000.00	1000.00	1		
	0.03803710E+02	0.02253567E-01	-0.07704535E-05	0.01316294E-08	-0.08694264E-13			2	
	0.09736135E+06	0.06128063E+02	0.04345528E+02	0.01264466E-01	-0.04652557E-04			3	
	0.08695856E-07	-0.04243536E-10	0.09731403E+06	0.03519437E+02				4	
C3H2	102193H	2C	3	G	0150.00	4000.00	1000.00	1	
	0.07670981E+02	0.02748749E-01	-0.04370943E-05	-0.06455599E-09	0.01663887E-12			2	
	0.06259722E+06	-0.01236890E+03	0.03166714E+02	0.02482572E+00	-0.04591637E-03			3	
	0.04268019E-06	-0.01482152E-09	0.06350421E+06	0.08869446E+02				4	
C3H2 (S)	101993H	2C	3	G	0300.00	4000.00	1400.00	1	
	0.08351312E+02	0.02672278E-01	-0.02129404E-05	-0.01478218E-08	0.02583689E-12			2	
	0.06800690E+06	-0.01950884E+03	0.04749475E+02	0.08520229E-01	-0.01160268E-04			3	
	-0.02494954E-07	0.09921004E-11	0.06939979E+06	0.05437792E+01				4	
C3H4	101993H	4C	3	G	0300.00	4000.00	1400.00	1	
	0.09776256E+02	0.05302138E-01	-0.03701118E-05	-0.03026386E-08	0.05089581E-12			2	
	0.01954972E+06	-0.03077061E+03	0.02539831E+02	0.01633437E+00	-0.01764950E-04			3	
	-0.04647365E-07	0.01729131E-10	0.02251243E+06	0.09935702E+02				4	
C3H4C	101993H	4C	3	G	0300.00	4000.00	1400.00	1	
	0.09708652E+02	0.05344939E-01	-0.03953553E-05	-0.03111764E-08	0.05369406E-12			2	
	0.02967722E+06	-0.03073273E+03	0.01056162E+02	0.01905236E+00	-0.02317048E-04			3	
	-0.05933690E-07	0.02307128E-10	0.03309110E+06	0.01761927E+03				4	
C3H4P	101993H	4C	3	G	0300.00	4000.00	1400.00	1	
	0.09768102E+02	0.05219151E-01	-0.03753140E-05	-0.02992191E-08	0.05107878E-12			2	

0.01860277E+06-0.03020678E+03	0.03029730E+02	0.01498961E+00-0.01398500E-04	3					
-0.03969619E-07	0.01388217E-10	0.02148408E+06	0.08004594E+02	4				
C3H6	120186C	3H	6	G	0300.00	5000.00	1000.00	1
0.06732257E+02	0.01490834E+00-0.04949899E-04	0.07212022E-08-0.03766204E-12	2					
-0.09235703E+04-0.01331335E+03	0.01493307E+02	0.02092518E+00	0.04486794E-04	3				
-0.01668912E-06	0.07158146E-10	0.01074826E+05	0.01614534E+03	4				
C3H8	120186C	3H	8	G	0300.00	5000.00	1000.00	1
0.07525217E+02	0.01889034E+00-0.06283924E-04	0.09179373E-08-0.04812410E-12	2					
-0.01646455E+06-0.01784390E+03	0.08969208E+01	0.02668986E+00	0.05431425E-04	3				
-0.02126001E-06	0.09243330E-10-0.01395492E+06	0.01935533E+03		4				
C3O2	121286C	3O	2	G	0300.00	5000.00	1000.00	1
0.08098897E+02	0.05560040E-01-0.02312265E-04	0.04340709E-08-0.03036387E-12	2					
-0.01421435E+06-0.01521974E+03	0.04018127E+02	0.01836661E+00-0.01907148E-03	3					
0.01185587E-06-0.03418748E-10-0.01312824E+06	0.05582084E+02		4					
C4	121286C	4		G	0300.00	5000.00	1000.00	1
0.06500180E+02	0.04228632E-01-0.01790718E-04	0.03404813E-08-0.02403978E-12	2					
0.01143401E+07-0.01148889E+03	0.02343028E+02	0.01642981E+00-0.01527986E-03	3					
0.07343826E-07-0.01582274E-10	0.01154538E+07	0.09826204E+02	4					
C4H	121686C	4H	1	G	0300.00	5000.00	1000.00	1
0.06242882E+02	0.06193683E-01-0.02085932E-04	0.03082203E-08-0.01636483E-12	2					
0.07568019E+06-0.07210806E+02	0.05023247E+02	0.07092375E-01-0.06073762E-07	3					
-0.02275752E-07	0.08086994E-11	0.07623813E+06-0.06942594E+00	4					
C4H10	62090C	4H	10	G	0300.00	4000.00	1500.00	1
0.01998785E+03	0.01037281E+00-0.09610818E-05-0.04623018E-08	0.08202828E-12	2					
-0.02625571E+06-0.08837907E+03-0.02256618E+02	0.05881732E+00-0.04525783E-03	3						
0.02037115E-06-0.04079458E-10-0.01760233E+06	0.03329595E+03	4						
C4H2	121686C	4H	2	G	0300.00	5000.00	1000.00	1
0.09031407E+02	0.06047253E-01-0.01948789E-04	0.02754863E-08-0.01385608E-12	2					
0.05294736E+06-0.02385068E+03	0.04005192E+02	0.01981000E+00-0.09865877E-04	3					
-0.06635158E-07	0.06077413E-10	0.05424065E+06	0.01845737E+02	4				
C4H6	120186C	4H	6	G	0300.00	5000.00	1000.00	1
0.08046583E+02	0.01648525E+00-0.05522227E-04	0.08123593E-08-0.04295078E-12	2					
0.01370130E+06-0.01800458E+03	0.03197108E+02	0.02025592E+00	0.06510192E-04	3				
-0.01658442E-06	0.06400282E-10	0.01571520E+06	0.09895660E+02	4				
C4H8	120386C	4H	8	G	0300.00	5000.00	1000.00	1
0.02053584E+02	0.03435051E+00-0.01588320E-03	0.03308966E-07-0.02536104E-11	2					
-0.02139723E+05	0.01554320E+03	0.01181138E+02	0.03085338E+00	0.05086525E-04	3			
-0.02465489E-06	0.01111019E-09-0.01790400E+05	0.02106247E+03	4					
C5	121286C	5		G	0300.00	5000.00	1000.00	1
0.08078081E+02	0.05743464E-01-0.02436405E-04	0.04638916E-08-0.03278910E-12	2					
0.01147022E+07-0.01953024E+03	0.02115274E+02	0.02326332E+00-0.02109499E-03	3					
0.09072734E-07-0.01540093E-10	0.01162738E+07	0.01097603E+03	4					
C5H	20387C	5H	1	G	0300.00	5000.00	1000.00	1
0.08695749E+02	0.06054301E-01-0.02016011E-04	0.02892893E-08-0.01470100E-12	2					
0.09031069E+06-0.02101595E+03	0.01634825E+02	0.02509538E+00-0.01206636E-03	3					
-0.01046511E-06	0.08809988E-10	0.09212488E+06	0.01512194E+03	4				
C5H12	20387C	5H	12	G	0300.00	4000.00	1000.00	1
0.01667798E+03	0.02114483E+00-0.03533321E-04-0.05742202E-08	0.01515948E-11	2					
-0.02553670E+06-0.06372940E+03	0.01877908E+02	0.04121646E+00	0.01253234E-03	3				
-0.03701537E-06	0.01525569E-09-0.02003816E+06	0.01877257E+03	4					
C5H2	20587C	5H	2	G	0300.00	5000.00	1000.00	1
0.01132917E+03	0.07424057E-01-0.02628189E-04	0.04082541E-08-0.02301333E-12	2					
0.07878706E+06-0.03617117E+03	0.03062322E+02	0.02709998E+00-0.01009170E-03	3					
-0.01272745E-06	0.09167219E-10	0.08114969E+06	0.07071078E+02	4				
C5H5	101993H	5C	5	G	0300.00	4000.00	1400.00	1
0.01531094E+03	0.07473806E-01-0.05837458E-05-0.04386651E-08	0.07696839E-12	2					
0.02525890E+06-0.05951593E+03	0.01007316E+02	0.03189880E+00-0.04748189E-04	3					
-0.01102390E-06	0.04584681E-10	0.03047390E+06	0.01934168E+03	4				
C5H6	20387C	5H	6	G	0300.00	5000.00	1000.00	1
0.09689815E+02	0.01838262E+00-0.06264884E-04	0.09393377E-08-0.05087708E-12	2					
0.01102124E+06-0.03122908E+03-0.03196739E+02	0.04081361E+00	0.06816505E-05	3					
-0.03137459E-06	0.01577223E-09	0.01529068E+06	0.03869939E+03	4				
C6H	121686C	6H	1	G	0300.00	5000.00	1000.00	1
0.01158735E+03	0.07295363E-01-0.02466008E-04	0.03407046E-08-0.01498185E-12	2					
0.01031448E+07-0.03172578E+03	0.04769848E+02	0.02457279E+00-0.07561252E-04	3					
-0.01480691E-06	0.09768054E-10	0.01048523E+07	0.03241530E+02	4				

C6H10	20387C	6H	10	G	0300.00	5000.00	1000.00	1	
0.01592777E+03	0.02374413E+00	-0.06908672E-04	0.08109777E-08	-0.02683123E-12				2	
-0.08642656E+05	-0.06525186E+03	-0.01394228E+02	0.04720693E+00	0.01196042E-03				3	
-0.04162896E-06	0.01740336E-09	-0.02217790E+05	0.03129604E+03					4	
C6H14	20387C	6H	14	G	0300.00	4000.00	1000.00	1	
0.02280472E+03	0.02097989E+00	-0.03530674E-04	-0.05466245E-08	0.01478950E-11				2	
-0.03073757E+06	-0.09583162E+03	0.01836174E+02	0.05098461E+00	0.01259586E-03				3	
-0.04428362E-06	0.01872237E-09	-0.02292750E+06	0.02088145E+03					4	
C6H2	121686C	6H	2	G	0300.00	5000.00	1000.00	1	
0.01275652E+03	0.08034381E-01	-0.02618215E-04	0.03725060E-08	-0.01878851E-12				2	
0.08075469E+06	-0.04041263E+03	0.05751085E+02	0.02636720E+00	-0.01166760E-03				3	
-0.01071450E-06	0.08790297E-10	0.08262013E+06	-0.04335532E+02					4	
C6H3	20387C	6H	3	G	0300.00	5000.00	1000.00	1	
0.01276118E+03	0.01038557E+00	-0.03479193E-04	0.05109733E-08	-0.02690965E-12				2	
0.07477706E+06	-0.03891745E+03	0.05007090E+02	0.02692852E+00	-0.05919866E-04				3	
-0.01527233E-06	0.09408310E-10	0.07713200E+06	0.02225621E+02					4	
C6H4	111293H	4C	6	G	0300.00	4000.00	1000.00	1	
0.01401625E+03	0.08242769E-01	-0.08099664E-05	-0.04654132E-08	0.08748122E-12				2	
0.04410396E+06	-0.05139376E+03	0.01520024E+02	0.02876611E+00	0.01417725E-04				3	
-0.01650589E-06	0.05873157E-10	0.04844894E+06	0.01719034E+03					4	
C6H5	82489C	6H	5	G	0300.00	4000.00	1000.00	1	
0.01577589E+03	0.09651109E-01	-0.09429416E-05	-0.05469111E-08	0.01026522E-11				2	
0.03302698E+06	-0.06176280E+03	0.01143557E+01	0.03627325E+00	0.01158286E-04				3	
-0.02196965E-06	0.08463556E-10	0.03836054E+06	0.02380117E+03					4	
C6H5 (L)	82489C	6H	5	G	0300.00	4000.00	1000.00	1	
0.01721540E+03	0.08621068E-01	-0.08221340E-05	-0.04752164E-08	0.08844086E-12				2	
0.06385819E+06	-0.06139128E+03	0.04854269E+02	0.03031659E+00	0.01742893E-05				3	
-0.01811010E-06	0.07392511E-10	0.06798734E+06	0.05854935E+02					4	
C6H5O	82489C	6H	5O	1	G	0300.00	4000.00	1000.00	1
0.01822639E+03	0.01003985E+00	-0.09915668E-05	-0.05672804E-08	0.01068372E-11				2	
-0.02620846E+05	-0.07361391E+03	0.01107497E+02	0.03956946E+00	0.08497295E-05				3	
-0.02436311E-06	0.09650660E-10	0.03159672E+05	0.01973496E+03					4	
C6H5OH	82489C	6H	6O	1	G	0300.00	4000.00	1000.00	1
0.01821633E+03	0.01142427E+00	-0.01096684E-04	-0.06427442E-08	0.01198893E-11				2	
-0.02053664E+06	-0.07304234E+03	0.01391456E+02	0.03931958E+00	0.01777096E-04				3	
-0.02277673E-06	0.08309659E-10	-0.01472181E+06	0.01917813E+03					4	
C6H6	20387C	6H	6	G	0300.00	5000.00	1000.00	1	
0.01291074E+03	0.01723297E+00	-0.05024211E-04	0.05893497E-08	-0.01947521E-12				2	
0.03664512E+05	-0.05002699E+03	-0.03138012E+02	0.04723103E+00	-0.02962208E-04				3	
-0.03262819E-06	0.01718692E-09	0.08890031E+05	0.03657573E+03					4	
C6H7	82489C	6H	7	G	0300.00	4000.00	1000.00	1	
0.01755221E+03	0.01227080E+00	-0.01185742E-04	-0.06959661E-08	0.01301326E-11				2	
0.01624581E+06	-0.07166589E+03	0.04639166E+01	0.03975928E+00	0.02529095E-04				3	
-0.02223792E-06	0.07557053E-10	0.02225169E+06	0.02235387E+03					4	
C8H	121686C	8H	1	G	0300.00	5000.00	1000.00	1	
0.01474991E+03	0.09931501E-01	-0.03374841E-04	0.04687593E-08	-0.02073536E-12				2	
0.01399448E+07	-0.04892690E+03	0.04489508E+02	0.03521521E+00	-0.01019390E-03				3	
-0.02197025E-06	0.01421416E-09	0.01425992E+07	0.03996225E+02					4	
C8H2	121686C	8H	2	G	0300.00	5000.00	1000.00	1	
0.01568021E+03	0.01115461E+00	-0.03724373E-04	0.05197891E-08	-0.02375550E-12				2	
0.01081123E+07	-0.05571437E+03	0.04630427E+02	0.03937080E+00	-0.01148035E-03				3	
-0.02562214E-06	0.01670791E-09	0.01108285E+07	0.08077425E+01					4	
CA	80792CA	1	G	0300.00	5000.00	1000.00		1	
0.01636990E+02	0.01938281E-01	-0.01464011E-04	0.04278257E-08	-0.03581686E-12				2	
0.02109799E+06	0.08990615E+02	0.01563120E+02	0.06228361E-01	-0.01415732E-03				3	
0.01323968E-06	-0.04370569E-10	0.02092191E+06	0.08370537E+02					4	
CA (A)	81092CA	1	S	0300.00	1500.00	1000.00		1	
0.03344424E+02	-0.06129555E-04	-0.02048549E-05	0.02199575E-08	-0.06498067E-12				2	
-0.01020624E+05	-0.01410880E+03	0.02492826E+02	0.03921280E-01	-0.07242436E-04				3	
0.05919276E-07	-0.01802531E-10	-0.08641901E+04	-0.01010018E+03					4	
CA (B)	81092CA	1	S	0300.00	2000.00	1000.00		1	
0.02149662E+02	0.02293734E-01	0.03948384E-05	-0.01813978E-08	0.03060995E-12				2	
-0.06970589E+04	-0.07862350E+02	0.02013343E+02	0.02718935E-01	-0.01374494E-05				3	
0.01528553E-08	-0.06023681E-12	-0.06613041E+04	-0.07168449E+02					4	
CA (L)	81092CA	1	L	0300.00	3000.00	1000.00		1	
0.03623553E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2	



0.02310016E+04-0.01455354E+03	0.03623553E+02	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	0.02310016E+04-0.01455354E+03		4
CA+	80792CA 1E -1	G	0300.00 5000.00 1000.00	1
0.02415423E+02	0.03140053E-02-0.03458031E-05	0.01350163E-08-0.01342160E-12		2
0.09252434E+06	0.05468189E+02	0.02276338E+02	0.01581988E-01-0.03878953E-04	3
0.03953701E-07-0.01427856E-10	0.09253536E+06	0.06008258E+02		4
CA2	80792CA 2	G	0300.00 5000.00 1000.00	1
0.04174798E+02-0.07401838E-02	0.03131196E-05-0.05885577E-09	0.04296578E-13		2
0.04052221E+06	0.07582380E+02	0.05604867E+02-0.04044408E-01	0.02454638E-04	3
-0.01495064E-08-0.01724184E-11	0.04008842E+06	0.01167234E+00		4
CABR	80792BR 1CA 1	G	0300.00 5000.00 1000.00	1
0.04312008E+02	0.04246804E-02-0.02536360E-05	0.07082421E-09-0.05508239E-13		2
-0.07242509E+05	0.05721414E+02	0.04004020E+02	0.01927770E-01-0.02749388E-04	3
0.01785012E-07-0.04190442E-11-0.07199987E+05	0.07125700E+02			4
CABR2	80792BR 2CA 1	G	0300.00 5000.00 1000.00	1
0.07388434E+02	0.01393017E-02-0.06561619E-06	0.01342748E-09-0.09993272E-14		2
-0.04852787E+06-0.04337760E+02	0.06902053E+02	0.01599316E-01-0.01154723E-04		3
-0.02428795E-08	0.03707822E-11-0.04841873E+06-0.01900929E+02			4
CABR2(S)	81292BR 2CA 1	S	0300.00 1500.00 1000.00	1
0.01076200E+03-0.02979247E-01	0.06950511E-05	0.03569778E-07-0.01382224E-10		2
-0.08542235E+06-0.04524895E+03	0.05478536E+02	0.02209325E+00-0.04544460E-03		3
0.04176543E-06-0.01322726E-09-0.08447516E+06-0.02052538E+03				4
CACL	80792CA 1CL 1	G	0300.00 5000.00 1000.00	1
0.04272197E+02	0.04612770E-02-0.02684554E-05	0.07233022E-09-0.05565813E-13		2
-0.01387933E+06	0.04556153E+02	0.03810549E+02	0.02372144E-01-0.02939380E-04	3
0.01528166E-07-0.02396962E-11-0.01379994E+06	0.06742955E+02			4
CACL2	80792CA 1CL 2	G	0300.00 5000.00 1000.00	1
0.07322969E+02	0.02201546E-02-0.01035664E-05	0.02117574E-09-0.01575201E-13		2
-0.05893953E+06-0.06959426E+02	0.06595983E+02	0.02364235E-01-0.01611807E-04		3
-0.04866457E-08	0.05973912E-11-0.05877467E+06-0.03308009E+02			4
CACL2(S)	81092CA 1CL 2	S	0300.00 2000.00 1000.00	1
0.06749013E+02	0.03694542E-01-0.02199980E-05	0.01165549E-08-0.02193898E-12		2
-0.09759255E+06-0.02629777E+03	0.05722155E+02	0.01836100E+00-0.03597296E-03		3
0.03173054E-06-0.09522563E-10-0.09798464E+06-0.02415730E+03				4
CAF	80792CA 1F 1	G	0300.00 5000.00 1000.00	1
0.04150489E+02	0.05746086E-02-0.03081448E-05	0.07585468E-09-0.05641270E-13		2
-0.03400290E+06	0.03725193E+02	0.03309446E+02	0.03419155E-01-0.03357208E-04	3
0.01004510E-07	0.01112627E-11-0.03382332E+06	0.07876121E+02		4
CAF2	80792CA 1F 2	G	0300.00 5000.00 1000.00	1
0.06575083E+02	0.05172194E-02-0.02403804E-05	0.04876347E-09-0.03608526E-13		2
-0.09641588E+06-0.04868362E+02	0.05023320E+02	0.04921285E-01-0.03129418E-04		3
-0.01178313E-07	0.01260201E-10-0.09604913E+06	0.02984363E+02		4
CAH202	81292CA 1H 20 2	G	0300.00 5000.00 1000.00	1
0.08627170E+02	0.03353668E-01-0.01123553E-04	0.01801642E-08-0.01122696E-12		2
-0.07617877E+06-0.01582838E+03	0.05634984E+02	0.01431225E+00-0.01160774E-03		3
0.02415328E-08	0.02445194E-10-0.07567777E+06-0.01510141E+02			4
CAH202(S)	81292CA 1H 20 2	S	0300.00 1000.00 1000.00	1
0.01418556E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.01237066E+07-0.07268995E+03-0.07906910E+01	0.06795647E+00-0.01329918E-02			3
0.01211862E-05-0.04117456E-09-0.01204396E+07-0.07999789E+01				4
CAI	80792CA 1I 1	G	0300.00 5000.00 1000.00	1
0.04316128E+02	0.04138589E-02-0.02776385E-05	0.08074141E-09-0.06592826E-13		2
-0.01903879E+05	0.06725163E+02	0.04078205E+02	0.01812968E-01-0.02972846E-04	3
0.02225520E-07-0.06173497E-11-0.01881151E+05	0.07754936E+02			4
CAI2	80792CA 1I 2	G	0300.00 5000.00 1000.00	1
0.07403366E+02	0.01208762E-02-0.05698306E-06	0.01167152E-09-0.08696049E-14		2
-0.03328039E+06-0.02870204E+02	0.06975307E+02	0.01413683E-01-0.01046359E-04		3
-0.01757655E-08	0.03111958E-11-0.03318450E+06-0.07269292E+01			4
CAO	80792CA 1O 1	G	0300.00 5000.00 1000.00	1
0.08665723E+02-0.09857255E-01	0.07277137E-04-0.01813874E-07	0.01477538E-11		2
0.02566423E+05-0.02151985E+03	0.07277069E+02-0.02477194E+00	0.06313166E-03		3
-0.06322423E-06	0.02200693E-09	0.03774998E+05-0.09934620E+02		4
CAO(S)	81092CA 1O 1	S	0300.00 3600.00 1000.00	1
0.05184497E+02	0.01938337E-01-0.08932525E-05	0.02410689E-08-0.02389613E-12		2
-0.07806390E+06-0.02562669E+03	0.02964466E+02	0.09464719E-01-0.07948131E-04		3
0.06517958E-08	0.01313902E-10-0.07762567E+06-0.01476156E+03			4

CAOH	80792CA	1H	1O	1	G	0300.00	5000.00	1000.00	1
	0.05164977E+02	0.01974644E-01	-0.07757403E-05	0.01507385E-08	-0.01048831E-12				2
	-0.02493597E+06	-0.01690344E+02	0.03596803E+02	0.08182874E-01	-0.07863515E-04				3
	0.01974293E-07	0.06136755E-11	-0.02469004E+06	0.05713983E+02					4
CAOH+	80792CA	1H	1O	1E	-1G	0300.00	5000.00	1000.00	1
	0.05293390E+02	0.01697953E-01	-0.05704847E-05	0.09169199E-09	-0.05724155E-13				2
	0.04274157E+06	-0.03041255E+02	0.03766022E+02	0.07251869E-01	-0.05903957E-04				3
	0.02063514E-08	0.01186538E-10	0.04300269E+06	0.04285959E+02					4
CAS	80792CA	1S	1		G	0300.00	5000.00	1000.00	1
	0.04077726E+02	-0.02148896E-01	0.03595164E-04	-0.01167272E-07	0.01101218E-11				2
	0.01401038E+06	0.05797750E+02	0.05045918E+02	-0.09248234E-01	0.03176027E-03				3
	-0.04007223E-06	0.01698112E-09	0.01355553E+06	0.08770679E+01					4
CCL	40992C	1CL	1		G	0300.00	4000.00	1500.00	1
	0.04306010E+02	0.01816861E-02	-0.07184326E-06	0.01354479E-09	-0.01002479E-13				2
	0.05198808E+06	0.01558593E+02	0.02871441E+02	0.04709268E-01	-0.05629052E-04				3
	0.03086609E-07	-0.06379756E-11	0.05237631E+06	0.08859373E+02					4
CCL2	40992C	1CL	2		G	0300.00	4000.00	1500.00	1
	0.06632435E+02	0.03558831E-02	-0.01507592E-05	0.03116243E-09	-0.02546496E-13				2
	0.02443636E+06	-0.06590137E+02	0.03329579E+02	0.01112853E+00	-0.01375891E-03				3
	0.07726329E-07	-0.01624070E-10	0.02530408E+06	0.01010975E+03					4
CCL2CCLO	40992C	2 O	1CL	3	G	0300.00	4000.00	1500.00	1
	0.01497380E+03	0.09004180E-02	-0.03714287E-05	0.05602716E-09	-0.02392170E-13				2
	-0.01781718E+06	-0.04510704E+03	0.05066114E+02	0.02846673E+00	-0.03113001E-03				3
	0.01605483E-06	-0.03208502E-10	-0.01474354E+06	0.06663101E+02					4
CCL2CCLOH	53090C	2H	1O	1CL	3G	0300.00	5000.00	1500.00	1
	0.01567259E+03	0.02218766E-01	-0.04425239E-05	0.06261725E-10	0.03673507E-13				2
	-0.02855361E+06	-0.05085224E+03	0.04602117E+02	0.03408842E+00	-0.03836909E-03				3
	0.02120271E-06	-0.04527143E-10	-0.02507945E+06	0.06859776E+02					4
CCL2CH	40992H	1C	2CL	2	G	0300.00	4000.00	1500.00	1
	0.01101223E+03	0.01364477E-01	-0.03497001E-05	0.01107466E-09	0.03844298E-13				2
	0.02706218E+06	-0.02886258E+03	0.02961736E+02	0.02429423E+00	-0.02731403E-03				3
	0.01493184E-06	-0.03162966E-10	0.02960233E+06	0.01317486E+03					4
CCL2HOO	53090C	1H	1O	2CL	2G	0300.00	5000.00	1500.00	1
	0.01273967E+03	0.01671789E-01	-0.03280073E-05	0.09239024E-10	0.02183938E-13				2
	-0.05665041E+05	-0.03552584E+03	0.03425417E+02	0.02745544E+00	-0.02973832E-03				3
	0.01588391E-06	-0.03309428E-10	-0.02675529E+05	0.01333474E+03					4
CCL2OHCH2	53090C	2H	3O	1CL	2G	0300.00	5000.00	1500.00	1
	0.01606355E+03	0.02856412E-01	-0.05564238E-05	0.02056416E-09	0.02871365E-13				2
	-0.01756115E+06	-0.05438455E+03	0.02870959E+02	0.04462273E+00	-0.05377946E-03				3
	0.03093185E-06	-0.06719238E-10	-0.01379636E+06	0.01305466E+03					4
CCL2OHCHL	53090C	2H	2O	1CL	3G	0300.00	5000.00	1500.00	1
	0.01681474E+03	0.02433421E-01	-0.04717311E-05	0.01595327E-09	0.02647197E-13				2
	-0.02217115E+06	-0.05406904E+03	0.05487264E+02	0.03719540E+00	-0.04391386E-03				3
	0.02501465E-06	-0.05417859E-10	-0.01882134E+06	0.04237537E+02					4
CCL3	40992C	1CL	3		G	0300.00	4000.00	1500.00	1
	0.09375859E+02	0.05723237E-02	-0.02242398E-05	0.04238666E-09	-0.03174834E-13				2
	0.05113147E+05	-0.01813304E+03	0.04292822E+02	0.01682379E+00	-0.02044420E-03				3
	0.01135805E-06	-0.02371493E-10	0.06477756E+05	0.07677874E+02					4
CCL3CCLH2	53090C	2H	2CL	4	G	0300.00	5000.00	1500.00	1
	0.01788619E+03	0.02281235E-01	-0.04746598E-05	0.01962667E-09	0.02451768E-13				2
	-0.02496335E+06	-0.06312883E+03	0.03463508E+02	0.04144805E+00	-0.04421053E-03				3
	0.02320525E-06	-0.04772525E-10	-0.02028144E+06	0.01275956E+03					4
CCL3CCLO	40992C	2 O	1CL	4	G	0300.00	4000.00	1500.00	1
	0.01687401E+03	0.01341876E-01	-0.04555006E-05	0.07178333E-09	-0.04348641E-13				2
	-0.03442278E+06	-0.05295025E+03	0.06334167E+02	0.03461171E+00	-0.04173791E-03				3
	0.02324686E-06	-0.04882451E-10	-0.03152121E+06	0.07697654E+01					4
CCL3CH2	53090C	2H	2CL	3	G	0300.00	5000.00	1500.00	1
	0.01468243E+03	0.02202649E-01	-0.03960690E-05	0.02319280E-10	0.03655521E-13				2
	0.03875531E+05	-0.04495230E+03	0.05008132E+02	0.03031103E+00	-0.03453620E-03				3
	0.01951049E-06	-0.04245840E-10	0.06936588E+05	0.05474640E+02					4
CCL3CHL	53090C	2H	1CL	4	G	0300.00	5000.00	1500.00	1
	0.01610198E+03	0.01597223E-01	-0.04069892E-05	0.04158083E-09	-0.01105635E-13				2
	-0.02318814E+04	-0.04936573E+03	0.05761929E+02	0.03433482E+00	-0.04163980E-03				3
	0.02362341E-06	-0.05054182E-10	0.02663920E+05	0.03399588E+02					4
CCL3CHO	53090C	2H	1O	1CL	3G	0300.00	5000.00	1500.00	1
	0.01532135E+03	0.01914228E-01	-0.03622777E-05	0.05526564E-10	0.03016202E-13				2

-0.02886499E+06-0.04774516E+03 0.05016867E+02 0.02961902E+00-0.03140321E-03 3  
0.01666643E-06-0.03481662E-10-0.02544921E+06 0.06644422E+02 4  
CCL300 53090C 1O 2CL 3 G 0300.00 5000.00 1500.00 1  
0.01473249E+03 0.08345102E-02-0.03627944E-05 0.07101159E-09-0.05165897E-13 2  
-0.05526644E+05-0.04381961E+03 0.04317420E+02 0.03486414E+00-0.04287094E-03 3  
0.02371950E-06-0.04903871E-10-0.02855912E+05 0.08720693E+02 4  
CCL4 40992C 1CL 4 G 0300.00 4000.00 1500.00 1  
0.01222570E+03 0.07440275E-02-0.03141658E-05 0.06499383E-09-0.05330319E-13 2  
-0.01439931E+06-0.03133566E+03 0.05107111E+02 0.02402469E+00-0.02980593E-03 3  
0.01678331E-06-0.03535253E-10-0.01253198E+06 0.04640845E+02 4  
CCLH200 53090C 1H 2O 2CL 1G 0300.00 5000.00 1500.00 1  
0.01131351E+03 0.02330645E-01-0.03546376E-05-0.02064087E-09 0.06154082E-13 2  
-0.04225590E+05-0.03183829E+03 0.01583541E+02 0.02745395E+00-0.02803155E-03 3  
0.01491598E-06-0.03172720E-10-0.08340802E+04 0.01999023E+03 4  
CH 121286C 1H 1 G 0300.00 5000.00 1000.00 1  
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2  
0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04 3  
0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331588E+02 4  
CH+ 121286C 1H 1E -1 G 0300.00 5000.00 1000.00 1  
0.02753358E+02 0.01552900E-01-0.05368453E-05 0.08921772E-09-0.05416801E-13 2  
0.01948467E+07 0.04654892E+02 0.03327207E+02 0.01347051E-01-0.03895861E-04 3  
0.05129390E-07-0.02054576E-10 0.01946452E+07 0.01408474E+02 4  
CH2 120186C 1H 2 G 0250.00 4000.00 1000.00 1  
0.03636408E+02 0.01933057E-01-0.01687016E-05-0.01009899E-08 0.01808256E-12 2  
0.04534134E+06 0.02156561E+02 0.03762237E+02 0.01159819E-01 0.02489585E-05 3  
0.08800836E-08-0.07332435E-11 0.04536791E+06 0.01712578E+02 4  
CH2(S) 31287C 1H 2 G 0300.00 4000.00 1000.00 1  
0.03552889E+02 0.02066788E-01-0.01914116E-05-0.01104673E-08 0.02021350E-12 2  
0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699089E-02 0.01025369E-04 3  
0.02492551E-07-0.01981266E-10 0.04989368E+06 0.05753207E+00 4  
CH2CCL 53090C 2H 2CL 1 G 0300.00 5000.00 1500.00 1  
0.09117805E+02 0.02336015E-01-0.03466390E-05-0.03584809E-09 0.08154328E-13 2  
0.02697366E+06-0.02251742E+03 0.01553177E+02 0.02243159E+00-0.02366950E-03 3  
0.01323270E-06-0.02931823E-10 0.02962339E+06 0.01769303E+03 4  
CH2CCL2 53090C 2H 2CL 2 G 0300.00 5000.00 1500.00 1  
0.01169451E+03 0.02435982E-01-0.03733045E-05-0.01419412E-09 0.05199337E-13 2  
-0.04601975E+05-0.03547415E+03 0.01527166E+02 0.02983780E+00-0.03171097E-03 3  
0.01728380E-06-0.03709638E-10-0.01173986E+05 0.01827540E+03 4  
CH2CCLOH 53090C 2H 3O 1CL 1G 0300.00 5000.00 1500.00 1  
0.01267601E+03 0.03201392E-01-0.04788878E-05-0.02136104E-09 0.07030796E-13 2  
-0.02402379E+06-0.04128498E+03 0.06647840E+01 0.03723168E+00-0.04115206E-03 3  
0.02307135E-06-0.05021609E-10-0.02012318E+06 0.02165270E+03 4  
CH2CHCCH 82489C 4H 4 G 0300.00 4000.00 1000.00 1  
0.01069777E+03 0.06982014E-01-0.06567747E-05-0.03884517E-08 0.07200946E-12 2  
0.03034803E+06-0.03128430E+03 0.03233893E+02 0.01865634E+00 0.01270320E-04 3  
-0.09410096E-07 0.02956111E-10 0.03301097E+06 0.09922676E+02 4  
CH2CHCCH2 82489C 4H 5 G 0300.00 4000.00 1000.00 1  
0.01199776E+03 0.07990580E-01-0.08098173E-05-0.04568733E-08 0.08636910E-12 2  
0.03228493E+06-0.03528495E+03 0.03879443E+02 0.01997664E+00 0.01872777E-04 3  
-0.09306953E-07 0.02386116E-10 0.03526859E+06 0.09842152E+02 4  
CH2CHCH2 82489C 3H 5 G 0300.00 4000.00 1000.00 1  
0.09651539E+02 0.08075596E-01-0.07965424E-05-0.04650696E-08 0.08603280E-12 2  
0.01530096E+06-0.02686774E+03 0.02276486E+02 0.01985564E+00 0.01123842E-04 3  
-0.01014576E-06 0.03441342E-10 0.01789497E+06 0.01372515E+03 4  
CH2CHCHCH 82489C 4H 5 G 0300.00 4000.00 1000.00 1  
0.01286597E+03 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12 2  
0.03783552E+06-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04 3  
-0.01148245E-06 0.03197824E-10 0.04142218E+06 0.01289454E+03 4  
CH2CHCHCH2 120189C 4H 6 G 0300.00 4000.00 1000.00 1  
0.01254437E+03 0.09596525E-01-0.09187012E-05-0.05429640E-08 0.01005364E-11 2  
0.08597330E+05-0.04217451E+03 0.01931624E+02 0.02479030E+00 0.03018071E-04 3  
-0.01154686E-06 0.02586623E-10 0.01255468E+06 0.01701999E+03 4  
CH2CHCL 53090C 2H 3CL 1 G 0300.00 5000.00 1500.00 1  
0.01029820E+03 0.03042926E-01-0.03881390E-05-0.04925565E-09 0.01005072E-12 2  
-0.02492899E+05-0.03108614E+03 0.01118026E+01 0.02796358E+00-0.02726559E-03 3  
0.01463257E-06-0.03204075E-10 0.01287844E+05 0.02381617E+03 4

CH2CL	53090C	1H	2CL	1	G	0300.00	5000.00	1500.00	1
	0.06822515E+02	0.01659744E-01	-0.02075515E-05	-0.02793518E-09	0.05509087E-13				2
	0.01080454E+06	-0.01090504E+03	0.02419924E+02	0.01303317E+00	-0.01356559E-03				3
	0.07836108E-07	-0.01800535E-10	0.01243112E+06	0.01269845E+03					4
CH2CL2	112989C	1H	2CL	2	G	0300.00	5000.00	1000.00	1
	0.05917327E+02	0.06762395E-01	-0.02676163E-04	0.04856687E-08	-0.03316974E-12				2
	-0.01385926E+06	-0.03877739E+02	0.01423284E+02	0.02116658E+00	-0.02178088E-03				3
	0.01345873E-06	-0.03811649E-10	-0.01268664E+06	0.01893445E+03					4
CH2CLCCL2	53090C	2H	2CL	3	G	0300.00	5000.00	1500.00	1
	0.01438156E+03	0.02379635E-01	-0.04167426E-05	-0.02445116E-10	0.04499574E-13				2
	-0.02746720E+05	-0.04351762E+03	0.03351194E+02	0.03297633E+00	-0.03604139E-03				3
	0.01977453E-06	-0.04233823E-10	0.08620011E+04	0.01444760E+03					4
CH2CLCCLO	53090C	2H	2O	1CL	2G	0300.00	5000.00	1500.00	1
	0.01392027E+03	0.02589602E-01	-0.04141892E-05	-0.01643169E-09	0.06237174E-13				2
	-0.03517257E+06	-0.04389503E+03	0.02705995E+02	0.03210128E+00	-0.03357727E-03				3
	0.01814310E-06	-0.03890009E-10	-0.03130905E+06	0.01566013E+03					4
CH2CLCH2	53090C	2H	4CL	1	G	0300.00	5000.00	1500.00	1
	0.01167011E+03	0.03554722E-01	-0.04124241E-05	-0.07276110E-09	0.01316756E-12				2
	0.06201629E+05	-0.03604549E+03	0.01635864E+02	0.02680201E+00	-0.02491421E-03				3
	0.01349235E-06	-0.03046571E-10	0.01014294E+06	0.01864248E+03					4
CH2CLCH2CL	53090C	2H	4CL	2	G	0300.00	5000.00	1500.00	1
	0.01443143E+03	0.03836770E-01	-0.05299122E-05	-0.05165412E-09	0.01177636E-12				2
	-0.02296285E+06	-0.05130124E+03	-0.02436500E+01	0.04032574E+00	-0.03956993E-03				3
	0.02074245E-06	-0.04412604E-10	-0.01767830E+06	0.02741366E+03					4
CH2CLCHCL	53090C	2H	3CL	2	G	0300.00	5000.00	1500.00	1
	0.01295593E+03	0.03001689E-01	-0.04165162E-05	-0.03909055E-09	0.09041090E-13				2
	0.09932077E+04	-0.03925387E+03	0.02276185E+02	0.03011401E+00	-0.03047664E-03				3
	0.01654880E-06	-0.03613198E-10	0.04836340E+05	0.01792166E+03					4
CH2CLCHCL2	53090C	2H	3CL	3	G	0300.00	5000.00	1500.00	1
	0.01618739E+03	0.03047681E-01	-0.05011496E-05	-0.01596701E-09	0.07107547E-13				2
	-0.02474417E+06	-0.05695454E+03	0.01239011E+02	0.04148444E+00	-0.04188654E-03				3
	0.02163214E-06	-0.04467364E-10	-0.01960717E+06	0.02257856E+03					4
CH2CLCHO	53090C	2H	3O	1CL	1G	0300.00	5000.00	1500.00	1
	0.01227955E+03	0.03320979E-01	-0.04106710E-05	-0.06199826E-09	0.01190594E-12				2
	-0.02678416E+06	-0.03762356E+03	0.06553003E+01	0.02959046E+00	-0.02635056E-03				3
	0.01327545E-06	-0.02838288E-10	-0.02227005E+06	0.02576797E+03					4
CH2CO	121686C	1H	2O	1	G	0300.00	5000.00	1000.00	1
	0.06038817E+02	0.05804840E-01	-0.01920954E-04	0.02794485E-08	-0.01458868E-12				2
	-0.08583402E+05	-0.07657581E+02	0.02974971E+02	0.01211871E+00	-0.02345046E-04				3
	-0.06466685E-07	0.03905649E-10	-0.07632637E+05	0.08673553E+02					4
CH2F2	82489C	1H	2F	2	G	0300.00	5000.00	1000.00	1
	0.04730052E+02	0.07997300E-01	-0.03186045E-04	0.05801160E-08	-0.03967925E-12				2
	-0.05637288E+06	-0.04954843E+01	0.03669434E+01	0.02168917E+00	-0.02441913E-03				3
	0.01942310E-06	-0.06978343E-10	-0.05510103E+06	0.02202215E+03					4
CH2HCO	110393O	1H	3C	2	G	0300.00	5000.00	1000.00	1
	0.05975670E+02	0.08130591E-01	-0.02743624E-04	0.04070304E-08	-0.02176017E-12				2
	0.04903218E+04	-0.05045251E+02	0.03409062E+02	0.01073857E+00	0.01891492E-04				3
	-0.07158583E-07	0.02867385E-10	0.01521477E+05	0.09558290E+02					4
CH2O	121286C	1H	2O	1	G	0300.00	5000.00	1000.00	1
	0.02995606E+02	0.06681321E-01	-0.02628955E-04	0.04737153E-08	-0.03212517E-12				2
	-0.01532037E+06	0.06912572E+02	0.01652731E+02	0.01263144E+00	-0.01888168E-03				3
	0.02050031E-06	-0.08413237E-10	-0.01486540E+06	0.01378482E+03					4
CH2OH	120186H	3C	1O	1	G	0250.00	4000.00	1000.00	1
	0.06327520E+02	0.03608271E-01	-0.03201547E-05	-0.01938750E-08	0.03509705E-12				2
	-0.04474509E+05	-0.08329366E+02	0.02862628E+02	0.01001527E+00	-0.05285436E-05				3
	-0.05138540E-07	0.02246041E-10	-0.03349679E+05	0.01039794E+03					4
CH2OHCL2	53090C	2H	3O	1CL	2G	0300.00	5000.00	1500.00	1
	0.01602181E+03	0.02846352E-01	-0.04974218E-05	-0.02167450E-10	0.05246046E-13				2
	-0.01829579E+06	-0.05402134E+03	0.01922940E+02	0.04158207E+00	-0.04427505E-03				3
	0.02343015E-06	-0.04851868E-10	-0.01375512E+06	0.02001902E+03					4
CH2OHCHCL	53090C	2H	4O	1CL	1G	0300.00	5000.00	1500.00	1
	0.01446298E+03	0.03569514E-01	-0.05419118E-05	-0.02862176E-09	0.08920560E-13				2
	-0.01475559E+06	-0.04942815E+03	0.03505696E+01	0.04212749E+00	-0.04493839E-03				3
	0.02448187E-06	-0.05236589E-10	-0.01007314E+06	0.02495261E+03					4
CH2SICL	40992H	2C	1SI	1CL	1G	0300.00	4000.00	1500.00	1
	0.09915966E+02	0.01896319E-01	-0.03304238E-05	-0.03882353E-09	0.01089169E-12				2

0.01906587E+06-0.02389137E+03 0.03514077E+02 0.01959495E+00-0.02147274E-03	3
0.01214017E-06-0.02691323E-10 0.02123280E+06 0.09882836E+02	4
CH2SICL3 40992H 2C 1SI 1CL 3G 0300.00 4000.00 1500.00	1
0.01476240E+03 0.02289499E-01-0.04148337E-05-0.01526182E-09 0.07724698E-13	2
-0.04947703E+06-0.04020475E+03 0.06718170E+02 0.02712662E+00-0.03168529E-03	3
0.01809641E-06-0.03938906E-10-0.04710183E+06 0.01167360E+02	4
CH2SIH2CL 40992H 4C 1SI 1CL 1G 0300.00 4000.00 1500.00	1
0.01260561E+03 0.03468476E-01-0.04606434E-05-0.09748147E-09 0.02077681E-12	2
-0.05748538E+05-0.03743183E+03 0.02426229E+02 0.03028056E+00-0.03039200E-03	3
0.01612599E-06-0.03425629E-10-0.02268891E+05 0.01657736E+03	4
CH2SIHCL2 40992H 3C 1SI 1CL 2G 0300.00 4000.00 1500.00	1
0.01360592E+03 0.02909029E-01-0.04521180E-05-0.05274788E-09 0.01389320E-12	2
-0.02781262E+06-0.03810353E+03 0.04180967E+02 0.03005761E+00-0.03288772E-03	3
0.01822025E-06-0.03925700E-10-0.02480330E+06 0.01134845E+03	4
CH3 121286C 1H 3 G 0300.00 5000.00 1000.00	1
0.02844052E+02 0.06137974E-01-0.02230345E-04 0.03785161E-08-0.02452159E-12	2
0.01643781E+06 0.05452697E+02 0.02430443E+02 0.01112410E+00-0.01680220E-03	3
0.01621829E-06-0.05864953E-10 0.01642378E+06 0.06789794E+02	4
CH3C(O)CL 53090C 2H 3O 1CL 1G 0300.00 5000.00 1500.00	1
0.01240568E+03 0.03210496E-01-0.03737157E-05-0.06739592E-09 0.01219122E-12	2
-0.03432420E+06-0.03909195E+03 0.02275117E+02 0.02518533E+00-0.02152420E-03	3
0.01084005E-06-0.02369191E-10-0.03024376E+06 0.01657016E+03	4
CH3CC 82489C 3H 3 G 0300.00 4000.00 1000.00	1
0.07640221E+02 0.05233556E-01-0.05053635E-05-0.02919772E-08 0.05445700E-12	2
0.05909763E+06-0.01629573E+03 0.03798751E+02 0.08749062E-01 0.02523014E-04	3
-0.01529373E-07-0.01410562E-10 0.06077425E+06 0.05989223E+02	4
CH3CCCH2 82489C 4H 5 G 0300.00 4000.00 1000.00	1
0.01156506E+03 0.08030297E-01-0.07649450E-05-0.04476534E-08 0.08313260E-12	2
0.03256813E+06-0.03014066E+03 0.05068450E+02 0.01571747E+00 0.02968975E-04	3
-0.04990587E-07-0.02984224E-11 0.03518855E+06 0.06791893E+02	4
CH3CCCH3 120189C 4H 6 G 0300.00 4000.00 1000.00	1
0.01133658E+03 0.01005764E+00-0.09511323E-05-0.05660497E-08 0.01049451E-11	2
0.01547659E+06-0.03350867E+03 0.04077105E+02 0.01703159E+00 0.04707490E-04	3
-0.03767240E-07-0.02066963E-10 0.01859757E+06 0.08444801E+02	4
CH3CCH2 82489C 3H 5 G 0300.00 4000.00 1000.00	1
0.09101018E+02 0.07964168E-01-0.07884945E-05-0.04562036E-08 0.08529212E-12	2
0.02670680E+06-0.02150559E+03 0.03385811E+02 0.01404534E+00 0.03204127E-04	3
-0.03824120E-07-0.09053742E-11 0.02909066E+06 0.01126649E+03	4
CH3CCL 53090C 2H 3CL 1 G 0300.00 5000.00 1500.00	1
0.01023962E+03 0.02767116E-01-0.03228853E-05-0.05752548E-09 0.01043430E-12	2
0.02633607E+06-0.02806184E+03 0.01687397E+02 0.02164347E+00-0.01891466E-03	3
0.09699015E-07-0.02134580E-10 0.02975387E+06 0.01882236E+03	4
CH3CCL2 53090C 2H 3CL 2 G 0300.00 5000.00 1500.00	1
0.01300035E+03 0.02940485E-01-0.03746456E-05-0.05040644E-09 0.01006332E-12	2
-0.04228816E+04-0.03979863E+03 0.03213473E+02 0.02587378E+00-0.02419993E-03	3
0.01273817E-06-0.02788481E-10 0.03325663E+05 0.01333320E+03	4
CH3CCL3 53090C 2H 3CL 3 G 0300.00 5000.00 1500.00	1
0.01637160E+03 0.02935021E-01-0.04836108E-05-0.01454723E-09 0.06731691E-13	2
-0.02378095E+06-0.05941864E+03 0.02484363E+02 0.03909474E+00-0.04013637E-03	3
0.02110179E-06-0.04418213E-10-0.01902540E+06 0.01435603E+03	4
CH3CCLO 53090C 2H 3O 1CL 1G 0300.00 5000.00 1500.00	1
0.01240595E+03 0.03210266E-01-0.03736397E-05-0.06740236E-09 0.01219081E-12	2
-0.03432283E+06-0.03909605E+03 0.02277402E+02 0.02517912E+00-0.02151632E-03	3
0.01083524E-06-0.02368079E-10-0.03024308E+06 0.01655556E+03	4
CH3CH2CCH 120189C 4H 6 G 0300.00 4000.00 1000.00	1
0.01200695E+03 0.09576069E-01-0.08995018E-05-0.05369808E-08 0.09934174E-12	2
0.01729420E+06-0.03802692E+03 0.03726043E+02 0.02053493E+00 0.03021439E-04	3
-0.08131813E-07 0.01095280E-10 0.02048821E+06 0.08538826E+02	4
CH3CH2CH2CH3 120293H 10C 4 G 0300.00 4000.00 1500.00	1
0.01945335E+03 0.01072566E+00-0.07261518E-05-0.06282734E-08 0.01058386E-11	2
-0.02519408E+06-0.08439214E+03 0.01384451E+02 0.03682875E+00-0.04264044E-04	3
-0.09300217E-07 0.03294447E-10-0.01734385E+06 0.01829556E+03	4
CH3CH2CL 53090C 2H 5CL 1 G 0300.00 5000.00 1500.00	1
0.01301118E+03 0.04448941E-01-0.05200473E-05-0.09119710E-09 0.01658842E-12	2
-0.02013503E+06-0.04677847E+03-0.06981899E+01 0.03567705E+00-0.03230260E-03	3
0.01689622E-06-0.03727523E-10-0.01476054E+06 0.02802219E+03	4

CH3CH2O	103190C	2H	5O	1	G	0300.00	4000.00	1500.00	1
0.01187115E+03	0.05390415E-01-0.04990159E-05-0.02399585E-08	0.04255456E-12	2						
-0.05950457E+05-0.03996585E+03	0.06904570E+01	0.02951398E+00-0.02245116E-03	3						
0.01011600E-06-0.02044101E-10-0.01559918E+05	0.02130230E+03	4							
CH3CHCH	82489C	3H	5	G	0300.00	4000.00	1000.00	1	
0.09209764E+02	0.07871413E-01-0.07724523E-05-0.04497357E-08	0.08377272E-12	2						
0.02853967E+06-0.02232370E+03	0.03161863E+02	0.01518100E+00	0.02722659E-04	3					
-0.05177112E-07	0.05435286E-12	0.03095548E+06	0.01197973E+03	4					
CH3CHCL	53090C	2H	4CL	1	G	0300.00	5000.00	1500.00	1
0.01166291E+03	0.03539284E-01-0.03858423E-05-0.08186871E-09	0.01407549E-12	2						
0.03696642E+05-0.03616108E+03	0.01903574E+02	0.02438193E+00-0.02062779E-03	3						
0.01068382E-06-0.02414461E-10	0.07722870E+05	0.01768152E+03	4						
CH3CHCL2	53090C	2H	4CL	2	G	0300.00	5000.00	1500.00	1
0.01454311E+03	0.03772378E-01-0.05189301E-05-0.05141063E-09	0.01163076E-12	2						
-0.02277045E+06-0.05147426E+03	0.04510764E+01	0.03884901E+00-0.03832912E-03	3						
0.02029502E-06-0.02391420E-10-0.01767234E+06	0.02414546E+03	4							
CH3CHOH	103190C	2H	4O	1	G	0300.00	4000.00	1500.00	1
0.01161148E+03	0.05173117E-01-0.04856685E-05-0.02202895E-08	0.03913721E-12	2						
-0.01248811E+06-0.03688213E+03	0.01415940E+02	0.02870648E+00-0.02373820E-03	3						
0.01148886E-06-0.02391420E-10-0.08638718E+05	0.01844256E+03	4							
CH3CL	112989C	1H	3CL	1	G	0300.00	5000.00	1000.00	1
0.03633876E+02	0.08664625E-01-0.03343871E-04	0.05950130E-08-0.04001401E-12	2						
-0.01177659E+06	0.04430651E+02	0.04621901E+01	0.02068247E+00-0.02553133E-03	3					
0.02160311E-06-0.07706816E-10-0.01093667E+06	0.02032977E+03	4							
CH3CO	120186C	2H	3O	1	G	0300.00	5000.00	1000.00	1
0.05612279E+02	0.08449886E-01-0.02854147E-04	0.04238376E-08-0.02268404E-12	2						
-0.05187863E+05-0.03274949E+02	0.03125278E+02	0.09778220E-01	0.04521448E-04	3					
-0.09009462E-07	0.03193718E-10-0.04108508E+05	0.01122885E+03	4						
CH3F	82489C	1H	3F	1	G	0300.00	5000.00	1000.00	1
0.03014978E+02	0.09314397E-01-0.03611697E-04	0.06443728E-08-0.04339594E-12	2						
-0.02977838E+06	0.06323815E+02	0.02600911E+01	0.02000788E+00-0.02662585E-03	3					
0.02561177E-06-0.09935237E-10-0.02896233E+06	0.02031799E+03	4							
CH3HCO	120186C	2O	1H	4	G	0300.00	5000.00	1000.00	1
0.05868650E+02	0.01079424E+00-0.03645530E-04	0.05412912E-08-0.02896844E-12	2						
-0.02264569E+06-0.06012946E+02	0.02505695E+02	0.01336991E+00	0.04671953E-04	3					
-0.01128140E-06	0.04263566E-10-0.02124589E+06	0.01335089E+03	4						
CH3NO	103190C	1H	3N	1O	1G	0300.00	4000.00	1500.00	1
0.08820547E+02	0.03706233E-01-0.02894741E-05-0.01897910E-08	0.03237544E-12	2						
0.05362862E+05-0.02213220E+03	0.02109955E+02	0.01517822E+00-0.07071789E-04	3						
0.01510611E-07-0.01604204E-11	0.08293612E+05	0.01569702E+03	4						
CH3NO2	103190C	1H	3N	1O	2G	0300.00	4000.00	1500.00	1
0.01090158E+03	0.04326381E-01-0.04203548E-05-0.01893071E-08	0.03417444E-12	2						
-0.01370862E+06-0.03073183E+03	0.03224717E+01	0.02665147E+00-0.01930574E-03	3						
0.07762620E-07-0.01398746E-10-0.09597527E+05	0.02726156E+03	4							
CH3O	121686C	1H	3O	1	G	0300.00	3000.00	1000.00	1
0.03770800E+02	0.07871497E-01-0.02656384E-04	0.03944431E-08-0.02112616E-12	2						
0.01278325E+04	0.02929575E+02	0.02106204E+02	0.07216595E-01	0.05338472E-04	3				
-0.07377636E-07	0.02075611E-10	0.09786011E+04	0.01315218E+03	4					
CH3OCH3	103190C	1H	6O	1	G	0300.00	4000.00	1500.00	1
0.01228100E+03	0.06711031E-01-0.04726871E-05-0.03636409E-08	0.06084545E-12	2						
-0.02839743E+06-0.04434692E+03	0.01245246E+02	0.02381198E+00-0.08266949E-04	3						
0.03068452E-08	0.01909248E-11-0.02335996E+06	0.01855817E+03	4						
CH3OCL	53090C	1H	3O	1CL	1G	0300.00	5000.00	1500.00	1
0.01022518E+03	0.02780047E-01-0.03331582E-05-0.05437858E-09	0.01012799E-12	2						
-0.01172886E+06-0.02912014E+03	0.01575392E+02	0.02255642E+00-0.02052644E-03	3						
0.01075312E-06-0.02371140E-10-0.08346834E+05	0.01804593E+03	4							
CH3OH	121686C	1H	4O	1	G	0300.00	5000.00	1000.00	1
0.04029061E+02	0.09376593E-01-0.03050254E-04	0.04358793E-08-0.02224723E-12	2						
-0.02615791E+06	0.02378196E+02	0.02660115E+02	0.07341508E-01	0.07170051E-04	3				
-0.08793194E-07	0.02390570E-10-0.02535348E+06	0.01123263E+03	4						
CH3ONO	103190C	1H	3N	1O	2G	0300.00	4000.00	1500.00	1
0.01136129E+03	0.04159349E-01-0.04145670E-05-0.01695140E-08	0.03028732E-12	2						
-0.01281482E+06-0.03545435E+03	0.01490345E+02	0.02645433E+00-0.02112332E-03	3						
0.09414399E-07-0.01811205E-10-0.09125782E+05	0.01813766E+03	4							
CH3ONO2	103190C	1H	3N	1O	3G	0300.00	4000.00	1500.00	1
0.01436189E+03	0.04112243E-01-0.05113052E-05-0.01496436E-08	0.03012156E-12	2						

-0.01972440E+06-0.05131842E+03 0.07803354E+01 0.03454204E+00-0.02822328E-03	3
0.01232324E-06-0.02302164E-10-0.01465346E+06 0.02245752E+03	4
CH3SICL 10891C 1H 3CL 1SI 1G 0300.00 4000.00 1500.00	1
0.01001981E+03 0.03098227E-01-0.03223524E-05-0.01222654E-08 0.02254960E-12	2
-0.05427416E+05-0.02357211E+03 0.03485139E+02 0.01833182E+00-0.01573128E-03	3
0.07856310E-07-0.01670946E-10-0.02954042E+05 0.01186948E+03	4
CH3SIH2SIH 10891C 2H 10SI 2 G 0300.00 4000.00 1500.00	1
0.02302241E+03 0.08819047E-01-0.08859755E-05-0.03700889E-08 0.06746256E-12	2
-0.01577058E+06-0.09458104E+03 0.02492915E+02 0.05396367E+00-0.04281663E-03	3
0.01967585E-06-0.03981630E-10-0.07813141E+05 0.01758364E+03	4
CH3SIH2SIH2CH3 61991H 10C 2SI 2 G 0300.00 2500.00 1500.00	1
0.01948332E+03 0.01195163E+00-0.02653155E-05-0.01489522E-07 0.03049901E-11	2
-0.01405639E+06-0.07368209E+03 0.03129493E+02 0.05016930E+00-0.03522061E-03	3
0.01354295E-06-0.02274339E-10-0.08303932E+05 0.01426819E+03	4
CH3SIHCL2 10891C 1CL 2H 4SI 1G 0300.00 4000.00 1500.00	1
0.01459367E+03 0.04005638E-01-0.04816391E-05-0.01336359E-08 0.02648177E-12	2
-0.05325682E+06-0.04689839E+03 0.04156949E+02 0.02994072E+00-0.02797859E-03	3
0.01431829E-06-0.03010165E-10-0.04952345E+06 0.09043929E+02	4
CH4 121286C 1H 4 G 0300.00 5000.00 1000.00	1
0.01683479E+02 0.01023724E+00-0.03875129E-04 0.06785585E-08-0.04503423E-12	2
-0.01008079E+06 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03	3
0.03049708E-06-0.01223931E-09-0.09825229E+05 0.01372219E+03	4
CHCL 112989C 1H 1CL 1 G 0300.00 5000.00 1200.00	1
0.03216518E+02 0.05976969E-01-0.02918238E-04 0.05912801E-08-0.04297945E-12	2
0.03879839E+06 0.07793842E+02 0.02781263E+02 0.07805384E-01-0.01063711E-03	3
0.01065441E-06-0.03916797E-10 0.03916144E+06 0.01045515E+03	4
CHCL2 40992H 1C 1CL 2 G 0300.00 4000.00 1500.00	1
0.06912875E+02 0.01251733E-01-0.01973086E-05-0.02153722E-09 0.05853635E-13	2
0.07229632E+05-0.07968135E+02 0.02809820E+02 0.01295936E+00-0.01392392E-03	3
0.07533319E-07-0.01588448E-10 0.08515305E+05 0.01343798E+03	4
CHCL2CCL2 40992H 1C 2CL 4 G 0300.00 4000.00 1500.00	1
0.01530640E+03 0.02140772E-01-0.04619954E-05 0.08299157E-10 0.05236928E-13	2
-0.01524306E+05-0.04358303E+03 0.04207169E+02 0.03437580E+00-0.03802411E-03	3
0.02026572E-06-0.04164115E-10 0.01811422E+05 0.01398021E+03	4
CHCL2CCLO 40992H 1C 2 O 1CL 3G 0300.00 4000.00 1500.00	1
0.01488775E+03 0.02323698E-01-0.04365744E-05-0.01680889E-09 0.08613253E-13	2
-0.03483792E+06-0.04504932E+03 0.04593886E+02 0.03118954E+00-0.03338775E-03	3
0.01763042E-06-0.03630728E-10-0.03160866E+06 0.08756166E+02	4
CHCL2CH2 53090C 2H 3CL 2 G 0300.00 5000.00 1500.00	1
0.01306632E+03 0.02964322E-01-0.04303601E-05-0.03173131E-09 0.08244908E-13	2
0.04594697E+05-0.03814765E+03 0.02234889E+02 0.03152885E+00-0.03307990E-03	3
0.01825221E-06-0.03994163E-10 0.08375531E+05 0.01944506E+03	4
CHCL2CHCL 53090C 2H 2CL 3 G 0300.00 5000.00 1500.00	1
0.01445051E+03 0.02336553E-01-0.04132107E-05-0.05243785E-11 0.04204775E-13	2
-0.05183250E+04-0.04362699E+03 0.03789098E+02 0.03243338E+00-0.03598339E-03	3
0.01993302E-06-0.04287482E-10 0.02920910E+05 0.01221991E+03	4
CHCL2CHCL2 53090C 2H 2CL 4 G 0300.00 5000.00 1500.00	1
0.01745859E+03 0.02484178E-01-0.05127803E-05 0.02266909E-09 0.02371932E-13	2
-0.02510699E+06-0.06065213E+03 0.02711746E+02 0.04441279E+00-0.04905962E-03	3
0.02632472E-06-0.05466293E-10-0.02052421E+06 0.01624857E+03	4
CHCL3 40992H 1C 1CL 3 G 0300.00 4000.00 1500.00	1
0.01034980E+03 0.01690302E-01-0.03209168E-05-0.09502160E-10 0.05845725E-13	2
-0.01567029E+06-0.02558805E+03 0.02905633E+02 0.02315061E+00-0.02534675E-03	3
0.01356724E-06-0.02810882E-10-0.01339798E+06 0.01310749E+03	4
CHCLCCL 40992H 1C 2CL 2 G 0300.00 4000.00 1500.00	1
0.01027647E+03 0.01733039E-01-0.03161161E-05-0.08153494E-10 0.05443014E-13	2
0.02418877E+06-0.02436862E+03 0.02625129E+02 0.02366908E+00-0.02583240E-03	3
0.01383374E-06-0.02870111E-10 0.02654214E+06 0.01545629E+03	4
CHCLCCLOH 53090C 2H 2O 1CL 2G 0300.00 5000.00 1500.00	1
0.01412206E+03 0.02583764E-01-0.04576900E-05 0.05215675E-10 0.03521300E-13	2
-0.02752482E+06-0.04544297E+03 0.02020547E+02 0.03810981E+00-0.04280147E-03	3
0.02343806E-06-0.04934735E-10-0.02385982E+06 0.01729375E+03	4
CHCLCH 53090C 2H 2CL 1 G 0300.00 5000.00 1500.00	1
0.09924881E+02 0.01618108E-01-0.02995768E-05-0.09718417E-11 0.03296695E-13	2
0.02834312E+06-0.02704593E+03 0.01190122E+02 0.02432800E+00-0.02555965E-03	3
0.01375158E-06-0.02941848E-10 0.03138157E+06 0.01944186E+03	4

CHCLCHCL 53090C 2H 2CL 2 G 0300.00 5000.00 1500.00 1  
0.01163648E+03 0.02461981E-01-0.03900520E-05-0.01521677E-09 0.05853766E-13 2  
-0.05593248E+05-0.03507354E+03 0.01054340E+02 0.03076645E+00-0.03252549E-03 3  
0.01763454E-06-0.03774444E-10-0.02006846E+05 0.02094011E+03 4  
CHCLCHOH 53090C 2H 3O 1CL 1G 0300.00 5000.00 1500.00 1  
0.01285464E+03 0.03107712E-01-0.04837735E-05-0.02088657E-09 0.07393125E-13 2  
-0.02505588E+06-0.04274804E+03-0.02073397E+01 0.03868022E+00-0.04104567E-03 3  
0.02211252E-06-0.04680556E-10-0.02074261E+06 0.02608356E+03 4  
CHCLOH 53090C 1H 2O 1CL 1G 0300.00 5000.00 1500.00 1  
0.09427376E+02 0.01722643E-01-0.02912707E-05-0.03765845E-10 0.03354461E-13 2  
-0.01224575E+06-0.02330123E+03 0.01319372E+02 0.02406119E+00-0.02560105E-03 3  
0.01356738E-06-0.02812530E-10-0.09640457E+05 0.01925640E+03 4  
CHCLOHCH2 53090C 2H 4O 1CL 1G 0300.00 5000.00 1500.00 1  
0.01438435E+03 0.03552541E-01-0.05033147E-05-0.04051247E-09 0.01001172E-12 2  
-0.01383899E+06-0.04819745E+03 0.01473757E+02 0.03764188E+00-0.03898776E-03 3  
0.02112109E-06-0.04543830E-10-0.09395106E+05 0.02033823E+03 4  
CHCLOHCHCL 53090C 2H 3O 1CL 2G 0300.00 5000.00 1500.00 1  
0.01567240E+03 0.02970040E-01-0.04827588E-05-0.01366600E-09 0.06500296E-13 2  
-0.01896002E+06-0.05132923E+03 0.02626025E+02 0.03856175E+00-0.04091474E-03 3  
0.02190241E-06-0.04603080E-10-0.01468188E+06 0.01735864E+03 4  
CHF 82489C 1H 1F 1 G 0300.00 5000.00 1000.00 1  
0.04242812E+02 0.02066316E-01-0.06527951E-05 0.01388700E-08-0.01213336E-12 2  
0.01355982E+06 0.01680197E+02 0.03029061E+02 0.04850873E-01-0.04971679E-04 3  
0.05277968E-07-0.02403154E-10 0.01401435E+06 0.08324101E+02 4  
CHF3 82489C 1H 1F 3 G 0300.00 5000.00 1000.00 1  
0.06834333E+02 0.06248731E-01-0.02575750E-04 0.04809112E-08-0.03352074E-12 2  
-0.08663771E+06-0.01062741E+03 0.08725142E+01 0.02308432E+00-0.02123718E-03 3  
0.01114428E-06-0.02909229E-10-0.08496391E+06 0.02021499E+03 4  
CHOHCLCCL2 53090C 2H 2O 1CL 3G 0300.00 5000.00 1500.00 1  
0.01681824E+03 0.02450153E-01-0.04706624E-05 0.01313263E-09 0.03046283E-13 2  
-0.02253368E+06-0.05396958E+03 0.04216444E+02 0.03898554E+00-0.04360467E-03 3  
0.02374677E-06-0.04984764E-10-0.01867017E+06 0.01152520E+03 4  
CHSICL 40992H 1C 1SI 1CL 1G 0300.00 4000.00 1500.00 1  
0.08205361E+02 0.01092172E-01-0.02021812E-05-0.04611367E-10 0.03306854E-13 2  
0.04201323E+06-0.01240589E+03 0.04575767E+02 0.01266147E+00-0.01507699E-03 3  
0.08704482E-07-0.01902710E-10 0.04304864E+06 0.06132926E+02 4  
CHSICL2 40992H 1C 1SI 1CL 2G 0300.00 4000.00 1500.00 1  
0.01071823E+03 0.01148355E-01-0.02625783E-05 0.01567972E-09 0.01085455E-13 2  
0.01124882E+06-0.02053734E+03 0.05945817E+02 0.01709681E+00-0.02135360E-03 3  
0.01252863E-06-0.02749860E-10 0.01253413E+06 0.03573691E+02 4  
CHSICL3 40992H 1C 1SI 1CL 3G 0300.00 4000.00 1500.00 1  
0.01359698E+03 0.01283679E-01-0.03320724E-05 0.03292615E-09-0.05463635E-14 2  
-0.02236189E+06-0.03349768E+03 0.07368467E+02 0.02227384E+00-0.02809218E-03 3  
0.01644147E-06-0.03590729E-10-0.02071740E+06-0.02118077E+02 4  
CHSIH2CL 40992H 3C 1SI 1CL 1G 0300.00 4000.00 1500.00 1  
0.01142815E+03 0.02475732E-01-0.03864817E-05-0.04667547E-09 0.01222497E-12 2  
0.02085332E+06-0.03033129E+03 0.02869509E+02 0.02622702E+00-0.02794178E-03 3  
0.01516891E-06-0.03231519E-10 0.02364000E+06 0.01462055E+03 4  
CHSIHCL 40992H 2C 1SI 1CL 1G 0300.00 4000.00 1500.00 1  
0.09716450E+02 0.01691882E-01-0.02846288E-05-0.02130090E-09 0.06948758E-13 2  
0.03056780E+06-0.02079822E+03 0.04045980E+02 0.01850072E+00-0.02095734E-03 3  
0.01185107E-06-0.02580401E-10 0.03232392E+06 0.08632908E+02 4  
CHSIHCL2 40992H 2C 1SI 1CL 2G 0300.00 4000.00 1500.00 1  
0.01246646E+03 0.01911555E-01-0.03687550E-05-0.05466318E-10 0.05749803E-13 2  
-0.09679288E+04-0.03163481E+03 0.04853917E+02 0.02509790E+00-0.02916486E-03 3  
0.01649649E-06-0.03563598E-10 0.01297543E+05 0.07606296E+02 4  
CL 42189CL 1 G 0300.00 5000.00 1000.00 1  
0.02920237E+02-0.03597985E-02 0.01294294E-05-0.02162776E-09 0.01376517E-13 2  
0.01371338E+06 0.03262690E+02 0.02381577E+02 0.08891079E-02 0.04070476E-05 3  
-0.02168943E-07 0.01160827E-10 0.01383999E+06 0.06021818E+02 4  
CL(CH3)SICH2 40992H 5C 2SI 1CL 1G 0300.00 4000.00 1500.00 1  
0.01496923E+03 0.05605854E-01-0.06191278E-05-0.02134591E-08 0.03977673E-12 2  
-0.01304066E+06-0.05036296E+03 0.02980753E+02 0.03627511E+00-0.03428566E-03 3  
0.01799146E-06-0.03853029E-10-0.08814405E+05 0.01362870E+03 4  
CL2 42189CL 2 G 0300.00 5000.00 1000.00 1  
0.04274587E+02 0.03717337E-02-0.01893490E-05 0.05337465E-09-0.05057602E-13 2



-0.01331149E+05	0.02256947E+02	0.03439587E+02	0.02870774E-01	-0.02385871E-04	3
0.02892918E-08	0.02915057E-11	-0.01131787E+05	0.06471359E+02		4
CL2CCCL2	40992C	2CL 4	G	0300.00 4000.00 1500.00	1
0.01440000E+03	0.01269397E-01	-0.03525286E-05	0.04493620E-09	-0.02348053E-13	2
-0.08039017E+05	-0.04321878E+03	0.05557831E+02	0.02778255E+00	-0.03176769E-03	3
0.01706054E-06	-0.03492940E-10	-0.05495042E+05	0.02293508E+02		4
CL2CCHCL	40992H	1C 2CL 3	G	0300.00 4000.00 1500.00	1
0.01278204E+03	0.02068630E-01	-0.03764411E-05	-0.09077792E-10	0.06116574E-13	2
-0.06934337E+05	-0.03655991E+03	0.03457684E+02	0.02848717E+00	-0.03070062E-03	3
0.01624951E-06	-0.03341401E-10	-0.04047205E+05	0.01206381E+03		4
CL2CCCHO	40992H	1C 2 O 1CL 2G	G	0300.00 4000.00 1500.00	1
0.01294627E+03	0.02168144E-01	-0.04244587E-05	-0.03590986E-09	0.01220303E-12	2
-0.01144361E+06	-0.03783814E+03	0.03400952E+02	0.02760695E+00	-0.02843245E-03	3
0.01470263E-06	-0.03017427E-10	-0.08287517E+05	0.01257321E+03		4
CL2CHOH	53090C	1H 2O 1CL 2G	G	0300.00 5000.00 1500.00	1
0.01129114E+03	0.02286704E-01	-0.03461513E-05	-0.01814480E-09	0.05661342E-13	2
-0.03803060E+06	-0.03079831E+03	0.02619078E+02	0.02601286E+00	-0.02784252E-03	3
0.01528682E-06	-0.03294008E-10	-0.03513998E+06	0.01492462E+03		4
CL2CO	40992C	1 O 1CL 2	G	0300.00 4000.00 1500.00	1
0.08764773E+02	0.08919938E-02	-0.02237590E-05	0.01486621E-09	0.09630870E-14	2
-0.02973390E+06	-0.01732025E+03	0.03460242E+02	0.01632331E+00	-0.01828304E-03	3
0.09805656E-07	-0.02024319E-10	-0.02813622E+06	0.01019127E+03		4
CL2COH	53090C	1O 1H 1CL 2G	G	0300.00 5000.00 1500.00	1
0.01026215E+03	0.01316796E-01	-0.02754008E-05	0.01630771E-09	0.06472563E-14	2
-0.01511655E+06	-0.02298315E+03	0.03800719E+02	0.02204678E+00	-0.02673857E-03	3
0.01531854E-06	-0.03305323E-10	-0.01332053E+06	0.09915879E+02		4
CL2HCO	53090C	1H 1O 1CL 2G	G	0300.00 5000.00 1500.00	1
0.01051838E+03	0.01499316E-01	-0.02927670E-05	0.07898750E-10	0.01988433E-13	2
-0.06272394E+05	-0.02634097E+03	0.02241202E+02	0.02456990E+00	-0.02682371E-03	3
0.01443170E-06	-0.03023080E-10	-0.03624526E+05	0.01703508E+03		4
CL2SI (CH3)2	40992H	6C 2SI 1CL 2G	G	0300.00 4000.00 1500.00	1
0.01890988E+03	0.06245385E-01	-0.06370532E-05	-0.02508388E-08	0.04589637E-12	2
-0.06523166E+06	-0.06829627E+03	0.05958770E+02	0.03632045E+00	-0.03098078E-03	3
0.01545683E-06	-0.03292671E-10	-0.06031232E+06	0.01996401E+02		4
CL2SI (CH3)CH2	40992H	5C 2SI 1CL 2G	G	0300.00 4000.00 1500.00	1
0.01795078E+03	0.05155757E-01	-0.06049094E-05	-0.01717793E-08	0.03355529E-12	2
-0.03961749E+06	-0.05949218E+03	0.05993815E+02	0.03621806E+00	-0.03546358E-03	3
0.01906128E-06	-0.04137511E-10	-0.03541814E+06	0.04216162E+02		4
CL2SICH2	40992H	2C 1SI 1CL 2G	G	0300.00 4000.00 1500.00	1
0.01186709E+03	0.02689241E-01	-0.04231139E-05	-0.05555102E-09	0.01367174E-12	2
-0.02169965E+06	-0.03225026E+03	0.04111900E+02	0.02637445E+00	-0.02985130E-03	3
0.01679309E-06	-0.03625511E-10	-0.01940307E+06	0.07695176E+02		4
CL2SICH3	40992H	3C 1SI 1CL 2G	G	0300.00 4000.00 1500.00	1
0.01285090E+03	0.03239360E-01	-0.03774509E-05	-0.01111777E-08	0.02163712E-12	2
-0.03164727E+06	-0.03531424E+03	0.05273286E+02	0.02205797E+00	-0.02049425E-03	3
0.01060061E-06	-0.02257829E-10	-0.02891555E+06	0.05340218E+02		4
CL2SISI	40992SI	2CL 2	G	0300.00 4000.00 1500.00	1
0.09706403E+02	0.03323652E-02	-0.01679851E-05	0.04061274E-09	-0.03746093E-13	2
0.01334060E+06	-0.01565614E+03	0.06576632E+02	0.01105568E+00	-0.01422816E-03	3
0.08199114E-07	-0.01752833E-10	0.01412004E+06	0.06538601E-02		4
CL2SISICL	40992SI	2CL 3	G	0300.00 4000.00 1500.00	1
0.01304318E+03	-0.01847658E-03	-0.02187635E-05	0.08817012E-09	-0.01004063E-12	2
-0.01640770E+06	-0.02832289E+03	0.08389457E+02	0.01629172E+00	-0.02138192E-03	3
0.01207431E-06	-0.02508349E-10	-0.01534318E+06	-0.05268396E+02		4
CL2SISICL2	40992SI	2CL 4	G	0300.00 4000.00 1500.00	1
0.01620538E+03	0.08400587E-04	-0.02457560E-05	0.08992196E-09	-0.09639101E-13	2
-0.05343016E+06	-0.04193027E+03	0.01077595E+03	0.01717615E+00	-0.02131386E-03	3
0.01172528E-06	-0.02417202E-10	-0.05196762E+06	-0.01431634E+03		4
CL3CCO	81092C	2O 1CL 3	G	0300.00 5000.00 1400.00	1
0.01383246E+03	0.01240141E-01	-0.03510210E-05	0.04103960E-09	-0.01475220E-13	2
0.07499342E+07	-0.03691505E+03	0.05016825E+02	0.02899350E+00	-0.03563990E-03	3
0.02082488E-06	-0.04661957E-10	0.07524076E+07	0.08141487E+02		4
CL3CO	53090C	1O 1CL 3	G	0300.00 5000.00 1500.00	1
0.01208526E+03	0.07759038E-02	-0.02700075E-05	0.04346263E-09	-0.02671642E-13	2
-0.06464079E+05	-0.03099432E+03	0.04548646E+02	0.02463303E+00	-0.02974898E-03	3
0.01647154E-06	-0.03433021E-10	-0.04416522E+05	0.07360693E+02		4

CL3COH	53090C	1O	1H	1CL	3G	0300.00	5000.00	1500.00	1
0.01285985E+03	0.01588083E-01	-0.03377500E-05	0.02031362E-09	0.08017922E-14					2
-0.03807818E+06	-0.03561945E+03	0.04269172E+02	0.02791723E+00	-0.03272753E-03					3
0.01828272E-06	-0.03882978E-10	-0.03558880E+06	0.08521096E+02						4
CL3SICH3	40992H	3C	1SI	1CL	3G	0300.00	4000.00	1500.00	1
0.01572988E+03	0.03373817E-01	-0.04472970E-05	-0.09359551E-09	0.01995442E-12					2
-0.07539927E+06	-0.05017697E+03	0.06708039E+02	0.02724465E+00	-0.02730290E-03					3
0.01457864E-06	-0.03116460E-10	-0.07231476E+06	-0.02328694E+02						4
CL3SISI	40992SI	2CL	3		G	0300.00	4000.00	1500.00	1
0.01263015E+03	0.04310339E-02	-0.02248369E-05	0.05573034E-09	-0.05229996E-13					2
-0.01723335E+06	-0.02767933E+03	0.08429942E+02	0.01496243E+00	-0.01942087E-03					3
0.01125326E-06	-0.02414611E-10	-0.01619796E+06	-0.06711706E+02						4
CL3SISICL	40992SI	2CL	4		G	0300.00	4000.00	1500.00	1
0.01503498E+03	0.05376136E-02	-0.02788507E-05	0.06889626E-09	-0.06454867E-13					2
-0.05496076E+06	-0.03460735E+03	0.09721335E+02	0.01889709E+00	-0.02451039E-03					3
0.01419597E-06	-0.03045164E-10	-0.05364875E+06	-0.08073287E+02						4
CLCCCL	40992C	2CL	2		G	0300.00	4000.00	1500.00	1
0.09105373E+02	0.09281996E-02	-0.01948371E-05	0.01590377E-10	0.02472937E-13					2
0.02507216E+06	-0.02072870E+03	0.05118707E+02	0.01243668E+00	-0.01386540E-03					3
0.07609302E-07	-0.01615959E-10	0.02631398E+06	0.03298777E+00						4
CLCCO	53090C	2O	1CL	1	G	0300.00	5000.00	1500.00	1
0.09368609E+02	0.03733935E-02	-0.01286981E-05	0.01206469E-09	0.09220283E-15					2
0.01762808E+06	-0.02046752E+03	0.04417443E+02	0.01129365E+00	-0.01013488E-03					3
0.04661357E-07	-0.09098661E-11	0.01952423E+06	0.06539246E+02						4
CLCH2OH	53090C	1H	3O	1CL	1G	0300.00	5000.00	1500.00	1
0.09750194E+02	0.02974385E-01	-0.03450482E-05	-0.06010047E-09	0.01089784E-12					2
-0.03248678E+06	-0.02345467E+03	0.08330910E+01	0.02358999E+00	-0.02137297E-03					3
0.01105808E-06	-0.02402402E-10	-0.02905351E+06	0.02503745E+03						4
CLCO	40992C	1O	1CL	1	G	0300.00	4000.00	1500.00	1
0.06134827E+02	0.05369294E-02	-0.07583742E-06	-0.01514557E-09	0.03376080E-13					2
-0.05363338E+05	-0.03198172E+02	0.04790425E+02	0.03165209E-01	-0.02098201E-04					3
0.07703306E-08	-0.01346351E-11	-0.04812905E+05	0.04257480E+02						4
CLCOH	53090C	1H	1O	1CL	1G	0300.00	5000.00	1500.00	1
0.07642908E+02	0.01507814E-01	-0.02651581E-05	-0.01466785E-09	0.04797316E-13					2
-0.02511908E+05	-0.01405046E+03	0.02037663E+02	0.01733328E+00	-0.01936443E-03					3
0.01099366E-06	-0.02427341E-10	-0.06596141E+04	0.01538422E+03						4
CLH2CO	53090C	1H	2O	1CL	1G	0300.00	5000.00	1500.00	1
0.09104530E+02	0.02130629E-01	-0.02994563E-05	-0.02733652E-09	0.06437597E-13					2
-0.05255641E+05	-0.02258799E+03	0.08437505E+01	0.02258903E+00	-0.02217447E-03					3
0.01165204E-06	-0.02487574E-10	-0.02264707E+05	0.02176388E+03						4
CLHCO	40992H	1C	1O	1CL	1G	0300.00	4000.00	1500.00	1
0.07132409E+02	0.01686027E-01	-0.02034320E-05	-0.05804520E-09	0.01152902E-12					2
-0.02522232E+06	-0.01150137E+03	0.02378612E+02	0.01278870E+00	-0.01094130E-03					3
0.05089666E-07	-0.09985544E-11	-0.02348305E+06	0.01417749E+03						4
CLO	40992O	1CL	1		G	0300.00	4000.00	1500.00	1
0.04320627E+02	0.01730970E-02	-0.07157875E-06	0.01424639E-09	-0.01115543E-13					2
0.01328601E+06	0.01764362E+02	0.02918696E+02	0.04664857E-01	-0.05654826E-04					3
0.03131108E-07	-0.06515478E-11	0.01365989E+06	0.08877238E+02						4
CLOCL	53090O	1CL	2		G	0300.00	5000.00	1500.00	1
0.06635186E+02	0.03284434E-02	-0.01225328E-05	0.02123621E-09	-0.01404377E-13					2
0.07672352E+05	-0.06410996E+02	0.03397880E+02	0.01080127E+00	-0.01324655E-03					3
0.07392960E-07	-0.01546583E-10	0.08527797E+05	0.09981834E+02						4
CLOO	40992O	2CL	1		G	0300.00	4000.00	1500.00	1
0.06500858E+02	0.04259430E-02	-0.01471496E-05	0.02312042E-09	-0.01357033E-13					2
0.01465068E+06	-0.05831007E+02	0.03097113E+02	0.01088530E+00	-0.01274586E-03					3
0.06909658E-07	-0.01419679E-10	0.01560137E+06	0.01159355E+03						4
CLSI (CH3) 2	40992H	6C	2SI	1CL	1G	0300.00	4000.00	1500.00	1
0.01602072E+03	0.06121766E-01	-0.05697358E-05	-0.02685516E-08	0.04764446E-12					2
-0.02023771E+06	-0.05448286E+03	0.04366292E+02	0.03146501E+00	-0.02442313E-03					3
0.01155763E-06	-0.02441972E-10	-0.01561856E+06	0.09415220E+02						4
CLSI (CH3) 2CH2	40992H	8C	3SI	1CL	1G	0300.00	4000.00	1500.00	1
0.02115100E+03	0.08018265E-01	-0.07924248E-05	-0.03295050E-08	0.05955233E-12					2
-0.02795355E+06	-0.07954995E+03	0.05283182E+02	0.04510586E+00	-0.03881938E-03					3
0.01972924E-06	-0.04266615E-10	-0.02191153E+06	0.06553031E+02						4
CLSI (CH3) 3	40992H	9C	3SI	1CL	1G	0300.00	4000.00	1500.00	1
0.02209311E+03	0.09120019E-01	-0.08258094E-05	-0.04093090E-08	0.07203542E-12					2

-0.05338834E+06-0.08746922E+03 0.05151450E+02 0.04536455E+00-0.03440035E-03	3
0.01610968E-06-0.03411234E-10-0.04659624E+06 0.05658041E+02	4
CLSICH3 40992H 3C 1SI 1CL 1G 0300.00 4000.00 1500.00	1
0.01002062E+03 0.03097435E-01-0.03221687E-05-0.01222123E-08 0.02253457E-12	2
-0.05623578E+05-0.02357626E+03 0.03485850E+02 0.01832800E+00-0.01572477E-03	3
0.07852071E-07-0.01669997E-10-0.03149803E+05 0.01186709E+03	4
CLSISI 40992SI 2CL 1 G 0300.00 4000.00 1500.00	1
0.06847303E+02 0.01844250E-02-0.09793979E-06 0.02440659E-09-0.02287823E-13	2
0.04772443E+06-0.03339368E+02 0.05234557E+02 0.05788035E-01-0.07516996E-04	3
0.04356402E-07-0.09346885E-11 0.04811932E+06 0.04702599E+02	4
CLSISICL 40992SI 2CL 2 G 0300.00 4000.00 1500.00	1
0.01008343E+03-0.01216815E-02-0.01555866E-05 0.07247150E-09-0.08633006E-13	2
0.01376083E+06-0.01644862E+03 0.07022588E+02 0.01136420E+00-0.01558778E-03	3
0.08961882E-07-0.01874769E-10 0.01437523E+06-0.01570360E+02	4
CN 121286C 1N 1 G 0300.00 5000.00 1000.00	1
0.03720120E+02 0.01518351E-02 0.01987381E-05-0.03798371E-09 0.01328230E-13	2
0.05111626E+06 0.02888597E+02 0.03663204E+02-0.01156529E-01 0.02163409E-04	3
0.01854208E-08-0.08214695E-11 0.05128118E+06 0.03739016E+02	4
CN+ 121286C 1N 1E -1 G 0300.00 5000.00 1000.00	1
0.03701463E+02 0.07482931E-02-0.01790173E-05 0.02366368E-09-0.01437037E-13	2
0.02155966E+07 0.04108678E+02 0.03118657E+02 0.01553258E-01-0.09487764E-05	3
0.01479501E-07-0.09096763E-11 0.02158512E+07 0.07456254E+02	4
CN- 121286C 1N 1E 1 G 0300.00 5000.00 1000.00	1
0.02981277E+02 0.01464773E-01-0.05672737E-05 0.01017623E-08-0.06870931E-13	2
0.06346098E+05 0.06171693E+02 0.03278995E+02 0.01464192E-01-0.03925899E-04	3
0.05629875E-07-0.02473497E-10 0.06279509E+05 0.04568972E+02	4
CN2 121686C 1N 2 G 0300.00 5000.00 1000.00	1
0.05567064E+02 0.02100501E-01-0.09010517E-05 0.01718572E-08-0.01206255E-12	2
0.05489968E+06-0.05630054E+02 0.03039964E+02 0.08812105E-01-0.07605508E-04	3
0.03554357E-07-0.08746100E-11 0.05563268E+06 0.07555298E+02	4
CNN 121286C 1N 2 G 0300.00 5000.00 1000.00	1
0.04785930E+02 0.02559554E-01-0.01003133E-04 0.01807149E-08-0.01227383E-12	2
0.06870411E+06-0.02953957E+01 0.03524436E+02 0.07271923E-01-0.08272698E-04	3
0.05628705E-07-0.01641576E-10 0.06899647E+06 0.05932445E+02	4
CNO 103190C 1N 1O 1 G 0300.00 4000.00 1500.00	1
0.06328598E+02 0.07390401E-02-0.01110761E-05-0.01846498E-09 0.04400816E-13	2
0.04683387E+06-0.09091839E+02 0.03819863E+02 0.06416255E-01-0.05303312E-04	3
0.02308211E-07-0.04256414E-11 0.04775979E+06 0.04507300E+02	4
CO 121286C 1O 1 G 0300.00 5000.00 1000.00	1
0.03025078E+02 0.01442689E-01-0.05630828E-05 0.01018581E-08-0.06910952E-13	2
-0.01426835E+06 0.06108218E+02 0.03262452E+02 0.01511941E-01-0.03881755E-04	3
0.05581944E-07-0.02474951E-10-0.01431054E+06 0.04848897E+02	4
CO2 121286C 1O 2 G 0300.00 5000.00 1000.00	1
0.04453623E+02 0.03140169E-01-0.01278411E-04 0.02393997E-08-0.01669033E-12	2
-0.04896696E+06-0.09553959E+01 0.02275725E+02 0.09922072E-01-0.01040911E-03	3
0.06866687E-07-0.02117280E-10-0.04837314E+06 0.01018849E+03	4
CO2- 121286C 1O 2E 1 G 0300.00 5000.00 1000.00	1
0.04610574E+02 0.02532962E-01-0.01070165E-04 0.02026771E-08-0.01424958E-12	2
-0.05479882E+06 0.01449630E+02 0.02637077E+02 0.07803230E-01-0.08196187E-04	3
0.06537897E-07-0.02520220E-10-0.05416773E+06 0.01188955E+03	4
COS 121286C 1O 1S 1 G 0300.00 5000.00 1000.00	1
0.05191925E+02 0.02506123E-01-0.01024396E-04 0.01943914E-08-0.01370800E-12	2
-0.01846210E+06-0.02825755E+02 0.02858531E+02 0.09515458E-01-0.08884915E-04	3
0.04220994E-07-0.08557340E-11-0.01785145E+06 0.09081989E+02	4
CS 121686C 1S 1 G 0300.00 5000.00 1000.00	1
0.03737431E+02 0.08180451E-02-0.03178918E-05 0.05356801E-09-0.02886195E-13	2
0.03247725E+06 0.03576557E+02 0.02938623E+02 0.02724352E-01-0.02397707E-04	3
0.01689501E-07-0.06665050E-11 0.03273992E+06 0.07848720E+02	4
CS2 121286C 1S 2 G 0300.00 5000.00 1000.00	1
0.05930515E+02 0.01813645E-01-0.07492172E-05 0.01445892E-08-0.01032638E-12	2
0.01205117E+06-0.06093910E+02 0.03566139E+02 0.08374928E-01-0.06835704E-04	3
0.02091214E-07-0.06737193E-12 0.01268848E+06 0.06085967E+02	4
CSICL 40992C 1SI 1CL 1 G 0300.00 4000.00 1500.00	1
0.06817655E+02 0.02139344E-02-0.01117811E-05 0.02768133E-09-0.02593011E-13	2
0.07133105E+06-0.04934821E+02 0.04809756E+02 0.07155653E-01-0.09274105E-04	3
0.05368218E-07-0.01150991E-10 0.07182609E+06 0.05089754E+02	4

CSICL2	40992C	1SI	1CL	2	G	0300.00	4000.00	1500.00	1
	0.09603536E+02	0.04212005E-02	0.02008617E-05	0.04653654E-09	0.04174779E-13				2
	0.04167197E+06	-0.01686119E+03	0.05482765E+02	0.01432904E+00	-0.01824531E-03				3
	0.01044588E-06	-0.02224179E-10	0.04271677E+06	0.03823593E+02					4
CSICL3	40992C	1SI	1CL	3	G	0300.00	4000.00	1500.00	1
	0.01250544E+03	0.05339218E-02	0.02588613E-05	0.06075307E-09	0.05497769E-13				2
	0.04346089E+04	-0.02851950E+03	0.07246579E+02	0.01837148E+00	-0.02348583E-03				3
	0.01347935E-06	-0.02874547E-10	0.01760441E+05	-0.02151092E+02					4
CSIH2CL	40992H	2C	1SI	1CL	1G	0300.00	4000.00	1500.00	1
	0.01027485E+03	0.01774759E-01	0.03308189E-05	-0.01554251E-09	0.07008815E-13				2
	0.04915449E+06	-0.02589174E+03	0.02180376E+02	0.02405210E+00	-0.02551666E-03				3
	0.01345591E-06	-0.02782039E-10	0.05175432E+06	0.01659754E+03					4
CSIHCL	40992H	1C	1SI	1CL	1G	0300.00	4000.00	1500.00	1
	0.08584251E+02	0.09503299E-02	0.01990512E-05	0.07276089E-11	0.02697011E-13				2
	0.05701632E+06	-0.01616263E+03	0.04195792E+02	0.01336658E+00	-0.01458110E-03				3
	0.07822924E-07	-0.01632113E-10	0.05839343E+06	0.06755654E+02					4
CSIHCL2	40992H	1C	1SI	1CL	2G	0300.00	4000.00	1500.00	1
	0.01133022E+03	0.01200867E-01	0.03112842E-05	0.02565133E-09	0.05146234E-14				2
	0.02764986E+06	-0.02737920E+03	0.04205701E+02	0.02278870E+00	-0.02653546E-03				3
	0.01465130E-06	-0.03083816E-10	0.02972624E+06	0.09294144E+02					4
D	41494D	1			G	0300.00	5000.00	1000.00	1
	0.02500252E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.02592392E+06	0.05785570E+01	0.02500252E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.02592392E+06	0.05785570E+01					4
D2	41494D	2			G	0300.00	5000.00	1000.00	1
	0.02723347E+02	0.01505752E-01	0.05015062E-05	0.08571456E-09	0.05569090E-13				2
	-0.07954394E+04	0.01664985E+02	0.03321112E+02	0.01402023E-01	-0.03851314E-04				3
	0.04705450E-07	-0.01769535E-10	0.01026878E+05	-0.01784515E+02					4
DH	41494D	1H	1		G	0300.00	5000.00	1000.00	1
	0.02824097E+02	0.01100398E-01	0.02642150E-05	0.03340498E-09	0.01499951E-13				2
	-0.07536879E+04	0.01092907E+02	0.03371353E+02	0.09388205E-02	-0.02213857E-04				3
	0.02228393E-07	-0.06325260E-11	0.09928156E+04	-0.02124907E+02					4
DIOXANE	103190C	4H	8O	2	G	0300.00	4000.00	1500.00	1
	0.02168170E+03	0.01049644E+00	-0.01053878E-04	-0.04473945E-08	0.08168288E-12				2
	-0.04922005E+06	-0.09955139E+03	-0.05862900E+02	0.07081444E+00	-0.05458695E-03				3
	0.02315148E-06	-0.04289514E-10	-0.03876477E+06	0.05061959E+03					4
E	120186E	1			G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-0.07453749E+04	-0.01173403E+03	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.07453750E+04	-0.01173403E+03					4
F	121286F	1			G	0300.00	5000.00	1000.00	1
	0.02687459E+02	-0.02010358E-02	0.08597957E-06	-0.01644974E-09	0.01166160E-13				2
	0.08722883E+05	0.03882212E+02	0.02913905E+02	-0.07336339E-02	0.05571015E-05				3
	-0.02666871E-08	0.08643255E-12	0.08651201E+05	0.02677115E+02					4
F2	121286F	2			G	0300.00	5000.00	1000.00	1
	0.04018308E+02	0.06221479E-02	-0.02420845E-05	0.04742076E-09	0.03418141E-13				2
	-0.01300713E+05	0.01126327E+02	0.02940287E+02	0.03491492E-01	-0.02458208E-04				3
	0.01837073E-08	0.02850917E-11	-0.01010430E+05	0.06694194E+02					4
F2SINH	42489SI	1N	1F	2H	1G	0300.00	3000.00	1000.00	1
	0.01004830E+03	0.01983144E-01	-0.02703169E-05	-0.01767853E-08	0.04444368E-12				2
	-0.07739741E+06	-0.02303889E+03	0.04951547E+02	0.01329636E+00	-0.02098648E-04				3
	-0.01007276E-06	0.05552286E-10	-0.07597541E+06	0.03690891E+02					4
F3SIN	22790F	3SI	1N	1	G	0300.00	4000.00	1000.00	1
	0.01151242E+03	0.01115029E-01	-0.01605465E-05	-0.05271933E-09	0.01160900E-12				2
	-0.01045919E+07	-0.02981224E+03	0.06028419E+02	0.01278681E+00	-0.01878856E-04				3
	-0.09695426E-07	0.05184848E-10	-0.01029950E+07	-0.08217831E+01					4
FNNF	42489F	2N	2		G	0300.00	3000.00	1000.00	1
	0.07255211E+02	0.02274410E-01	-0.02793346E-05	-0.02203844E-08	0.05359234E-12				2
	0.06360353E+05	-0.01094248E+03	0.03127143E+02	0.01057134E+00	-0.09746112E-05				3
	-0.07208357E-07	0.03567978E-10	0.07615831E+05	0.01107465E+03					4
FNO3	121286F	1N	1O	3	G	0300.00	5000.00	1000.00	1
	0.09176275E+02	0.04219072E-01	-0.01835576E-04	0.03553718E-08	-0.02541078E-12				2
	-0.02118639E+05	-0.01934397E+03	0.02985786E+02	0.02094642E+00	-0.01652733E-03				3
	0.04318770E-07	0.01660784E-11	-0.04237215E+04	0.01266793E+03					4
FO	121286F	1O	1		G	0300.00	5000.00	1000.00	1
	0.03913735E+02	0.07210714E-02	-0.02796614E-05	0.05337821E-09	0.03720184E-13				2

0.01180141E+06	0.03346368E+02	0.02879578E+02	0.03399121E-01	0.02572855E-04	3
0.07422381E-08	-0.04328053E-12	0.01209663E+06	0.08738887E+02		4
FO2	121286F	1O 2	G	0300.00 5000.00	1
0.05678971E+02	0.01442455E-01	-0.06229546E-05	0.01199612E-08	-0.08543416E-13	2
-0.03861836E+04	-0.01941812E+02	0.03872542E+02	0.06409974E-01	-0.05517785E-04	3
0.02232771E-07	-0.03876157E-11	0.01157076E+04	0.07406950E+02		4
FSIN	42489SI	1N 1F 1	G	0300.00 3000.00	1
0.06269572E+02	0.06747867E-02	-0.01241976E-05	-0.04970158E-09	0.01424452E-12	2
0.02533350E+06	-0.04201141E+02	0.04269969E+02	0.05298358E-01	-0.01103802E-04	3
-0.03962805E-07	0.02282982E-10	0.02587238E+06	0.06215038E+02		4
GA	62987GA	1	G	0300.00 1500.00	1
0.02679919E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
0.03368804E+06	0.06788109E+02	0.02679919E+02	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	0.03368804E+06	0.06788109E+02		4
GA2H6	62987GA	2H 6	G	0300.00 1500.00	1
0.06016247E+02	0.01788370E+00	-0.01204229E-05	-0.06487881E-07	0.02075367E-10	2
0.01312548E+06	-0.05228030E+02	-0.03914561E+02	0.04965434E+00	0.07401904E-04	3
-0.01124137E-05	0.08726339E-09	0.01493079E+06	0.04274883E+03		4
GAAS	62987GA	1AS 1	G	0300.00 1500.00	1
0.04471149E+02	0.04238449E-02	-0.02279405E-05	-0.04441172E-10	0.02618952E-12	2
0.04313359E+06	0.06212471E+02	0.03967474E+02	0.02318966E-01	-0.01145452E-04	3
-0.03411431E-07	0.03365821E-10	0.04321919E+06	0.08599628E+02		4
GAAS(3,C)	62987GA	3AS 3	G	0300.00 1500.00	1
0.01485247E+03	0.02959435E-01	-0.07124246E-05	-0.05316048E-08	0.01287321E-11	2
0.01191262E+07	-0.03514144E+03	0.01470189E+03	0.03827728E-01	-0.02945747E-04	3
0.02465370E-07	-0.01520598E-10	0.01191496E+07	-0.03445955E+03		4
GAAS(3,L)	62987GA	3AS 3	G	0300.00 1500.00	1
0.01356850E+03	0.02802435E-01	-0.07969918E-05	-0.06437098E-08	0.01560255E-11	2
0.01248005E+07	-0.01381063E+03	0.01341276E+03	0.03617689E-01	-0.02726209E-04	3
0.01877183E-07	-0.01259178E-10	0.01248265E+07	-0.01309195E+03		4
GAAS(5,C)	62987GA	5AS 5	G	0300.00 1500.00	1
0.02573672E+03	0.05523956E-01	-0.01203468E-04	-0.01043743E-07	0.02528931E-11	2
0.01721381E+07	-0.08254488E+03	0.02546512E+03	0.07014337E-01	-0.04881356E-04	3
0.03825484E-07	-0.02450420E-10	0.01721819E+07	-0.08130267E+03		4
GAAS(5,L)	62987GA	5AS 5	G	0300.00 1500.00	1
0.03045793E+03	0.05403152E-01	-0.01649477E-04	-0.09968842E-08	0.02413154E-11	2
0.02020691E+07	-0.07768010E+03	0.03015255E+03	0.07234394E-01	-0.06497994E-04	3
0.05559585E-07	-0.03339653E-10	0.02021151E+07	-0.07630866E+03		4
GAET	62987GA	1C 2H 5	G	0300.00 1500.00	1
0.05932970E+02	0.01342454E+00	0.04110518E-05	-0.04286069E-07	0.01238710E-10	2
0.06504863E+05	0.03090838E+02	0.01846399E+02	0.02592050E+00	0.05522394E-04	3
-0.04977960E-06	0.03654362E-09	0.07264445E+05	0.02294639E+03		4
GAET2	62987GA	1C 4H 10	G	0300.00 1500.00	1
0.07213832E+02	0.03055228E+00	0.01249451E-04	-0.09990274E-07	0.02881966E-10	2
-0.01392119E+05	-0.07795098E+00	-0.02162930E+02	0.05892512E+00	0.01447145E-03	3
-0.01168602E-05	0.08526654E-09	0.03561841E+04	0.04552626E+03		4
GAET3	62987GA	1C 6H 15	G	0300.00 1500.00	1
0.08436453E+02	0.04804950E+00	0.02119157E-04	-0.01581685E-06	0.04571178E-10	2
-0.01346996E+06	-0.06196490E+02	-0.06544289E+02	0.09332246E+00	0.02364121E-03	3
-0.01874104E-05	0.01367721E-08	-0.01067659E+06	0.06666796E+03		4
GAH	62987GA	1H 1	G	0300.00 1500.00	1
0.03232142E+02	0.01343247E-01	-0.04325499E-06	-0.02791841E-08	0.04973590E-12	2
0.02656060E+06	0.05947896E+02	0.03524579E+02	0.03386213E-02	-0.02064014E-05	3
0.03220999E-07	-0.02936132E-10	0.02651074E+06	0.04554067E+02		4
GAH2	62987GA	1H 2	G	0300.00 1500.00	1
0.03762385E+02	0.03210792E-01	0.02180096E-06	-0.08908393E-08	0.02219063E-11	2
0.01936647E+06	0.05783398E+02	0.03559710E+02	0.03676742E-01	0.06484499E-05	3
-0.03109349E-07	0.01585414E-10	0.01940976E+06	0.06803082E+02		4
GAH3	62987GA	1H 3	G	0300.00 1500.00	1
0.03345476E+02	0.06399313E-01	0.01122996E-05	-0.02065900E-07	0.05780202E-11	2
0.01228185E+06	0.06394842E+02	0.01726154E+02	0.01124739E+00	0.02447527E-04	3
-0.02026314E-06	0.01447000E-09	0.01258620E+06	0.01428445E+03		4
GAME	62987GA	1C 1H 3	G	0300.00 1500.00	1
0.04809857E+02	0.06824207E-01	0.02258235E-05	-0.02018341E-07	0.05736453E-11	2
0.07558677E+05	0.02595904E+02	0.03054537E+02	0.01218640E+00	0.02332213E-04	3
-0.02121866E-06	0.01544226E-09	0.07885869E+05	0.01112878E+03		4

GAME2	62987GA	1C	2H	6	G	0300.00	1500.00	0600.00	1
	0.07068373E+02	0.01421602E+00	0.05120694E-05	-0.04421986E-07	0.01309641E-10				2
	0.05453790E+05	-0.04173960E+02	0.02257655E+02	0.02916446E+00	0.05669861E-04				3
	-0.05709755E-06	0.04268905E-09	0.06341297E+05	0.01915435E+03					4
GAME3	62987GA	1C	3H	9	G	0300.00	1500.00	0600.00	1
	0.08410636E+02	0.02262803E+00	0.01043019E-04	-0.07049611E-07	0.02015308E-10				2
	-0.09087271E+05	-0.01072250E+03	0.02120239E+02	0.04161029E+00	0.09959505E-04				3
	-0.07846792E-06	0.05693396E-09	-0.07911968E+05	0.01988516E+03					4
H	120186H	1			G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.02547163E+06	-0.04601176E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.02547163E+06	-0.04601176E+01					4
H(CH3)SICH2	61991H	6C	2SI	1	G	0300.00	2500.00	1500.00	1
	0.01254527E+03	0.07143719E-01	-0.01146987E-05	-0.08100963E-08	0.01568740E-11				2
	0.07723628E+05	-0.04075435E+03	0.01206249E+02	0.03587271E+00	-0.02971970E-03				3
	0.01379675E-06	-0.02695736E-10	0.01156328E+06	0.01956017E+03					4
H+	120186H	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.01840334E+07	-0.01153862E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.01840334E+07	-0.01153862E+02					4
H-	120186H	1E	1		G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.01596104E+06	-0.01152449E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.01596104E+06	-0.01152449E+02					4
H2	121286H	2			G	0300.00	5000.00	1000.00	1
	0.02991423E+02	0.07000644E-02	-0.05633829E-06	-0.09231578E-10	0.01582752E-13				2
	-0.08350340E+04	-0.01355110E+02	0.03298124E+02	0.08249442E-02	-0.08143015E-05				3
	-0.09475434E-09	0.04134872E-11	-0.01012521E+05	-0.03294094E+02					4
H2ALME	62987AL	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.04898410E+02	0.01358223E+00	0.02611459E-05	-0.04575170E-07	0.01384802E-10				2
	0.08743072E+04	-0.01113117E+02	-0.06283259E+01	0.03089531E+00	0.05774090E-04				3
	-0.06488033E-06	0.04907111E-09	0.01889334E+05	0.02565779E+03					4
H2ASME	62987AS	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.05686213E+02	0.02154422E+00	0.08185248E-05	-0.07069951E-07	0.02101522E-10				2
	0.09331084E+05	-0.06513957E+02	-0.02113506E+02	0.04564229E+00	0.09983227E-04				3
	-0.09399697E-06	0.07014021E-09	0.01077170E+06	0.03132611E+03					4
H2C4O	120189H	2C	4O	1	G	0300.00	4000.00	1000.00	1
	0.01026888E+03	0.04896164E-01	-0.04885081E-05	-0.02708566E-08	0.05107013E-12				2
	0.02346903E+06	-0.02815985E+03	0.04810971E+02	0.01313999E+00	0.09865073E-05				3
	-0.06120720E-07	0.01640003E-10	0.02545803E+06	0.02113424E+02					4
H2CCC	102093H	2C	3		G	0300.00	4000.00	1400.00	1
	0.08266525E+02	0.02728619E-01	-0.02160829E-05	-0.01515161E-08	0.02641695E-12				2
	0.07757192E+06	-0.01864937E+03	0.04212193E+02	0.08954521E-01	-0.01050721E-04				3
	-0.02578513E-07	0.09722836E-11	0.07922349E+06	0.04134299E+02					4
H2CCC(S)	102093H	2C	3		G	0300.00	4000.00	1400.00	1
	0.07904213E+02	0.02907464E-01	-0.02219731E-05	-0.01620844E-08	0.02796013E-12				2
	0.06385167E+06	-0.01810882E+03	0.03794178E+02	0.08761049E-01	-0.07975878E-05				3
	-0.02308045E-07	0.07911151E-11	0.06563580E+06	0.05264196E+02					4
H2CCCCCH	101993H	3C	5		G	0300.00	4000.00	1400.00	1
	0.01440736E+03	0.04424058E-01	-0.03618245E-05	-0.02456408E-08	0.04327859E-12				2
	0.05896103E+06	-0.04775145E+03	0.07441421E+02	0.01585165E+00	-0.02219895E-04				3
	-0.04928038E-07	0.01984559E-10	0.06162266E+06	-0.09047891E+02					4
H2CCCCH	82489C	4H	3		G	0300.00	4000.00	1000.00	1
	0.01131409E+03	0.05014414E-01	-0.05350445E-05	-0.02825309E-08	0.05403279E-12				2
	0.05181211E+06	-0.03062434E+03	0.06545799E+02	0.01242477E+00	0.05603226E-05				3
	-0.05631141E-07	0.01665218E-10	0.05352503E+06	-0.04264082E+02					4
H2CCCCH2	82489C	4H	4		G	0300.00	4000.00	1000.00	1
	0.01062083E+03	0.07199370E-01	-0.06806234E-05	-0.04021185E-08	0.07378498E-12				2
	0.03358798E+06	-0.03193583E+03	0.03849007E+02	0.01713169E+00	0.01644270E-04				3
	-0.07761590E-07	0.01947860E-10	0.03608372E+06	0.05732121E+02					4
H2CCH	82489C	3H	3		G	0300.00	4000.00	1000.00	1
	0.08831047E+02	0.04357195E-01	-0.04109067E-05	-0.02368723E-08	0.04376520E-12				2
	0.03847420E+06	-0.02177919E+03	0.04754200E+02	0.01108028E+00	0.02793323E-05				3
	-0.05479212E-07	0.01949629E-10	0.03988883E+06	0.05854549E+01					4
H2CCCL	53090C	2H	2O	1CL	1G	0300.00	5000.00	1500.00	1
	0.01240462E+03	0.02067658E-01	-0.03889952E-05	-0.03138121E-10	0.04625008E-13				2

-0.01114503E+06-0.03928723E+03 0.01680422E+02 0.03020642E+00-0.03234256E-03	3
0.01779343E-06-0.03877221E-10-0.07395297E+05 0.01777265E+03	4
H2CCH(SICL2H) 40992H 4C 2SI 1CL 2G 0300.00 4000.00 1500.00	1
0.01680247E+03 0.04516342E-01-0.05794312E-05-0.01367868E-08 0.02833862E-12	2
-0.04037858E+06-0.05763375E+03 0.03640801E+02 0.03803764E+00-0.03641732E-03	3
0.01855101E-06-0.03834642E-10-0.03581475E+06 0.01252145E+03	4
H2CCH2OH 103190C 2H 5O 1 G 0300.00 4000.00 1500.00	1
0.01144956E+03 0.05249185E-01-0.04887850E-05-0.02243250E-08 0.03973360E-12	2
-0.07554972E+05-0.03426083E+03 0.01304406E+02 0.02873214E+00-0.02387448E-03	3
0.01166988E-06-0.02450027E-10-0.03718933E+05 0.02078756E+03	4
H2CCHO 103190C 2H 3O 1 G 0300.00 4000.00 1500.00	1
0.09710060E+02 0.03854966E-01-0.04677825E-05-0.01505179E-08 0.02941428E-12	2
-0.02692492E+05-0.02810566E+03 0.02802205E+01 0.02740311E+00-0.02554683E-03	3
0.01306679E-06-0.02750425E-10 0.06682648E+04 0.02239731E+03	4
H2CCHSI 61991H 3C 2SI 1 G 0300.00 2500.00 1500.00	1
0.09386889E+02 0.03941784E-01-0.01316150E-05-0.04081553E-08 0.07971026E-12	2
0.04528924E+06-0.02340680E+03 0.01645904E+02 0.02461474E+00-0.02252401E-03	3
0.01105892E-06-0.02209069E-10 0.04779814E+06 0.01738303E+03	4
H2CCHSIH 61991H 4C 2SI 1 G 0300.00 2500.00 1500.00	1
0.01039415E+03 0.04987864E-01-0.01480904E-05-0.05650110E-08 0.01139073E-11	2
0.03263919E+06-0.02930385E+03 0.01989225E+02 0.02637566E+00-0.02197547E-03	3
0.09982490E-07-0.01893595E-10 0.03544082E+06 0.01531216E+03	4
H2CCHSIH2 61991H 5C 2SI 1 G 0300.00 2500.00 1500.00	1
0.01289871E+03 0.05366252E-01-0.02345064E-05-0.05622057E-08 0.01143224E-11	2
0.02373919E+06-0.04346106E+03 0.04606628E+01 0.03824847E+00-0.03490747E-03	3
0.01656684E-06-0.03180820E-10 0.02773639E+06 0.02208512E+03	4
H2CCHSIH3 61991H 6C 2SI 1 G 0300.00 2500.00 1500.00	1
0.01249653E+03 0.07666553E-01-0.02075339E-05-0.09569749E-08 0.01987112E-11	2
0.04799029E+05-0.04174850E+03 0.07686183E+01 0.03576322E+00-0.02634364E-03	3
0.01032868E-06-0.01717329E-10 0.08811836E+05 0.02100703E+03	4
H2CLSICH3 40992H 5C 1SI 1CL 1G 0300.00 4000.00 1500.00	1
0.01354344E+03 0.04577293E-01-0.04988032E-05-0.01758807E-08 0.03311232E-12	2
-0.03126783E+06-0.04541432E+03 0.02142669E+02 0.03103477E+00-0.02660368E-03	3
0.01286599E-06-0.02646554E-10-0.02699973E+06 0.01636317E+03	4
H2CLSIISICL3 40992H 2SI 2CL 4 G 0300.00 4000.00 1500.00	1
0.01871701E+03 0.01924360E-01-0.04472779E-05 0.02003132E-09 0.03268818E-13	2
-0.08047111E+06-0.05817685E+03 0.08945602E+02 0.03068227E+00-0.03483212E-03	3
0.01910354E-06-0.04027623E-10-0.07751434E+06-0.07537633E+02	4
H2CN 41687H 2C 1N 1 G 0300.00 4000.00 1000.00	1
0.05209703E+02 0.02969291E-01-0.02855589E-05-0.01635550E-08 0.03043259E-12	2
0.02767711E+06-0.04444478E+02 0.02851661E+02 0.05695233E-01 0.01071140E-04	3
-0.01622612E-07-0.02351108E-11 0.02863782E+06 0.08992751E+02	4
H2CNCH2 103190C 2H 4N 1 G 0300.00 4000.00 1500.00	1
0.01065385E+03 0.05191287E-01-0.05816522E-05-0.02206912E-08 0.04101341E-12	2
0.02345063E+06-0.03469895E+03-0.01203076E+01 0.03225369E+00-0.02968723E-03	3
0.01527290E-06-0.03242500E-10 0.02728820E+06 0.02297042E+03	4
H2CNCH2O 103190C 2H 4N 1O 1G 0300.00 4000.00 1500.00	1
0.01327652E+03 0.04830938E-01-0.04858949E-05-0.02009495E-08 0.03640181E-12	2
0.01624962E+06-0.04713094E+03-0.01978522E+01 0.03341279E+00-0.02432022E-03	3
0.09438643E-07-0.01604050E-10 0.02141154E+06 0.02658265E+03	4
H2CNCHO 103190C 2H 3N 1O 1G 0300.00 4000.00 1500.00	1
0.01196792E+03 0.03915428E-01-0.03860933E-05-0.01696877E-08 0.03041050E-12	2
-0.05902236E+05-0.03958545E+03 0.01096066E+02 0.02577215E+00-0.01711630E-03	3
0.05880104E-07-0.08956774E-11-0.01612063E+05 0.02032528E+03	4
H2CNH 41687C 1H 3N 1 G 0300.00 4000.00 1000.00	1
0.05221589E+02 0.04748526E-01-0.04179159E-05-0.02606612E-08 0.04703140E-12	2
0.08657219E+05-0.04500776E+02 0.02365879E+02 0.06780570E-01 0.02423000E-04	3
-0.06157824E-08-0.01615097E-10 0.09971141E+05 0.01230718E+03	4
H2CNNHO 103190C 1H 3N 2O 1G 0300.00 4000.00 1500.00	1
0.01157754E+03 0.04489180E-01-0.05033233E-05-0.01651066E-08 0.03069139E-12	2
0.01986783E+06-0.03656958E+03 0.05954945E+01 0.03239559E+00-0.02993966E-03	3
0.01489054E-06-0.03022863E-10 0.02364485E+06 0.02192790E+03	4
H2CNNO 103190C 1H 2N 2O 1G 0300.00 4000.00 1500.00	1
0.01016234E+03 0.03065936E-01-0.03082820E-05-0.01194424E-08 0.02169867E-12	2
0.02494088E+06-0.02762275E+03 0.02498334E+02 0.01993009E+00-0.01557879E-03	3
0.06838956E-07-0.01313250E-10 0.02786476E+06 0.01417025E+03	4

H2CNNO2	41687H	2C	1N	2O	2G	0300.00	4000.00	1000.00	1
	0.01140794E+03	0.04564542E-01	-0.04600304E-05	-0.02513539E-08	0.04782211E-12				2
	0.01242142E+06	-0.03165238E+03	0.03534317E+02	0.01811272E+00	0.02394018E-05				3
	-0.01080024E-06	0.04222725E-10	0.01509006E+06	0.01131138E+03					4
H2CNO	103190C	1H	2N	1O	1G	0300.00	4000.00	1500.00	1
	0.08485639E+02	0.02633277E-01	-0.03017498E-05	-0.08341916E-09	0.01593977E-12				2
	0.01716434E+06	-0.02052156E+03	0.01045856E+02	0.02126494E+00	-0.01962754E-03				3
	0.09659592E-07	-0.01941069E-10	0.01974611E+06	0.01919718E+03					4
H2CNO2	103190C	1H	2N	1O	2G	0300.00	4000.00	1500.00	1
	0.01127481E+03	0.02584711E-01	-0.03934331E-05	-0.05614969E-09	0.01392400E-12				2
	0.01360470E+06	-0.03461951E+03	0.01165696E+02	0.02890490E+00	-0.02817663E-03				3
	0.01387569E-06	-0.02727595E-10	0.01694546E+06	0.01888293E+03					4
H2CONO	103190C	1H	2N	1O	2G	0300.00	4000.00	1500.00	1
	0.01075754E+03	0.02983288E-01	-0.04123564E-05	-0.08096724E-09	0.01720195E-12				2
	0.01230253E+06	-0.02976009E+03	0.02120026E+02	0.02709056E+00	-0.02799616E-03				3
	0.01479145E-06	-0.03074997E-10	0.01504327E+06	0.01546092E+03					4
H2GAET	62987GA	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.07187273E+02	0.01867211E+00	0.06156157E-05	-0.06027764E-07	0.01797524E-10				2
	-0.04232757E+05	-0.04686699E+02	0.04124020E+01	0.03972972E+00	0.07979140E-04				3
	-0.08059234E-06	0.06040387E-09	-0.02983932E+05	0.02816148E+03					4
H2GAME	62987GA	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.05831604E+02	0.01222872E+00	0.03033669E-05	-0.03956941E-07	0.01225452E-10				2
	0.05189255E+05	-0.04446614E+02	0.05251130E+01	0.02904695E+00	0.04844148E-04				3
	-0.06097646E-06	0.04672763E-09	0.06158712E+05	0.02122149E+03					4
H2NF	42489H	2N	1F	1	G	0300.00	3000.00	1000.00	1
	0.04143658E+02	0.03805135E-01	-0.02771153E-05	-0.03589717E-08	0.07589549E-12				2
	-0.04891486E+05	0.02309362E+02	0.02597863E+02	0.05882104E-01	0.04938351E-05				3
	-0.01948600E-07	0.03634003E-11	-0.04301253E+05	0.01098289E+03					4
H2NNO	103190H	2N	2O	1	G	0300.00	4000.00	1500.00	1
	0.07759737E+02	0.03025701E-01	-0.02888916E-05	-0.01262990E-08	0.02195026E-12				2
	0.05894193E+05	-0.01647713E+03	0.02088916E+02	0.01684997E+00	-0.01428977E-03				3
	0.06830147E-07	-0.01368985E-10	0.07907340E+05	0.01394381E+03					4
H2NO	102290H	2N	1O	1	G	0300.00	4000.00	1500.00	1
	0.05673346E+02	0.02298837E-01	-0.01774446E-05	-0.01103482E-08	0.01859762E-12				2
	0.05569325E+05	-0.06153540E+02	0.02530590E+02	0.08596035E-01	-0.05471030E-04				3
	0.02276249E-07	-0.04648073E-11	0.06868030E+05	0.01126651E+03					4
H2NOH	103190H	3N	1O	1	G	0300.00	4000.00	1500.00	1
	0.06764633E+02	0.03047036E-01	-0.02777798E-05	-0.01250487E-08	0.02191094E-12				2
	-0.09026701E+05	-0.01269845E+03	0.01407003E+02	0.01658498E+00	-0.01463594E-03				3
	0.07318354E-07	-0.01511897E-10	-0.07158596E+05	0.01589649E+03					4
H2O	20387H	2O	1	G	0300.00	5000.00	1000.00	1	
	0.02672146E+02	0.03056293E-01	-0.08730260E-05	0.01200996E-08	-0.06391618E-13				2
	-0.02989921E+06	0.06862817E+02	0.03386842E+02	0.03474982E-01	-0.06354696E-04				3
	0.06968581E-07	-0.02506588E-10	0.03020811E+06	0.02590233E+02					4
H2O(L)	120186H	2O	1	L	0273.15	1000.00	1000.00	1	
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.00000000E+00	0.00000000E+00	0.01271278E+03	-0.01766279E+00	-0.02255666E-03				3
	0.02082091E-05	-0.02407861E-08	-0.03748320E+06	-0.05911535E+03					4
H2O(S)	120186H	2O	1	S	0200.00	0273.15	0273.15	1	
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.00000000E+00	0.00000000E+00	-0.03926933E+00	0.01692042E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.03594958E+06	0.05693378E+01					4
H2O2	120186H	2O	2	G	0300.00	5000.00	1000.00	1	
	0.04573167E+02	0.04336136E-01	-0.01474689E-04	0.02348904E-08	-0.01431654E-12				2
	-0.01800696E+06	0.05011370E+01	0.03388754E+02	0.06569226E-01	-0.01485013E-05				3
	-0.04625806E-07	0.02471515E-10	-0.01766315E+06	0.06785363E+02					4
H2S	121286H	2S	1	G	0300.00	5000.00	1000.00	1	
	0.02883147E+02	0.03827835E-01	-0.01423398E-04	0.02497999E-08	-0.01660273E-12				2
	-0.03480743E+05	0.07258162E+02	0.03071029E+02	0.05578261E-01	-0.01030967E-03				3
	0.01201953E-06	-0.04838370E-10	-0.03559826E+05	0.05935226E+02					4
H2SI(CH3)2	61991H	8C	2SI	1	G	0300.00	2500.00	1500.00	1
	0.01362000E+03	0.01024457E+00	-0.01528107E-05	-0.01329179E-07	0.02717974E-11				2
	-0.01781386E+06	-0.04695844E+03	0.02005893E+02	0.03638380E+00	-0.02273374E-03				3
	0.07691266E-07	-0.01156681E-10	-0.01364280E+06	0.01583265E+03					4
H2SI(CH3)CH2	61991H	7C	2SI	1	G	0300.00	2500.00	1500.00	1
	0.01388829E+03	0.07937538E-01	-0.01559644E-05	-0.09324826E-08	0.01847251E-11				2



0.06767195E+05-0.04464997E+03	0.01980449E+02	0.03727036E+00-0.02944759E-03	3
0.01312558E-06-0.02507859E-10	0.01087973E+06	0.01898102E+03	4
H2SI (NH2) 2	22790SI 1H 6N 2	G 0300.00 4000.00 1000.00	1
0.01302179E+03	0.06465444E-01-0.05816746E-05-0.03484493E-08	0.06340675E-12	2
-0.02357071E+06-0.04132570E+03	0.05615307E+02	0.02079854E+00-0.09999530E-05	3
-0.01288525E-06	0.06091866E-10-0.02126283E+06-0.01615658E+02		4
H2SIC	61991H 2C 1SI 1	G 0300.00 2500.00 1500.00	1
0.07319671E+02	0.01729952E-01-0.01346466E-05-0.01450487E-08	0.03000643E-12	2
0.08125478E+06-0.01320432E+03	0.02408167E+02	0.01437372E+00-0.01331203E-03	3
0.06387472E-07-0.01244523E-10	0.08289031E+06	0.01283748E+03	4
H2SICCH	61991H 3C 2SI 1	G 0300.00 2500.00 1500.00	1
0.01091422E+03	0.03001577E-01-0.01622344E-05-0.02466767E-08	0.04595260E-12	2
0.04137118E+06-0.03153165E+03	0.02952641E+02	0.02407857E+00-0.02313898E-03	3
0.01172227E-06-0.02393835E-10	0.04400800E+06	0.01054929E+03	4
H2SICH	61991H 3C 1SI 1	G 0300.00 2500.00 1500.00	1
0.08489276E+02	0.02348812E-01-0.01091163E-05-0.02027972E-08	0.03759264E-12	2
0.04973382E+06-0.01845097E+03	0.03442743E+02	0.01542521E+00-0.01429096E-03	3
0.07252204E-07-0.01507009E-10	0.05145786E+06	0.08363421E+02	4
H2SICH2	61991H 4C 1SI 1	G 0300.00 2500.00 1500.00	1
0.09303939E+02	0.04006038E-01-0.09702324E-06-0.03997739E-08	0.07350215E-12	2
0.01649066E+06-0.02623845E+03	0.01049782E+02	0.02562277E+00-0.02324392E-03	3
0.01142315E-06-0.02295441E-10	0.01922778E+06	0.01743860E+03	4
H2SICH3	61991H 5C 1SI 1	G 0300.00 2500.00 1500.00	1
0.08991115E+02	0.06006339E-01-0.01118591E-05-0.07745983E-08	0.01594429E-11	2
0.01270233E+06-0.02218700E+03	0.02094419E+02	0.02127010E+00-0.01294390E-03	3
0.04156964E-07-0.05854213E-11	0.01520143E+06	0.01518517E+03	4
H2SIN	22790H 2SI 1N 1	G 0300.00 4000.00 1000.00	1
0.06826533E+02	0.02125460E-01-0.02343132E-05-0.01166339E-08	0.02277273E-12	2
0.07253673E+06-0.01052162E+03	0.03549344E+02	0.07311005E-01	3
-0.03682945E-07	0.01121511E-10	0.07370656E+06	4
H2SINH	42489SI 1N 1H 3	G 0300.00 3000.00 1000.00	1
0.06588295E+02	0.04903194E-01-0.04944720E-05-0.05014630E-08	0.01139470E-11	2
0.01809794E+06-0.09522970E+02	0.02822196E+02	0.01245518E+00-0.08350819E-05	3
-0.07411814E-07	0.03579019E-10	0.01923616E+06	4
H2SINH2	42489SI 1N 1H 4	G 0300.00 3000.00 1000.00	1
0.07392047E+02	0.05476841E-01-0.04453276E-05-0.05236661E-08	0.01138390E-11	2
0.01136858E+06-0.01138050E+03	0.04053223E+02	0.01182231E+00-0.04348128E-05	3
-0.06225818E-07	0.02798829E-10	0.01241971E+06	4
H2SINH3	121386SI 1H 5N 1	G 0300.00 4000.00 1000.00	1
0.08711392E+02	0.05909106E-01-0.05436615E-05-0.03248350E-08	0.05960257E-12	2
0.08441694E+05-0.01933470E+03	0.04269730E+02	0.01125224E+00	3
-0.03578373E-07-0.08372202E-12	0.01022204E+06	0.05876736E+02	4
H2SISIH2	42489SI 2H 4	G 0300.00 3000.00 1000.00	1
0.08986817E+02	0.05405047E-01-0.05214022E-05-0.05313742E-08	0.01188727E-11	2
0.02832748E+06-0.02004478E+03	0.05133186E+02	0.01252855E+00-0.04620421E-05	3
-0.06606075E-07	0.02864345E-10	0.02956915E+06	4
H3ASGAET3	62987AS 1GA 1C 6H 18G	0300.00 1500.00 0600.00	1
0.08508501E+02	0.05632369E+00	0.02524140E-04-0.01861451E-06	2
-0.01085517E+06-0.03399858E+02-0.08974745E+02	0.01090516E+01	0.02811457E-03	3
-0.02195513E-05	0.01599734E-08-0.07592761E+05	0.08165459E+03	4
H3ASGAME3	62987AS 1GA 1C 3H 12G	0300.00 1500.00 0600.00	1
0.01125499E+03	0.03159753E+00	0.01177904E-04-0.01013352E-06	2
-0.07280344E+05-0.02238730E+03	0.01267161E+02	0.06214586E+00	3
-0.01220044E-05	0.08982019E-09-0.05425619E+05	0.02613306E+03	4
H3CONHO	103190C 1H 4N 1O 2G	0300.00 4000.00 1500.00	1
0.01249270E+03	0.04773900E-01-0.04717255E-05-0.01987935E-08	0.03599460E-12	2
-0.02354754E+05-0.03945442E+03	0.01930733E+02	0.02865910E+00-0.02313063E-03	3
0.01068402E-06-0.02139376E-10	0.01638891E+05	0.01796108E+03	4
H3SIC	61991H 3C 1SI 1	G 0300.00 2500.00 1500.00	1
0.08536022E+02	0.02944748E-01-0.01752614E-05-0.03061316E-08	0.06463710E-12	2
0.07066730E+06-0.02041360E+03	0.01037017E+02	0.02192253E+00-0.01926062E-03	3
0.08725014E-07-0.01615505E-10	0.07315849E+06	0.01939904E+03	4
H3SICCH	61991H 4C 2SI 1	G 0300.00 2500.00 1500.00	1
0.01193845E+03	0.04298239E-01-0.01882154E-05-0.04212272E-08	0.08245783E-12	2
0.02161639E+06-0.03978125E+03	0.01692389E+02	0.03078862E+00-0.02808630E-03	3
0.01359918E-06-0.02690423E-10	0.02503587E+06	0.01453670E+03	4

H3SICH	61991H	4C	1SI	1	G	0300.00	2500.00	1500.00	1
	0.09747808E+02	0.03532863E-01	-0.01540271E-05	-0.03539077E-08	0.06992248E-12				2
	0.04253036E+06	-0.02504347E+03	0.01710027E+02	0.02413212E+00	-0.02164005E-03				3
	0.01035470E-06	-0.02035579E-10	0.04522928E+06	0.01762908E+03					4
H3SICH2	61991H	5C	1SI	1	G	0300.00	2500.00	1500.00	1
	0.01050164E+03	0.04907525E-01	-0.01523178E-05	-0.05436598E-08	0.01082455E-11				2
	0.01632252E+06	-0.02911264E+03	0.01199673E+02	0.02828259E+00	-0.02394311E-03				3
	0.01103518E-06	-0.02125819E-10	0.01948167E+06	0.02041804E+03					4
H3SICH3	61991H	6C	1SI	1	G	0300.00	2500.00	1500.00	1
	0.01022214E+03	0.07221275E-01	-0.01482544E-05	-0.09419140E-08	0.01956175E-11				2
	-0.08301660E+05	-0.03163487E+03	0.01240228E+02	0.02729962E+00	-0.01707597E-03				3
	0.05502474E-07	-0.07521465E-11	-0.05090007E+05	0.01692759E+03					4
H3SIN	22790H	3SI	1N	1	G	0300.00	4000.00	1000.00	1
	0.07964213E+02	0.03355633E-01	-0.03579695E-05	-0.01889818E-08	0.03650912E-12				2
	0.01148697E+07	-0.01924110E+03	0.02790629E+02	0.01134566E+00	0.08321879E-05				3
	-0.05845045E-07	0.01685969E-10	0.01167357E+07	0.09384630E+02					4
H3SINH	42489SI	1N	1H	4	G	0300.00	3000.00	1000.00	1
	0.07697340E+02	0.05657943E-01	-0.05209306E-05	-0.05617966E-08	0.01263502E-11				2
	0.02282005E+06	-0.01330379E+03	0.02778390E+02	0.01510711E+00	-0.06734261E-05				3
	-0.08928515E-07	0.04115347E-10	0.02435913E+06	0.01309386E+03					4
H3SISIH	111191H	4SI	2	G	0300.00	4000.00	1500.00	1	
	0.01127202E+03	0.02538145E-01	-0.02998472E-05	-0.09465367E-09	0.01855053E-12				2
	0.03297169E+06	-0.03264598E+03	0.03698707E+02	0.01870180E+00	-0.01430704E-03				3
	0.06005836E-07	-0.01116293E-10	0.03590825E+06	0.08825191E+02					4
H3SISIH3	42489SI	2H	6	G	0300.00	3000.00	1000.00	1	
	0.01068273E+03	0.08221416E-01	-0.08096035E-05	-0.08337975E-08	0.01908205E-11				2
	0.05316920E+05	-0.03082188E+03	0.03898290E+02	0.01977415E+00	0.01791014E-05				3
	-0.01033168E-06	0.03931699E-10	0.07621719E+05	0.06227022E+02					4
HALME	62987AL	1C	1H	4	G	0300.00	1500.00	0600.00	1
	0.04812273E+02	0.01029645E+00	0.02582808E-05	-0.03323597E-07	0.09884584E-11				2
	0.01176673E+06	0.09557062E+01	0.01118789E+02	0.02180038E+00	0.04120785E-04				3
	-0.04366690E-06	0.03273825E-09	0.01244736E+06	0.01886107E+03					4
HALME2	62987AL	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.05705172E+02	0.01924317E+00	0.06377855E-05	-0.06346800E-07	0.01896800E-10				2
	-0.06049865E+05	-0.06331378E+01	-0.01494261E+02	0.04158568E+00	0.08686772E-04				3
	-0.08604142E-06	0.06447653E-09	-0.04722517E+05	0.03427725E+03					4
HASALME	62987AS	1AL	1C	1H	4G	0300.00	1500.00	0600.00	1
	0.06956539E+02	0.01061278E+00	0.02440154E-05	-0.03297737E-07	0.01020004E-10				2
	0.02582506E+06	-0.08625792E+01	0.02544859E+02	0.02465795E+00	0.03677808E-04				3
	-0.05008894E-06	0.03848384E-09	0.02663010E+06	0.02046859E+03					4
HASGAET	62987AS	1GA	1C	2H	6G	0300.00	1500.00	0600.00	1
	0.06336445E+02	0.02340603E+00	0.09066638E-05	-0.07519059E-07	0.01828115E-10				2
	0.03184605E+06	0.05812180E+02	0.05642724E+02	0.02296739E+00	0.01094867E-03				3
	-0.02449038E-06	0.09602701E-10	0.03204718E+06	0.09675533E+02					4
HASGAME	62987AS	1GA	1C	1H	4G	0300.00	1500.00	0600.00	1
	0.07507970E+02	0.09277900E-01	0.01891932E-05	-0.02769887E-07	0.07996070E-11				2
	0.03253908E+06	-0.01422608E+02	0.04859127E+02	0.01750423E+00	0.02831996E-04				3
	-0.03107937E-06	0.02299468E-09	0.03302941E+06	0.01142952E+03					4
HASME	62987AS	1C	1H	4	G	0300.00	1500.00	0600.00	1
	0.05753261E+02	0.01841813E+00	0.07493313E-05	-0.05919917E-07	0.01726247E-10				2
	0.01880057E+06	-0.05360325E+02	-0.01575095E+01	0.03649094E+00	0.08332940E-04				3
	-0.07234666E-06	0.05330928E-09	0.01989792E+06	0.02335316E+03					4
HASME2	62987AS	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.05850437E+02	0.01841766E+00	0.08066845E-05	-0.05868715E-07	0.01726428E-10				2
	0.06450535E+05	0.03909152E+01	-0.02908405E+01	0.03729577E+00	0.08335855E-04				3
	-0.07455611E-06	0.05527881E-09	0.07587766E+05	0.03020451E+03					4
HCCCHCCH	101993H	3C	5	G	0300.00	4000.00	1400.00	1	
	0.01412247E+03	0.04593411E-01	-0.03738175E-05	-0.02574329E-08	0.04539160E-12				2
	0.06249257E+06	-0.04722335E+03	0.06854796E+02	0.01699404E+00	-0.02582284E-04				3
	-0.05488765E-07	0.02281481E-10	0.06515364E+06	-0.07133854E+02					4
HCCCL	40992H	1C	2CL	1	G	0300.00	4000.00	1500.00	1
	0.07743241E+02	0.01618655E-01	-0.02465935E-05	-0.02909336E-09	0.07522752E-13				2
	0.02472494E+06	-0.01686593E+03	0.02969338E+02	0.01583152E+00	-0.01787078E-03				3
	0.01017728E-06	-0.02231985E-10	0.02620733E+06	0.07906791E+02					4
HCCHCCH	82489C	4H	3	G	0300.00	4000.00	1000.00	1	
	0.01075274E+03	0.05381153E-01	-0.05549638E-05	-0.03052266E-08	0.05761740E-12				2

0.06121419E+06-0.02973025E+03	0.04153882E+02	0.01726287E+00-0.02389374E-05	3
-0.01018700E-06	0.04340505E-10	0.06338071E+06	4
HCCO	32387H	1C 2O 1 G 0300.00 4000.00	1
0.06758073E+02	0.02000400E-01-0.02027607E-05-0.01041132E-08	0.01965165E-12	2
0.01901513E+06-0.09071262E+02	0.05047965E+02	0.04453478E-01	3
-0.01482095E-07	0.02250742E-11	0.01965892E+06	4
HCCOH	32387H	2C 2O 1 G 0300.00 4000.00	1
0.07328324E+02	0.03336416E-01-0.03024705E-05-0.01781106E-08	0.03245168E-12	2
0.07598258E+05-0.01401214E+03	0.03899465E+02	0.09701075E-01-0.03119309E-05	3
-0.05537732E-07	0.02465732E-10	0.08701190E+05	4
HCCSICL2H	40992H	2C 2SI 1CL 2G 0300.00 4000.00	1
0.01480501E+03	0.02600965E-01-0.04631204E-05-0.02401379E-09	0.09812397E-13	2
-0.02163059E+06-0.04610236E+03	0.04846840E+02	0.03181717E+00-0.03572068E-03	3
0.01983339E-06-0.04248036E-10-0.01856223E+06	0.05613645E+02		4
HCL	42189CL	1H 1 G 0300.00 5000.00	1
0.02755335E+02	0.01473581E-01-0.04971254E-05	0.08108658E-09-0.05072063E-13	2
-0.01191806E+06	0.06515116E+02	0.03338534E+02	3
0.04703992E-07-0.01836011E-10-0.01213151E+06	0.03193555E+02		4
HCL2SICH3	40992H	4C 1SI 1CL 2G 0300.00 4000.00	1
0.01459366E+03	0.04006211E-01-0.04818700E-05-0.01336338E-08	0.02648821E-12	2
-0.05346984E+06-0.04689795E+03	0.04155299E+02	0.02995026E+00-0.02799546E-03	3
0.01433046E-06-0.03013208E-10-0.04973616E+06	0.09051815E+02		4
HCL2SISICL2H	40992H	2SI 2CL 4 G 0300.00 4000.00	1
0.01863092E+03	0.01991871E-01-0.04703153E-05	0.02393378E-09	2
-0.07983306E+06-0.05812192E+03	0.08215700E+02	0.03290751E+00-0.03764294E-03	3
0.02071053E-06-0.04369767E-10-0.07671145E+06-0.04245506E+02			4
HCLCCLO	40992H	1C 2 O 1CL 2G 0300.00 4000.00	1
0.01282877E+03	0.02295631E-01-0.04601887E-05-0.02941710E-09	0.01148412E-12	2
-0.01481358E+06-0.03708152E+03	0.03082763E+02	0.03013466E+00-0.03298082E-03	3
0.01776354E-06-0.03720337E-10-0.01177928E+06	0.01372635E+03		4
HCLCCHO	53090C	2H 2O 1CL 1G 0300.00 5000.00	1
0.01228193E+03	0.02136310E-01-0.03756942E-05-0.01347374E-09	0.05834907E-13	2
-0.04235416E+05-0.03860056E+03	0.01544662E+02	0.02882431E+00-0.02921314E-03	3
0.01557811E-06-0.03358528E-10-0.04546644E+05	0.01905110E+03		4
HCLSI (CH3)2	40992H	7C 2SI 1CL 1G 0300.00 4000.00	1
0.01779932E+03	0.06864497E-01-0.06677913E-05-0.02916791E-08	0.05251096E-12	2
-0.04235416E+06-0.06627844E+03	0.03428693E+02	0.03880542E+00-0.03118298E-03	3
0.01483918E-06-0.03097758E-10-0.03676770E+06	0.01220014E+03		4
HCLSI (CH3)CH2	40992H	6C 2SI 1CL 1G 0300.00 4000.00	1
0.01684996E+03	0.05769153E-01-0.06362653E-05-0.02117805E-08	0.04004912E-12	2
-0.01692029E+06-0.05821970E+03	0.03518672E+02	0.03868692E+00-0.03578989E-03	3
0.01856940E-06-0.03976975E-10-0.01207708E+06	0.01340137E+03		4
HCLSICH2	40992H	3C 1SI 1CL 1G 0300.00 4000.00	1
0.01094639E+03	0.03063482E-01-0.04057563E-05-0.07933510E-09	0.01649546E-12	2
-0.03161099E+05-0.03101113E+03	0.02331473E+02	0.02712338E+00-0.02843577E-03	3
0.01542443E-06-0.03288710E-10-0.03745104E+04	0.01417701E+03		4
HCLSICH3	40992H	4C 1SI 1CL 1G 0300.00 4000.00	1
0.01183446E+03	0.03802168E-01-0.04054360E-05-0.01478932E-08	0.02756845E-12	2
-0.09669808E+05-0.03413556E+03	0.03061496E+02	0.02418432E+00-0.02072566E-03	3
0.01016711E-06-0.02124115E-10-0.06367089E+05	0.01342892E+03		4
HCLSISI	40992H	1SI 2CL 1 G 0300.00 4000.00	1
0.08766356E+02	0.08352699E-02-0.01828719E-05	0.04227080E-10	2
0.03066829E+06-0.01515527E+03	0.05006777E+02	0.01170423E+00-0.01308663E-03	3
0.07173085E-07-0.01520111E-10	0.03183531E+06	0.04414009E+02	4
HCN	110193H	1C 1N 1 G 0300.00 4000.00	1
0.03426457E+02	0.03924190E-01-0.01601138E-04	0.03161966E-08-0.02432850E-12	2
0.01485552E+06	0.03607795E+02	0.02417787E+02	3
0.07980141E-07-0.02311141E-10	0.01501044E+06	0.08222891E+02	4
HCNH	41687C	1H 2N 1 G 0300.00 4000.00	1
0.04923293E+02	0.03332897E-01-0.03370897E-05-0.01901619E-08	0.03531825E-12	2
0.03132669E+06-0.01632509E+02	0.02759456E+02	0.06103387E-01	3
-0.02063094E-07	0.01931920E-11	0.03217247E+06	4
HCNO	120186H	1C 1N 1O 1G 0250.00 4000.00	1
0.06692412E+02	0.02368360E-01-0.02371510E-05-0.01275503E-08	0.02407137E-12	2
0.01694737E+06-0.01245434E+03	0.03184859E+02	0.09752316E-01-0.01280203E-04	3
-0.06163104E-07	0.03226275E-10	0.01797907E+06	4

HCO	121286H	1C	1O	1	G	0300.00	5000.00	1000.00	1
	0.03557271E+02	0.03345573E-01	-0.01335006E-04	0.02470573E-08	-0.01713851E-12				2
	0.03916324E+05	0.05552299E+02	0.02898330E+02	0.06199147E-01	-0.09623084E-04				3
	0.01089825E-06	-0.04574885E-10	0.04159922E+05	0.08983614E+02					4
HCO+	121286H	1C	1O	1E	-1G	0300.00	5000.00	1000.00	1
	0.03692074E+02	0.03454732E-01	-0.01316524E-04	0.02323551E-08	-0.01554132E-12				2
	0.09890941E+06	0.02330722E+02	0.02496483E+02	0.08690658E-01	-0.01060445E-03				3
	0.07882791E-07	-0.02418385E-10	0.09915097E+06	0.08048178E+02					4
HCOOH	103190C	1H	2O	2	G	0300.00	4000.00	1500.00	1
	0.07959698E+02	0.03024532E-01	-0.03434242E-05	-0.01326767E-08	0.02520240E-12				2
	-0.05027445E+06	-0.01872208E+03	0.09326031E+01	0.01891002E+00	-0.01554964E-03				3
	0.07290031E-07	-0.01483695E-10	-0.04760071E+06	0.01950653E+03					4
HE	120186HE	1			G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-0.07453750E+04	0.09153489E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.09153488E+01					4
HE+	120186HE	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.02853427E+07	0.01608405E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.02853427E+07	0.01608405E+02					4
HF	121286H	1F	1		G	0300.00	5000.00	1000.00	1
	0.02956767E+02	0.07721015E-02	-0.09899833E-06	-0.04993521E-10	0.01429331E-13				2
	-0.03361061E+06	0.04011673E+02	0.03431841E+02	0.04404166E-02	-0.08828452E-05				3
	0.06574516E-08	-0.02055910E-12	-0.03381977E+06	0.01238270E+02					4
HG2BR2(S)	81292BR	2HG	2		S	0300.00	1500.00	1000.00	1
	0.01131527E+03	0.05176237E-01	-0.09149018E-05	-0.01774353E-07	0.08208311E-11				2
	-0.02812664E+06	-0.03960847E+03	0.09176256E+02	0.01716637E+00	-0.02379101E-03				3
	0.01656353E-06	-0.04492058E-10	-0.02787921E+06	-0.03016915E+03					4
HG2CL2(S)	81292CL	2HG	2		S	0300.00	1500.00	1000.00	1
	0.01170237E+03	0.03242224E-01	-0.01018772E-05	-0.03745899E-08	0.04682208E-12				2
	-0.03555571E+06	-0.04461773E+03	0.01002375E+03	0.01031694E+00	-0.01160577E-03				3
	0.08123549E-07	-0.02343515E-10	-0.03522627E+06	-0.03658009E+03					4
HG2F2(S)	81292F	2HG	2		S	0300.00	1500.00	1000.00	1
	0.01156086E+03	0.03513290E-01	-0.04228193E-06	-0.06265655E-08	0.01191005E-11				2
	-0.06207291E+06	-0.04780613E+03	0.01035013E+03	0.06139501E-01	-0.03674693E-05				3
	-0.03011902E-07	0.01414143E-10	-0.06172955E+06	-0.04143495E+03					4
HG2I2(S)	81292I	2HG	2		S	0300.00	1500.00	1000.00	1
	0.01104021E+03	0.05724188E-01	-0.09515335E-05	-0.02149612E-07	0.09793057E-11				2
	-0.01777374E+06	-0.03535439E+03	0.09788829E+02	0.01440390E+00	-0.01844748E-03				3
	0.01180869E-06	-0.02911372E-10	-0.01774167E+06	-0.03032197E+03					4
HGAET	62987GA	1C	2H	6	G	0300.00	1500.00	0600.00	1
	0.06580152E+02	0.01610132E+00	0.05009546E-05	-0.05185148E-07	0.01524085E-10				2
	0.08765131E+05	-0.04046067E+01	0.01163284E+02	0.03282213E+00	0.06765717E-04				3
	-0.06509541E-06	0.04835807E-09	0.09767174E+05	0.02588269E+03					4
HGAET2	62987GA	1C	4H	11	G	0300.00	1500.00	0600.00	1
	0.06511306E+02	0.02819754E+00	0.01418751E-04	-0.09000947E-07	0.02572894E-10				2
	-0.04482180E+05	0.04709022E+02	-0.01486576E+02	0.05217640E+00	0.01356342E-03				3
	-0.01011982E-05	0.07319854E-09	-0.02985242E+05	0.04364749E+03					4
HGAME	62987GA	1C	1H	4	G	0300.00	1500.00	0600.00	1
	0.05318279E+02	0.09490931E-01	0.02277164E-05	-0.03005070E-07	0.09037830E-11				2
	0.01253534E+06	-0.01065710E+01	0.01784750E+02	0.02058861E+00	0.03548509E-04				3
	-0.04111927E-06	0.03108978E-09	0.01318422E+06	0.01700702E+03					4
HGAME2	62987GA	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.06759398E+02	0.01426103E+00	-0.01174024E-05	-0.05001401E-07	0.01502785E-10				2
	-0.01473265E+05	-0.02967135E+02	0.09039155E+01	0.03264779E+00	0.05389244E-04				3
	-0.06814504E-06	0.05150323E-09	-0.03978242E+04	0.02539305E+03					4
HGBR	81292BR	1HG	1		G	0300.00	5000.00	1000.00	1
	0.04470182E+02	0.01740022E-02	-0.01782286E-06	0.03639776E-10	-0.02699461E-14				2
	0.01118634E+06	0.07116504E+02	0.04325519E+02	0.06429246E-02	-0.04527797E-05				3
	0.04543436E-09	0.06863204E-12	0.01121730E+06	0.07833202E+02					4
HGCL2	81292CL	2HG	1		G	0300.00	5000.00	1000.00	1
	0.07251462E+02	0.03082143E-02	-0.01447555E-05	0.02958294E-09	-0.02201214E-13				2
	-0.01981231E+06	-0.06061846E+02	0.06249130E+02	0.03221573E-01	-0.02109668E-04				3
	-0.07713536E-08	0.08526178E-11	-0.01958242E+06	-0.01015613E+02					4
HGCL2(S)	81292CL	2HG	1		S	0300.00	1500.00	1000.00	1
	0.07750329E+02	0.03529253E-01	0.03886646E-06	-0.08307839E-08	0.02781535E-11				2

-0.03009787E+06-0.02772331E+03	0.07611778E+02	0.05084911E-01-0.02887606E-04	3		
0.09093899E-08	0.04734468E-12-0.03015054E+06-0.02738100E+03		4		
HGF2	81292F 2HG 1	G 0300.00 5000.00 1000.00	1		
0.06970407E+02	0.06373497E-02-0.02938029E-05	0.05925826E-09-0.04366956E-13	2		
-0.03751535E+06-0.08137829E+02	0.05155538E+02	0.05733727E-01-0.03667157E-04	3		
-0.01223692E-07	0.01370429E-10-0.03707844E+06	0.01073098E+02	4		
HGF2 (S)	81292F 2HG 1	S 0300.00 2000.00 1000.00	1		
0.08322627E+02	0.02317361E-01	0.02103511E-05-0.09665973E-09	0.01631405E-12	2	
-0.05342179E+06-0.03414006E+03	0.08250103E+02	0.02543387E-01-0.07218619E-06	3		
0.08044224E-09-0.03175138E-12-0.05340276E+06-0.03377085E+03			4		
HGH	81292H 1HG 1	G 0300.00 5000.00 1000.00	1		
0.03674353E+02	0.01116618E-01-0.03728888E-05	0.07077644E-09-0.04984356E-13	2		
0.02745200E+06	0.04954799E+02	0.02859969E+02	0.03217363E-01-0.02993410E-04	3	
0.02267118E-07-0.08671660E-11	0.02771287E+06	0.09273314E+02	4		
HGI	81292HG 1I 1	G 0300.00 5000.00 1000.00	1		
0.04487935E+02	0.03041356E-02-0.07219846E-07	0.01468881E-10-0.01089820E-14	2		
0.01470042E+06	0.08086309E+02	0.04411734E+02	0.05799910E-02-0.03475217E-05	3	
0.01593090E-08-0.01730073E-12	0.01471610E+06	0.08458668E+02	4		
HGO	81292HG 1O 1	G 0300.00 5000.00 1000.00	1		
0.04192036E+02	0.04176084E-02-0.01658976E-05	0.03318185E-09-0.02429647E-13	2		
0.03713110E+05	0.04621457E+02	0.03235991E+02	0.03067171E-01-0.01992628E-04	3	
-0.04378690E-08	0.06018341E-11	0.03950193E+05	0.09495331E+02	4	
HGO (S)	81292HG 1O 1	S 0300.00 1000.00 1000.00	1		
0.07146808E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	2	
-0.01350616E+06-0.03327734E+03	0.02854835E+02	0.01115052E+00-0.01160794E-03	3		
0.06126729E-07-0.01377341E-10-0.01217635E+06-0.01067390E+03			4		
HMEGAET	62987GA 1C 3H 9	G 0300.00 1500.00 0600.00	1		
0.07025463E+02	0.02564787E+00	0.09619100E-05-0.08403699E-07	0.02488960E-10	2	
-0.01361377E+05-0.03319484E+02-0.02079143E+02	0.05373076E+00	0.01181036E-03	3		
-0.01099855E-05	0.08189554E-09	0.03216961E+04	0.04086070E+03	4	
HN (OH) 2	103190H 3N 1O 2	G 0300.00 4000.00 1500.00	1		
0.09963640E+02	0.02864737E-01-0.03812930E-05-0.07443356E-09	0.01610124E-12	2		
-0.01662184E+06-0.02871770E+03	0.03244199E+01	0.02850544E+00-0.02753934E-03	3		
0.01337294E-06-0.02571777E-10-0.01354499E+06	0.02201480E+03		4		
HN3	82687H 1N 3	G 0300.00 4000.00 1000.00	1		
0.06023015E+02	0.02454362E-01-0.02404279E-05-0.01322973E-08	0.02474146E-12	2		
0.03394051E+06-0.07015537E+02	0.03621003E+02	0.06030785E-01	0.04054460E-05	3	
-0.02545271E-07	0.06174280E-11	0.03482373E+06	0.06333769E+02	4	
HNC	92392H 1C 1N 1	G 0300.00 5000.00 1500.00	1		
0.05283464E+02	0.01092476E-01-0.01170865E-05-0.02308672E-09	0.03950673E-13	2		
0.02012958E+06-0.06388218E+02	0.03592377E+02	0.05561340E-01-0.05936823E-04	3		
0.03782329E-07-0.09365092E-11	0.02079803E+06	0.02732160E+02	4		
HNCN	62790C 1H 1N 2	G 0300.00 4000.00 1500.00	1		
0.07251951E+02	0.01587363E-01-0.01995579E-05-0.04841944E-09	0.09908280E-13	2		
0.03563666E+06-0.01312080E+03	0.02951908E+02	0.01245028E+00-0.01161611E-03	3		
0.05786108E-07-0.01175004E-10	0.03712483E+06	0.09811426E+02	4		
HNCNH	62790C 1H 2N 2	G 0300.00 4000.00 1500.00	1		
0.08374143E+02	0.02366143E-01-0.03502324E-05-0.04391102E-09	0.01096859E-12	2		
0.01461088E+06-0.02107393E+03	0.01001985E+02	0.02464016E+00-0.02759770E-03	3		
0.01532472E-06-0.03268280E-10	0.01679368E+06	0.01694325E+03	4		
HNCO	110193H 1C 1N 1O 1G	0300.00 4000.00 1400.00	1		
0.06545307E+02	0.01965760E-01-0.01562664E-05-0.01074318E-08	0.01874680E-12	2		
-0.01664773E+06-0.01003880E+03	0.03858467E+02	0.06390342E-01-0.09016628E-05	3		
-0.01898224E-07	0.07651380E-11-0.01562343E+06	0.04882493E+02	4		
HNF	42489H 1N 1F 1	G 0300.00 3000.00 1000.00	1		
0.04133219E+02	0.01912057E-01-0.01625330E-05-0.01726461E-08	0.03743691E-12	2		
0.01467052E+06	0.03292122E+02	0.03249761E+02	0.03261818E-01	0.04355642E-06	3
-0.01100277E-07	0.02926757E-11	0.01499126E+06	0.08187434E+02	4	
HNF2	42489H 1N 1F 2	G 0300.00 3000.00 1000.00	1		
0.05704866E+02	0.03049897E-01-0.02826803E-05-0.02923185E-08	0.06551055E-12	2		
-0.09107488E+05-0.03941332E+02	0.02572812E+02	0.08762144E-01-0.02326921E-05	3		
-0.05000826E-07	0.02143838E-10-0.08086760E+05	0.01300681E+03	4		
HNNHO	103190H 2N 2O 1	G 0300.00 4000.00 1500.00	1		
0.07462348E+02	0.03113521E-01-0.02614534E-05-0.01394601E-08	0.02363352E-12	2		
0.07517607E+05-0.01619293E+03	0.07974964E+01	0.01693171E+00-0.01141086E-03	3		
0.04201242E-07-0.06926417E-11	0.01010665E+06	0.02038765E+03	4		

HNNO	103190H	1N	2O	1	G	0300.00	4000.00	1500.00	1
	0.06991217E+02	0.01875970E-01	-0.02124584E-05	-0.06710472E-09	0.01230508E-12				2
	0.02497566E+06	-0.01123523E+03	0.02238298E+02	0.01359200E+00	-0.01179873E-03				3
	0.05392971E-07	-0.01010859E-10	0.02660259E+06	0.01413679E+03					4
HNNONO	10891H	1N	3O	2	G	0300.00	4000.00	1500.00	1
	0.01246747E+03	0.02018438E-01	-0.03674474E-05	-0.03459117E-09	0.01090810E-12				2
	0.02452278E+06	-0.03868309E+03	0.02642670E+02	0.02625418E+00	-0.02477878E-03				3
	0.01184374E-06	-0.02298757E-10	0.02793182E+06	0.01383705E+03					4
HNO	121286H	1N	1O	1	G	0300.00	5000.00	1000.00	1
	0.03615144E+02	0.03212486E-01	-0.01260337E-04	0.02267298E-08	-0.01536236E-12				2
	0.01066191E+06	0.04810264E+02	0.02784403E+02	0.06609646E-01	-0.09300223E-04				3
	0.09437980E-07	-0.03753146E-10	0.01091878E+06	0.09035629E+02					4
HNO2	103190H	1N	1O	2	G	0300.00	4000.00	1500.00	1
	0.06479630E+02	0.01995274E-01	-0.01740387E-05	-0.09695872E-09	0.01701480E-12				2
	-0.09999271E+05	-0.01067286E+03	0.01934838E+02	0.01010036E+00	-0.04964616E-04				3
	0.08701120E-08	-0.0324135E-13	-0.08105484E+05	0.01473250E+03					4
HNO3	121286H	1N	1O	3	G	0300.00	5000.00	1000.00	1
	0.07003845E+02	0.05811493E-01	-0.02333789E-04	0.04288814E-08	-0.02959385E-12				2
	-0.01889952E+06	-0.01047863E+03	0.01353185E+02	0.02220025E+00	-0.01978812E-03				3
	0.08773908E-07	-0.01658384E-10	-0.01738563E+06	0.01851868E+03					4
HNOH	102290H	2N	1O	1	G	0300.00	4000.00	1500.00	1
	0.06396134E+02	0.01821067E-01	-0.01870892E-05	-0.07844472E-09	0.01444855E-12				2
	0.07859615E+05	-0.01040479E+03	0.02125274E+02	0.01066282E+00	-0.07602589E-04				3
	0.03081642E-07	-0.05726498E-11	0.09553544E+05	0.01309672E+03					4
HO2	20387H	1O	2	G	0300.00	5000.00	1000.00	1	
	0.04072191E+02	0.02131296E-01	-0.05308145E-05	0.06112269E-09	-0.02841165E-13				2
	-0.01579727E+04	0.03476029E+02	0.02979963E+02	0.04996697E-01	-0.03790997E-04				3
	0.02354192E-07	-0.08089024E-11	0.01762274E+04	0.09222724E+02					4
HOCH2OH	103190C	1H	4O	2	G	0300.00	4000.00	1500.00	1
	0.01089048E+03	0.04000443E-01	-0.04729597E-05	-0.01295970E-08	0.02552658E-12				2
	-0.05347440E+06	-0.03540623E+03	-0.06548874E+01	0.03377715E+00	-0.03157595E-03				3
	0.01532216E-06	-0.02994259E-10	-0.04963411E+06	0.02579207E+03					4
HOCCL	40992H	1O	1CL	1	G	0300.00	4000.00	1500.00	1
	0.04953150E+02	0.01100053E-01	-0.01256296E-05	-0.03349951E-09	0.06464506E-13				2
	-0.01114737E+06	-0.06838384E+01	0.02861399E+02	0.07134484E-01	-0.07311028E-04				3
	0.03980236E-07	-0.08506421E-11	-0.01049306E+06	0.01021485E+03					4
HOCN	110193H	1C	1N	1O	1G	0300.00	4000.00	1400.00	1
	0.06022112E+02	0.01929530E-01	-0.01455029E-05	-0.01045811E-08	0.01794814E-12				2
	-0.04040321E+05	-0.05866433E+02	0.03789424E+02	0.05387981E-01	-0.06518270E-05				3
	-0.01420164E-07	0.05367969E-11	-0.03135335E+05	0.06667052E+02					4
HOCO	103190C	1H	1O	2	G	0300.00	4000.00	1500.00	1
	0.07517634E+02	0.01259029E-01	-0.01910901E-05	-0.03136391E-09	0.07547673E-13				2
	-0.02634121E+06	-0.01448392E+03	0.02285122E+02	0.01351435E+00	-0.01160407E-03				3
	0.05047011E-07	-0.09032231E-11	-0.02448416E+06	0.01367874E+03					4
HONO	31787H	1N	1O	2	G	0300.00	5000.00	1000.00	1
	0.05486893E+02	0.04218065E-01	-0.01649143E-04	0.02971877E-08	-0.02021148E-12				2
	-0.01126865E+06	-0.02997002E+02	0.02290413E+02	0.01409922E+00	-0.01367872E-03				3
	0.07498780E-07	-0.01876905E-10	-0.01043195E+06	0.01328077E+03					4
HONO2	103190H	1N	1O	3	G	0300.00	4000.00	1500.00	1
	0.09756148E+02	0.01900948E-01	-0.03240020E-05	-0.03976639E-09	0.01100334E-12				2
	-0.01942244E+06	-0.02690023E+03	0.07877668E+01	0.02382329E+00	-0.02205964E-03				3
	0.01034048E-06	-0.01972857E-10	-0.01630442E+06	0.02108964E+03					4
HSI (CH3)2	61991H	7C	3SI	1	G	0300.00	2500.00	1500.00	1
	0.01220942E+03	0.09173338E-01	-0.01186653E-05	-0.01188590E-07	0.02418110E-11				2
	0.03781464E+05	-0.03668250E+03	0.02568267E+02	0.03071446E+00	-0.01863911E-03				3
	0.06210373E-07	-0.09376544E-11	0.07271919E+05	0.01551808E+03					4
HSI (CH3)2CH2	61991H	9C	3SI	1	G	0300.00	2500.00	1500.00	1
	0.01723999E+03	0.01101475E+00	-0.01546410E-05	-0.01338650E-07	0.02653453E-11				2
	-0.02842083E+05	-0.06077749E+03	0.03367732E+02	0.04430759E+00	-0.03246598E-03				3
	0.01379387E-06	-0.02586752E-10	0.02041653E+05	0.01367000E+03					4
HSI (CH3)3	61991H	10C	3SI	1	G	0300.00	2500.00	1500.00	1
	0.01689903E+03	0.01338224E+00	-0.01538243E-05	-0.01746233E-07	0.03550375E-11				2
	-0.02740327E+06	-0.06121112E+03	0.03224459E+02	0.04373614E+00	-0.02597404E-03				3
	0.08415742E-07	-0.01236561E-10	-0.02243583E+06	0.01289306E+03					4
HSI (NH2)2	22790SI	1H	5N	2	G	0300.00	4000.00	1000.00	1
	0.01171677E+03	0.05339021E-01	-0.04667824E-05	-0.02824087E-08	0.05080916E-12				2

-0.01264169E+05-0.03245118E+03 0.06289699E+02 0.01675060E+00-0.01520878E-04	3
-0.01070065E-06 0.05538641E-10 0.03154771E+04-0.03746008E+02	4
HSI (NH2) 3 22790SI 1H 7N 3 G 0300.00 4000.00 1000.00	1
0.01661406E+03 0.07395874E-01-0.06440010E-05-0.03918887E-08 0.07045959E-12	2
-0.03859547E+06-0.05865318E+03 0.07070983E+02 0.02754435E+00-0.02603669E-04	3
-0.01874567E-06 0.09778511E-10-0.03582658E+06-0.08209675E+02	4
HSIC 61991H 1C 1SI 1 G 0300.00 2500.00 1500.00	1
0.05849544E+02 0.07628346E-02-0.09974130E-06-0.03811586E-09 0.08581471E-13	2
0.09097438E+06-0.04862062E+02 0.03761288E+02 0.06108070E-01-0.05721172E-04	3
0.02805116E-07-0.05597709E-11 0.09168219E+06 0.06236756E+02	4
HSICCH 61991H 2C 2SI 1 G 0300.00 2500.00 1500.00	1
0.09098096E+02 0.02292999E-01-0.01278589E-05-0.01869017E-08 0.03514532E-12	2
0.04933532E+06-0.02153271E+03 0.03799881E+02 0.01633703E+00-0.01551299E-03	3
0.07880591E-07-0.01619982E-10 0.05109468E+06 0.06475363E+02	4
HSICH2 61991H 3C 1SI 1 G 0300.00 2500.00 1500.00	1
0.08641686E+02 0.02535259E-01-0.01532829E-05-0.02418416E-08 0.04870000E-12	2
0.03962671E+06-0.02128790E+03 0.02376883E+02 0.01822864E+00-0.01641260E-03	3
0.07937691E-07-0.01590356E-10 0.04179768E+06 0.01215211E+03	4
HSICH3 61991H 4C 1SI 1 G 0300.00 2500.00 1500.00	1
0.07578257E+02 0.05000398E-01-0.08706991E-06-0.06516750E-08 0.01344446E-11	2
0.02138075E+06-0.01438961E+03 0.02658293E+02 0.01547950E+00-0.08319889E-04	3
0.02184355E-07-0.02302844E-11 0.02319822E+06 0.01240552E+03	4
HSICL 121986SI 1H 1CL 1 G 0300.00 2000.00 1000.00	1
0.04900628E+02 0.01981752E-01-0.03634647E-05-0.02285211E-08 0.07633527E-12	2
0.06914634E+05 0.01377004E+02 0.03072748E+02 0.09057843E-01-0.01159134E-03	3
0.08310477E-07-0.02483000E-10 0.07324210E+05 0.01033490E+03	4
HSIN 22790H 1SI 1N 1 G 0300.00 4000.00 1000.00	1
0.05746590E+02 0.01167119E-01-0.01360742E-05-0.05908617E-09 0.01174696E-12	2
0.04484671E+06-0.05931788E+02 0.04865176E+02 0.01775119E-01 0.04890870E-05	3
0.03922383E-08-0.07913276E-11 0.04526353E+06-0.07134509E+01	4
HSINH 42489SI 1H 2N 1 G 0300.00 3000.00 1000.00	1
0.06493435E+02 0.02567980E-01-0.03126526E-05-0.02577467E-08 0.06216479E-12	2
0.04035934E+06-0.07830112E+02 0.03566343E+02 0.08446736E-01-0.07699952E-05	3
-0.05270970E-07 0.02581065E-10 0.04124904E+06 0.07780791E+02	4
HSINH2 42489SI 1N 1H 3 G 0300.00 3000.00 1000.00	1
0.06177894E+02 0.04689964E-01-0.03583294E-05-0.04457980E-08 0.09379187E-12	2
0.01091277E+06-0.07006672E+02 0.02716144E+02 0.01204278E+00-0.09827195E-05	3
-0.07408477E-07 0.03789792E-10 0.01190771E+06 0.01126252E+03	4
HSISICL 40992H 1SI 2CL 1 G 0300.00 4000.00 1500.00	1
0.09242357E+02 0.07265211E-02-0.02039730E-05-0.03559737E-10 0.04236577E-13	2
0.03651789E+06-0.01714597E+03 0.05753464E+02 0.01000321E+00-0.01097056E-03	3
0.06117942E-07-0.01351102E-10 0.03773825E+06 0.01395110E+02	4
I*C3H7 120186C 3H 7 G 0300.00 5000.00 1000.00	1
0.08063369E+02 0.01574488E+00-0.05182392E-04 0.07477245E-08-0.03854422E-12	2
0.05313871E+05-0.02192647E+03 0.01713300E+02 0.02542616E+00 0.01580808E-04	3
-0.01821286E-06 0.08827710E-10 0.07535809E+05 0.01297901E+03	4
K 81092K 1 G 0300.00 5000.00 1000.00	1
0.02563720E+02-0.01453656E-02 0.01223794E-05-0.05337797E-09 0.01196251E-12	2
0.09958933E+05 0.04689090E+02 0.02599395E+02-0.06665192E-02 0.01537419E-04	3
-0.01462701E-07 0.04917226E-11 0.09968534E+05 0.04606125E+02	4
K(L) 81092K 1 L 0300.00 2000.00 1000.00	1
0.03274152E+02-0.08858241E-03 0.03862458E-05 0.01524701E-08-0.07158116E-12	2
-0.05365253E+04-0.09686786E+02 0.04883188E+02-0.05109876E-01 0.08368289E-04	3
-0.07183867E-07 0.02694974E-10-0.01014822E+05-0.01801753E+03	4
K+ 81092K 1E -1 G 0300.00 5000.00 1000.00	1
0.02500252E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
0.06110476E+06 0.04335097E+02 0.02500252E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00 0.06110476E+06 0.04335097E+02	4
K2 81092K 2 G 0300.00 5000.00 1000.00	1
0.04493744E+02 0.02561175E-02-0.03738461E-07 0.07392168E-11-0.05314252E-15	2
0.01393386E+06 0.04344696E+02 0.04445378E+02 0.04507960E-02-0.02923572E-05	3
0.01874060E-08-0.04441270E-12 0.01394330E+06 0.04577300E+02	4
K2B407(S) 81292B 4K 20 7 S 0300.00 2000.00 1000.00	1
0.02241821E+03 0.01632758E+00-0.03423961E-04-0.01996427E-07 0.07329643E-11	2
-0.04092750E+07-0.01095459E+04-0.02998519E+02 0.01131803E+01-0.01363625E-02	3
0.07498933E-06-0.01475027E-09-0.04041216E+07 0.01385206E+03	4

K2B6O10(S)	81292B	6K	20	10	S	0300.00	2000.00	1000.00	1
	0.03118760E+03	0.02605101E+00	-0.07109914E-04	-0.01524101E-07	0.08605891E-11				2
	-0.05702715E+07	-0.01601394E+04	0.08964822E+02	0.01355307E+01	-0.02844741E-02				3
	0.03136564E-05	-0.01242126E-08	-0.05641143E+07	-0.05121922E+03					4
K2B8O13(S)	81292B	8K	20	13	S	0300.00	2000.00	1000.00	1
	0.04112535E+03	0.02714051E+00	0.01343626E-04	-0.04965544E-07	0.09664300E-11				2
	-0.07315279E+07	-0.02135898E+04	0.02800687E+03	0.02363518E+00	0.05436592E-03				3
	-0.04802017E-06	0.07622581E-10	-0.07248984E+07	-0.01332889E+04					4
K2CO3(S)	81292C	1K	20	3	S	0300.00	2000.00	1000.00	1
	0.01170935E+03	0.01041619E+00	0.01020812E-04	-0.05155670E-08	0.09388472E-12				2
	-0.01424670E+07	-0.05154899E+03	0.06680495E+02	0.03154875E+00	-0.03258348E-03				3
	0.02341080E-06	-0.06331882E-10	-0.01414994E+07	-0.02751031E+03					4
K2H2O2	81292H	2K	20	2	G	0300.00	5000.00	1000.00	1
	0.09476007E+02	0.05520012E-01	-0.02003512E-04	0.03416984E-08	-0.02230089E-12				2
	-0.08204786E+06	-0.01665546E+03	0.06069657E+02	0.01657159E+00	-0.01641134E-03				3
	0.09628012E-07	-0.02546013E-10	-0.08118152E+06	0.05625929E+01					4
K2O(S)	81092K	2O	1		S	0300.00	2000.00	1000.00	1
	0.09200109E+02	0.04813529E-01	-0.01018656E-04	0.08972973E-08	-0.02121417E-11				2
	-0.04671154E+06	-0.04264142E+03	0.02640315E+02	0.04577225E+00	-0.09349357E-03				3
	0.08921012E-06	-0.03044898E-09	-0.04583697E+06	-0.01392763E+03					4
K2O2(S)	81092K	2O	2		S	0300.00	2000.00	1000.00	1
	0.01094138E+03	0.06102309E-01	0.08639951E-05	-0.02383978E-08	0.01021959E-12				2
	-0.06335114E+06	-0.05099447E+03	0.08940024E+02	0.01225014E+00	-0.08065365E-04				3
	0.07182271E-07	-0.02627561E-10	-0.06277485E+06	-0.04066683E+03					4
K2SO4	81092K	2O	4S	1	G	0300.00	5000.00	1000.00	1
	0.01526056E+03	0.04272701E-01	-0.01902870E-04	0.03745009E-08	-0.02710228E-12				2
	-0.01368994E+07	-0.04548655E+03	0.06620770E+02	0.02753542E+00	-0.01909671E-03				3
	-0.04668391E-08	0.03385142E-10	-0.01346318E+07	-0.01043411E+02					4
K2SO4(A)	81092K	2O	4S	1	S	0300.00	1200.00	1000.00	1
	0.01112054E+03	0.01688473E+00	0.02694884E-04	-0.06810694E-07	0.03326950E-10				2
	-0.01771853E+07	-0.04766545E+03	0.05610137E+02	0.05334319E+00	-0.08680538E-03				3
	0.08485600E-06	-0.02978756E-09	-0.01763645E+07	-0.02358624E+03					4
K2SO4(B)	81092K	2O	4S	1	S	0300.00	1500.00	1000.00	1
	0.01400625E+03	0.08639256E-01	0.01734839E-04	-0.01101018E-07	0.02493181E-11				2
	-0.01758863E+07	-0.05931899E+03	0.01384030E+03	0.09154258E-01	0.01580722E-04				3
	-0.01673984E-07	0.06273504E-11	-0.01758589E+07	-0.05851410E+03					4
K3CL6AL(S)	81292AL	1CL	6K	3	S	0300.00	2000.00	1000.00	1
	0.02692199E+03	0.01202448E+00	0.05058586E-06	-0.02459252E-07	0.06112274E-11				2
	-0.02602720E+07	-0.01118533E+04	0.02756025E+03	0.01980910E-01	0.02914285E-03				3
	-0.03306608E-06	0.01153111E-09	-0.02601182E+07	-0.01132925E+04					4
K3CL9AL2(S)	81292AL	2CL	9K	3	S	0300.00	1500.00	1000.00	1
	0.04789960E+03	-0.03698524E-01	0.01208277E-04	0.06439299E-07	-0.01714364E-10				2
	-0.03594776E+07	-0.02186357E+04	0.03685728E+03	0.02754220E-01	0.05087779E-03				3
	-0.06808868E-06	0.02773367E-09	-0.03554758E+07	-0.01561649E+04					4
K3F6AL(S)	81292AL	1F	6K	3	S	0300.00	2000.00	1000.00	1
	0.02557611E+03	0.01452585E+00	-0.02005301E-04	-0.01843642E-07	0.05259736E-11				2
	-0.04090259E+07	-0.01172057E+04	0.01633462E+03	0.05150368E+00	-0.07128115E-03				3
	0.06274052E-06	-0.02251868E-09	-0.04067185E+07	-0.07147460E+03					4
KBF4	81292B	1F	4K	1	G	0300.00	5000.00	1000.00	1
	0.01230182E+03	0.04142506E-01	-0.01820830E-04	0.03550730E-08	-0.02552394E-12				2
	-0.01910389E+07	-0.03449073E+03	0.05358002E+02	0.02295803E+00	-0.01721231E-03				3
	0.02466718E-07	0.01382599E-10	-0.01891819E+07	0.01299769E+02					4
KBO2	81292B	1K	10	2	G	0300.00	5000.00	1000.00	1
	0.07506115E+02	0.02663024E-01	-0.01134505E-04	0.02165299E-08	-0.01532624E-12				2
	-0.08364206E+06	-0.08262075E+02	0.04636629E+02	0.01088843E+00	-0.09865937E-04				3
	0.04481115E-07	-0.09043993E-11	-0.08286314E+06	0.06500684E+02					4
KBO2(S)	81292B	1K	10	2	S	0300.00	2000.00	1000.00	1
	0.07971486E+02	0.06730890E-01	-0.01544574E-04	-0.09972352E-08	0.04052630E-11				2
	-0.01227148E+07	-0.03858371E+03	0.01603821E+02	0.03275175E+00	-0.04757948E-03				3
	0.03848067E-06	-0.01269093E-09	-0.01212629E+07	-0.07486101E+02					4
KBR	81292BR	1K	1		G	0300.00	5000.00	1000.00	1
	0.04458711E+02	0.01473836E-02	-0.02499466E-06	0.05161851E-10	-0.03875234E-14				2
	-0.02300303E+06	0.04657488E+02	0.04270624E+02	0.07398923E-02	-0.05320569E-05				3
	-0.05894879E-10	0.01133094E-11	-0.02296215E+06	0.05593031E+02					4
KBR(L)	81292BR	1K	1		L	0300.00	2500.00	1000.00	1
	0.08404630E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2



-0.04779214E+06-0.03519115E+03 0.08404630E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00-0.04779214E+06-0.03519115E+03	4
KBR (S) 81292BR 1K 1 S 0300.00 1500.00	1
-0.05170830E+02 0.01746852E+00 0.01013392E-04-0.07494241E-07 0.02378879E-10	2
-0.04495981E+06 0.03946532E+03 0.05431605E+02 0.03845234E-01-0.03455247E-04	3
-0.09685064E-09 0.02470977E-10-0.04912882E+06-0.02040493E+03	4
KCL 81092CL 1K 1 G 0300.00 5000.00 1000.00	1
0.04434967E+02 0.01726721E-02-0.03865868E-06 0.07943251E-10-0.05932801E-14	2
-0.02716306E+06 0.03398542E+02 0.04149517E+02 0.01039142E-01-0.07034589E-05	3
-0.01200715E-08 0.02112200E-11-0.02709960E+06 0.04826011E+02	4
KCL (L) 81092CL 1K 1 L 0300.00 2000.00 1000.00	1
0.08852542E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
-0.05337392E+06-0.04001344E+03 0.08852542E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00-0.05337392E+06-0.04001344E+03	4
KCL (S) 81092CL 1K 1 S 0300.00 1500.00 1000.00	1
0.01391136E+01 0.07749002E-01 0.02100056E-04-0.01960861E-07 0.03813962E-12	2
-0.05188544E+06 0.09020889E+02 0.05818812E+02-0.05778791E-02 0.09593293E-04	3
-0.01468548E-06 0.07916702E-10-0.05429399E+06-0.02336092E+03	4
KCL4AL (S) 81292AL 1CL 4K 1 S 0300.00 2000.00 1000.00	1
0.02311946E+03 0.01525936E-01-0.06380630E-06-0.04176163E-08 0.01306884E-11	2
-0.01521618E+07-0.01113391E+04 0.01753111E+03-0.03647218E-01 0.03673018E-03	3
-0.03613268E-06 0.09813280E-10-0.01492592E+07-0.07647553E+03	4
KCLO4 (S) 81092CL 1K 1O 4 S 0300.00 1500.00 1000.00	1
0.01704025E+03 0.06660737E-01-0.06016704E-05 0.09785776E-08-0.05059647E-11	2
-0.05676480E+06-0.08085843E+03-0.08468085E+02 0.01228758E+01-0.02129487E-02	3
0.01790606E-05-0.05694776E-09-0.05181381E+06 0.04005509E+03	4
KCN 81092C 1K 1N 1 G 0300.00 5000.00 1000.00	1
0.05842749E+02 0.01653475E-01-0.06722096E-05 0.01241081E-08-0.08573718E-13	2
0.07711161E+05-0.03406482E+02 0.05315387E+02 0.03936776E-01-0.05387426E-04	3
0.04814072E-07-0.01739264E-10 0.07842257E+05-0.08199391E+01	4
KCN (L) 81092C 1K 1N 1 L 0300.00 3000.00 1000.00	1
0.09058883E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
-0.01522798E+06-0.03545687E+03 0.09058883E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00-0.01522798E+06-0.03545687E+03	4
KCN (S) 81092C 1K 1N 1 S 0300.00 2000.00 1000.00	1
0.07894013E+02 0.02150449E-02-0.01621315E-05 0.06831993E-09-0.01060712E-12	2
-0.01600422E+06-0.02964975E+03 0.08115453E+02-0.08847082E-02 0.01981085E-04	3
-0.01804607E-07 0.05974163E-11-0.01604356E+06-0.03067895E+03	4
KF 81292F 1K 1 G 0300.00 5000.00 1000.00	1
0.04357120E+02 0.02586241E-02-0.08236973E-06 0.01676907E-09-0.01243132E-13	2
-0.04063861E+06 0.02285054E+02 0.03798984E+02 0.01885430E-01-0.01210870E-04	3
-0.03741075E-08 0.04494632E-11-0.04051013E+06 0.05095577E+02	4
KF (L) 81292F 1K 1 L 0300.00 3000.00 1000.00	1
0.08656265E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
-0.06927377E+06-0.04118344E+03 0.08656265E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00-0.06927377E+06-0.04118344E+03	4
KF (S) 81292F 1K 1 S 0300.00 2000.00 1000.00	1
0.03272299E+01 0.08993195E-01-0.03094381E-06-0.02624963E-07 0.07101532E-11	2
-0.06804909E+06 0.05309298E+02 0.06190467E+02-0.05622034E-01 0.02294401E-03	3
-0.02818213E-06 0.01204436E-09-0.07014057E+06-0.02637925E+03	4
KH 81092H 1K 1 G 0300.00 5000.00 1000.00	1
0.03968138E+02 0.07086924E-02-0.02618517E-05 0.05096044E-09-0.03655452E-13	2
0.01350120E+06 0.08027413E+01 0.02900121E+02 0.03518317E-01-0.02544774E-04	3
0.04599961E-08 0.01286229E-11 0.01379667E+06 0.06342766E+02	4
KH (S) 81092H 1K 1 S 0300.00 1500.00 1000.00	1
0.05864564E+02 0.01204909E-01 0.02825877E-06 0.03559937E-08-0.02515747E-11	2
-0.09079129E+05-0.02848776E+03 0.05248775E+01 0.02016870E+00-0.02768125E-03	3
0.02024240E-06-0.06052568E-10-0.07796234E+05-0.01890097E+02	4
KI 81092I 1K 1 G 0300.00 5000.00 1000.00	1
0.04470767E+02 0.01359027E-02-0.01768799E-06 0.03648327E-10-0.02733674E-14	2
-0.01644198E+06 0.05528315E+02 0.04327901E+02 0.05945793E-02-0.04409470E-05	3
0.04559572E-09 0.06522621E-12-0.01641095E+06 0.06237795E+02	4
KI (L) 81092I 1K 1 L 0300.00 2500.00 1000.00	1
0.08706593E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
-0.04022598E+06-0.03588112E+03 0.08706593E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00-0.04022598E+06-0.03588112E+03	4

KI(S)	81092I	1K	1		S	0300.00	2000.00	1000.00	1
	0.01442913E+02	0.09802845E-01	-0.01380615E-04	-0.02325573E-07	0.07600708E-11				2
	-0.03988335E+06	0.02717618E+02	0.05114120E+02	0.08508960E-01	-0.02212545E-03				3
	0.02836093E-06	-0.01155892E-09	-0.04120049E+06	-0.01812497E+03					4
KO	81092K	1O	1		G	0300.00	5000.00	1000.00	1
	0.04400291E+02	0.02386787E-02	-0.05880047E-06	0.01206713E-09	-0.09006961E-14				2
	0.07217110E+05	0.03434775E+02	0.03985333E+02	0.01469353E-01	-0.09479054E-05				3
	-0.02419141E-08	0.03264700E-11	0.07311120E+05	0.05517902E+02					4
KO-	81092K	1O	1E	1	G	0300.00	5000.00	1000.00	1
	0.04394805E+02	0.02418371E-02	-0.06146423E-06	0.01255348E-09	-0.09326869E-14				2
	-0.01794565E+06	0.02053687E+02	0.03961007E+02	0.01526099E-01	-0.09806386E-05				3
	-0.02666917E-08	0.03470232E-11	-0.01784737E+06	0.04231682E+02					4
KO2(S)	81092K	1O	2		S	0300.00	1500.00	1000.00	1
	0.01049310E+03	0.01397618E-01	-0.06976643E-05	0.03477427E-08	-0.01222708E-11				2
	-0.03767516E+06	-0.04607321E+03	0.04023244E+02	0.02903561E+00	-0.04812416E-03				3
	0.03816613E-06	-0.01168231E-09	-0.03635805E+06	-0.01502191E+03					4
KOH	81092H	1K	1O	1	G	0300.00	2000.00	1000.00	1
	0.09996477E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-0.05262511E+06	-0.04533806E+03	0.09996477E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.05262511E+06	-0.04533805E+03					4
KOH+	81092H	1K	1O	1E	-1G	0300.00	5000.00	1000.00	1
	0.05583889E+02	0.01372118E-01	-0.04239710E-05	0.06231942E-09	-0.03548772E-13				2
	0.05821436E+06	-0.02017959E+02	0.05036081E+02	0.04278173E-01	-0.04213406E-04				3
	0.01114253E-07	0.03757057E-11	0.05823345E+06	0.03093667E+01					4
ME2GAET	62987GA	1C	4H	11	G	0300.00	1500.00	0600.00	1
	0.07174541E+02	0.03235532E+00	0.01495199E-04	-0.01048226E-06	0.03053962E-10				2
	-0.06383914E+05	-0.02026765E+02	-0.03218207E+02	0.06398884E+00	0.01554552E-03				3
	-0.01284710E-05	0.09441259E-09	-0.04451897E+05	0.04848091E+03					4
MEGAET	62987GA	1C	3H	8	G	0300.00	1500.00	0600.00	1
	0.06600990E+02	0.02284791E+00	0.01013375E-04	-0.07318046E-07	0.02140197E-10				2
	0.04071593E+05	0.05239052E+01	-0.08169937E+01	0.04554296E+00	0.01053133E-03				3
	-0.09079987E-06	0.06700564E-09	0.05448005E+05	0.03655502E+03					4
MEGAET2	62987GA	1C	5H	13	G	0300.00	1500.00	0600.00	1
	0.08123156E+02	0.03978908E+00	0.01690979E-04	-0.01308415E-06	0.03852599E-10				2
	-0.08091057E+05	-0.05039992E+02	-0.05607499E+02	0.08187357E+00	0.01920530E-03				3
	-0.01678979E-05	0.01243354E-08	-0.05546688E+05	0.06163371E+03					4
MG	81292MG	1			G	0300.00	5000.00	1000.00	1
	0.02392633E+02	0.02085925E-02	-0.01269898E-05	0.02553204E-09	-0.04502495E-14				2
	0.01704914E+06	0.04211876E+02	0.02416375E+02	0.05325518E-02	-0.01135514E-04				3
	0.09757325E-08	-0.02898280E-11	0.01701992E+06	0.03983786E+02					4
MG(L)	81292MG	1			L	0300.00	2500.00	1000.00	1
	0.02664314E+02	0.01304526E-01	-0.07547418E-07	0.06776047E-10	-0.01436523E-13				2
	0.02234430E+04	-0.01047801E+03	0.02161491E+02	0.04242991E-01	-0.06464607E-04				3
	0.06116790E-07	-0.02090033E-10	0.02996028E+04	-0.08229090E+02					4
MG(S)	81292MG	1			S	0300.00	2000.00	1000.00	1
	0.02318547E+02	0.01929427E-01	-0.01682130E-05	0.04131403E-09	-0.01669293E-13				2
	-0.07634172E+04	-0.09802473E+02	0.01505637E+02	0.09217769E-01	-0.01955590E-03				3
	0.02020331E-06	-0.07251403E-10	-0.07226661E+04	-0.06689818E+02					4
MG+	81292MG	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02504405E+02	-0.08920014E-04	0.06671727E-07	-0.02081615E-10	0.02311490E-14				2
	0.01064936E+07	0.04292208E+02	0.02498282E+02	0.01465863E-03	-0.03808341E-06				3
	0.04118195E-09	-0.01573362E-12	0.01064953E+07	0.04322873E+02					4
MG2	81292MG	2			G	0300.00	5000.00	1000.00	1
	0.03671278E+02	-0.02125120E-02	0.01013096E-05	-0.02144628E-09	0.01719351E-13				2
	0.03362331E+06	0.08548934E+02	0.04345606E+02	-0.02080614E-01	0.01110301E-04				3
	0.08675645E-08	-0.07025087E-11	0.03346530E+06	0.05134171E+02					4
MG2BR4	81292BR	4MG	2		G	0300.00	5000.00	1000.00	1
	0.01577579E+03	0.02832096E-02	-0.01343784E-05	0.02764443E-09	-0.02066139E-13				2
	-0.09710095E+06	-0.03457961E+03	0.01476089E+03	0.03361559E-01	-0.02433120E-04				3
	-0.05502974E-08	0.08111758E-11	-0.09687714E+06	-0.02950851E+03					4
MG2C3(S)	81292C	3MG	2		S	0300.00	2500.00	1000.00	1
	0.01239169E+03	0.04624400E-01	-0.02484800E-04	0.08656213E-08	-0.01151950E-11				2
	0.05393315E+05	-0.06051988E+03	-0.01026610E+02	0.07016433E+00	-0.01240220E-02				3
	0.01009934E-05	-0.03082738E-09	0.07664551E+05	0.01701243E+02					4
MG2F4	81292F	4MG	2		G	0300.00	5000.00	1000.00	1
	0.01441927E+03	0.01917749E-01	-0.08894670E-05	0.01801607E-08	-0.01331627E-12				2

-0.02113316E+07-0.04283410E+03 0.08770948E+02 0.01784847E+00-0.01109718E-03	3
-0.04603306E-07 0.04695460E-10-0.02099919E+07-0.01422645E+03	4
MGAL2O4 (S) 81292AL 2MG 1O 4 S 0300.00 2800.00 1000.00	1
0.01495895E+03 0.08818509E-01-0.03160711E-04 0.01013391E-07-0.01228526E-11	2
-0.02817956E+07-0.07811436E+03-0.04868005E+02 0.01055641E+01-0.01821902E-02	3
0.01481432E-05-0.04514191E-09-0.02784436E+07 0.01382603E+03	4
MGB2 (S) 81292B 2MG 1 S 0300.00 2000.00 1000.00	1
0.06619755E+02 0.01322195E-01 0.04697857E-05 0.03681802E-08-0.01739753E-11	2
-0.01346401E+06-0.03460640E+03 0.04176086E+02 0.06396544E-01-0.05616456E-04	3
0.07092297E-07-0.03442529E-10-0.01255609E+06-0.02118159E+03	4
MGBR 81292BR 1MG 1 G 0300.00 5000.00 1000.00	1
0.04385933E+02 0.01975075E-02-0.06117347E-06 0.01027103E-09-0.03876260E-14	2
-0.05584836E+05 0.04357095E+02 0.03932960E+02 0.01518559E-01-0.09413456E-05	3
-0.03806534E-08 0.04026288E-11-0.05481871E+05 0.06634707E+02	4
MGBR2 81292BR 2MG 1 G 0300.00 5000.00 1000.00	1
0.07282371E+02 0.02671005E-02-0.01246470E-05 0.02534839E-09-0.01878437E-13	2
-0.03865522E+06-0.05463838E+02 0.06436183E+02 0.02723204E-01-0.01828290E-04	3
-0.05509276E-08 0.06681264E-11-0.03845914E+06-0.01198273E+02	4
MGBR2+ 81292BR 2MG 1E -1 G 0300.00 5000.00 1000.00	1
0.07317323E+02 0.02252288E-02-0.01039562E-05 0.02025280E-09-0.01333602E-13	2
0.08575141E+06-0.03144653E+02 0.06600891E+02 0.02322271E-01-0.01575443E-04	3
-0.04621806E-08 0.05719750E-11 0.08591576E+06 0.04604670E+01	4
MGC2 (S) 81292C 2MG 1 S 0300.00 2500.00 1000.00	1
0.07427011E+02 0.02786444E-01-0.01500518E-04 0.05235992E-08-0.06981197E-12	2
0.08069270E+05-0.03697419E+03-0.06510206E+01 0.04230993E+00-0.07491559E-03	3
0.06109534E-06-0.01867195E-09 0.09434739E+05 0.04708862E+01	4
MGCL 81292CL 1MG 1 G 0300.00 5000.00 1000.00	1
0.04335941E+02 0.02574531E-02-0.09346352E-06 0.01898185E-09-0.01405830E-13	2
-0.06564693E+05 0.03214818E+02 0.03708081E+02 0.02069048E-01-0.01328293E-04	3
-0.04347061E-08 0.05033764E-11-0.06418555E+05 0.06382778E+02	4
MGCL2 81292CL 2MG 1 G 0300.00 5000.00 1000.00	1
0.07176871E+02 0.03917414E-02-0.01814155E-05 0.03670114E-09-0.02710187E-13	2
-0.04941693E+06-0.07830507E+02 0.06000831E+02 0.03745347E-01-0.02447708E-04	3
-0.07873749E-08 0.09100925E-11-0.04913880E+06-0.01880677E+02	4
MGCL2 (S) 81292CL 2MG 1 S 0300.00 2000.00 1000.00	1
0.08460549E+02 0.02204761E-01-0.06316590E-05 0.02617815E-08-0.05082748E-12	2
-0.07983216E+06-0.03816537E+03 0.04852236E+02 0.02102714E+00-0.03667994E-03	3
0.03032449E-06-0.09279303E-10-0.07928891E+06-0.02175204E+03	4
MGCO3 (S) 81292C 1MG 1O 3 S 0300.00 1000.00 1000.00	1
0.01585340E+03 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
-0.01402924E+07-0.08639698E+03 0.01344667E+02 0.03695912E+00-0.04452165E-03	3
0.03181716E-06-0.09745892E-10-0.01354278E+07-0.09041713E+02	4
MGF 81292F 1MG 1 G 0300.00 5000.00 1000.00	1
0.04166004E+02 0.04434929E-02-0.01720072E-05 0.03280565E-09-0.02190876E-13	2
-0.02980270E+06 0.02577443E+02 0.03172942E+02 0.03157075E-01-0.02008009E-04	3
-0.04636928E-08 0.06097890E-11-0.02955269E+06 0.07654193E+02	4
MGF2 81292F 2MG 1 G 0300.00 5000.00 1000.00	1
0.06314408E+02 0.08013760E-02-0.03622602E-05 0.07202929E-09-0.05250556E-13	2
-0.08944590E+06-0.05637362E+02 0.04365511E+02 0.06150098E-01-0.04077014E-04	3
-0.07490467E-08 0.01130754E-10-0.08895505E+06 0.04323487E+02	4
MGF2 (S) 81292F 2MG 1 S 0300.00 2000.00 1000.00	1
0.08170168E+02 0.02353222E-01-0.01060785E-04 0.02392788E-08-0.01594861E-12	2
-0.01379692E+07-0.04083052E+03 0.01762995E+02 0.03056669E+00-0.04933989E-03	3
0.03778577E-06-0.01108964E-09-0.01367476E+07-0.01039233E+03	4
MGF2+ 81292F 2MG 1E -1 G 0300.00 5000.00 1000.00	1
0.06819974E+02 0.08267521E-02-0.03871799E-05 0.07864547E-09-0.05589085E-13	2
0.06903427E+06-0.08313943E+02 0.04782002E+02 0.06580736E-01-0.04470059E-04	3
-0.08656625E-08 0.01305586E-10 0.06953005E+06 0.02038302E+02	4
MGH 81292H 1MG 1 G 0300.00 5000.00 1000.00	1
0.03501857E+02 0.01196289E-01-0.04870483E-05 0.09616032E-09-0.06566165E-13	2
0.01915847E+06 0.02762077E+02 0.02929127E+02 0.02881565E-01-0.03702138E-04	3
0.03761425E-07-0.01569289E-10 0.01935649E+06 0.05809553E+02	4
MGH2 (S) 81292H 2MG 1 S 0300.00 2000.00 1000.00	1
0.04503751E+02 0.05009365E-01-0.07076169E-05-0.09321345E-08 0.03016174E-11	2
-0.01106837E+06-0.02418625E+03-0.09052193E+00 0.01938007E+00-0.01936573E-03	3
0.01164904E-06-0.03397887E-10-0.09845471E+05-0.07606392E+01	4

MGH2O2	81292H	2MG	1O	2	G	0300.00	5000.00	1000.00	1
0.08302454E+02	0.03712996E-01	-0.01279645E-04	0.02102831E-08	-0.01337217E-12					2
-0.07153173E+06	-0.01640682E+03	0.04724303E+02	0.01611746E+00	-0.01291007E-03					3
0.05703660E-08	0.02430663E-10	-0.07085783E+06	0.09898885E+01						4
MGH2O2 (S)	81292H	2MG	1O	2	S	0300.00	1000.00	1000.00	1
0.01381001E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-0.01162998E+07	-0.07323205E+03	-0.04220693E+02	0.07726916E+00	-0.01383568E-02					3
0.01155986E-05	-0.03648025E-09	-0.01123883E+07	0.01381610E+03						4
MGN	81292MG	1N	1		G	0300.00	5000.00	1000.00	1
0.04177825E+02	0.04387980E-02	-0.01726040E-05	0.03444124E-09	-0.02516521E-13					2
0.03340716E+06	0.02969357E+02	0.03200092E+02	0.03139739E-01	-0.02045035E-04					3
-0.04125930E-08	0.05937391E-11	0.03365107E+06	0.07958522E+02						4
MGO (S)	81292MG	1O	1		S	0300.00	4000.00	1000.00	1
0.04857470E+02	0.01952289E-01	-0.08605956E-05	0.02101340E-08	-0.01886027E-12					2
-0.07394488E+06	-0.02524503E+03	0.01971740E+02	0.01095483E+00	-0.08169910E-04					3
0.06359402E-08	0.02019714E-10	-0.07332016E+06	-0.01088662E+03						4
MGOH	81292H	1MG	1O	1	G	0300.00	5000.00	1000.00	1
0.05156858E+02	0.01849251E-01	-0.06339213E-05	0.01026031E-08	-0.06282974E-13					2
-0.02145938E+06	-0.02774689E+02	0.03347871E+02	0.08101305E-01	-0.06443066E-04					3
0.02006805E-08	0.01261718E-10	-0.02111816E+06	0.06024177E+02						4
MGOH+	81292H	1MG	1O	1E	-1G	0300.00	5000.00	1000.00	1
0.05171484E+02	0.01835998E-01	-0.06314934E-05	0.01036229E-08	-0.06583402E-13					2
0.06865354E+06	-0.03526109E+02	0.03383351E+02	0.08055572E-01	-0.06452790E-04					3
0.02400212E-08	0.01246873E-10	0.06898753E+06	0.05158118E+02						4
MGS	81292MG	1S	1		G	0300.00	5000.00	1000.00	1
0.01071331E+03	-0.06086042E-01	0.02390833E-04	-0.04174042E-08	0.02737530E-12					2
0.01317442E+06	-0.03521998E+03	0.03789723E+02	-0.03985028E-01	0.02217192E-03					3
-0.01858825E-06	0.03239714E-10	0.01635406E+06	0.05868810E+02						4
MGS (S)	81292MG	1S	1		S	0300.00	3000.00	1000.00	1
0.05581918E+02	0.08031267E-02	-0.01812239E-05	0.04113088E-09	-0.02798069E-13					2
-0.04331716E+06	-0.02607368E+03	0.04076152E+02	0.07088011E-01	-0.09604458E-04					3
0.06056009E-07	-0.01373560E-10	-0.04304232E+06	-0.01890776E+03						4
MGSO4 (S)	81292MG	1O	4S	1	S	0300.00	2500.00	1000.00	1
0.08845820E+02	0.01221900E+00	-0.02141897E-04	-0.09580988E-08	0.02954552E-11					2
-0.01549512E+07	-0.04302983E+03	0.02258418E+02	0.04788929E+00	-0.07110586E-03					3
0.05630850E-06	-0.01709008E-09	-0.01540505E+07	-0.01345647E+03						4
N	120186N	1			G	0300.00	5000.00	1000.00	1
0.02450268E+02	0.01066146E-02	-0.07465337E-06	0.01879652E-09	-0.01025984E-13					2
0.05611604E+06	0.04448758E+02	0.02503071E+02	-0.02180018E-03	0.05420529E-06					3
-0.05647560E-09	0.02099904E-12	0.05609890E+06	0.04167566E+02						4
N*C3H7	120186C	3H	7		G	0300.00	5000.00	1000.00	1
0.07978291E+02	0.01576113E+00	-0.05173243E-04	0.07443892E-08	-0.03824978E-12					2
0.07579402E+05	-0.01935611E+03	0.01922537E+02	0.02478927E+00	0.01810249E-04					3
-0.01783266E-06	0.08582996E-10	0.09713281E+05	0.01399271E+03						4
N2	121286N	2			G	0300.00	5000.00	1000.00	1
0.02926640E+02	0.01487977E-01	-0.05684761E-05	0.01009704E-08	-0.06753351E-13					2
-0.09227977E+04	0.05980528E+02	0.03298677E+02	0.01408240E-01	-0.03963222E-04					3
0.05641515E-07	-0.02444855E-10	-0.01020900E+05	0.03950372E+02						4
N2H2	121286N	2H	2		G	0300.00	5000.00	1000.00	1
0.03371185E+02	0.06039968E-01	-0.02303854E-04	0.04062789E-08	-0.02713144E-12					2
0.02418172E+06	0.04980585E+02	0.01617999E+02	0.01306312E+00	-0.01715712E-03					3
0.01605608E-06	-0.06093639E-10	0.02467526E+06	0.01379467E+03						4
N2H3	120186N	2H	3		G	0300.00	5000.00	1000.00	1
0.04441846E+02	0.07214271E-01	-0.02495684E-04	0.03920565E-08	-0.02298950E-12					2
0.01664221E+06	-0.04275205E+01	0.03174204E+02	0.04715907E-01	0.01334867E-03					3
-0.01919685E-06	0.07487564E-10	0.01727270E+06	0.07557224E+02						4
N2H4	121286N	2H	4		G	0300.00	5000.00	1000.00	1
0.04977317E+02	0.09595519E-01	-0.03547639E-04	0.06124299E-08	-0.04029795E-12					2
0.09341219E+05	-0.02962990E+02	0.06442606E+00	0.02749730E+00	-0.02899451E-03					3
0.01745240E-06	-0.04422282E-10	0.01045192E+06	0.02127789E+03						4
N2H4 (L)	90589H	4N	2		L	0300.00	0600.00	0450.00	1
0.08890683E+02	0.08330343E-01	0.04945549E-04	-0.04909251E-08	-0.03355824E-10					2
0.03032250E+05	-0.03871433E+03	0.09047444E+02	0.09241592E-01	0.02263547E-04					3
-0.08952247E-07	0.01486863E-09	0.02970393E+05	-0.03974034E+03						4
N2O	121286N	2O	1		G	0300.00	5000.00	1000.00	1
0.04718977E+02	0.02873714E-01	-0.01197496E-04	0.02250552E-08	-0.01575337E-12					2

0.08165811E+05-0.01657250E+02	0.02543058E+02	0.09492193E-01-0.09792775E-04	3
0.06263845E-07-0.01901826E-10	0.08765100E+05	0.09511222E+02	4
N2O+	121286N 2O 1E -1	G 0300.00 5000.00 1000.00	1
0.05398516E+02	0.02249478E-01-0.09577057E-05	0.01823193E-08-0.01284422E-12	2
0.01584851E+07-0.03733146E+02	0.03187228E+02	0.08350714E-01-0.07894549E-04	3
0.04597445E-07-0.01381075E-10	0.01591279E+07	0.07779426E+02	4
N2O4	121286N 2O 4	G 0300.00 5000.00 1000.00	1
0.01048220E+03	0.05972272E-01-0.02564044E-04	0.04916885E-08-0.03490969E-12	2
-0.02849989E+05-0.02612289E+03	0.03624593E+02	0.02474708E+00-0.02172875E-03	3
0.09927104E-07-0.02222817E-10-0.09128241E+04	0.09457174E+02		4
N3	121286N 3	G 0300.00 5000.00 1000.00	1
0.05208505E+02	0.02444507E-01-0.01038941E-04	0.01977417E-08-0.01395644E-12	2
0.04796178E+06-0.03612756E+02	0.02882219E+02	0.08930338E-01-0.08539038E-04	3
0.05045585E-07-0.01521248E-10	0.04863468E+06	0.08481757E+02	4
NA	80792NA 1	G 0300.00 5000.00 1000.00	1
0.02574480E+02-0.01605880E-02	0.01250641E-05-0.04516576E-09	0.06941745E-13	2
0.01219129E+06	0.03830900E+02	0.02591348E+02-0.05961520E-02	3
-0.01211123E-07	0.03890067E-11	0.01220642E+06	4
NA(L)	81092NA 1	L 0300.00 2000.00 1000.00	1
0.04030581E+02-0.01320419E-01	0.04136604E-05	0.05486936E-08-0.01916626E-11	2
-0.07899189E+04-0.01548589E+03	0.04682137E+02-0.03624112E-01	0.04776195E-04	3
-0.03871514E-07	0.01518150E-10-0.09807172E+04-0.01881830E+03		4
NA+	80792NA 1E -1	G 0300.00 5000.00 1000.00	1
0.02500252E+02	0.00000000E+00	0.00000000E+00	2
0.07260903E+06	0.03538490E+02	0.02500252E+02	3
0.00000000E+00	0.00000000E+00	0.07260904E+06	4
NA2	80792NA 2	G 0300.00 5000.00 1000.00	1
0.04480669E+02	0.02178011E-02-0.01102830E-06	0.02208498E-10-0.01614866E-14	2
0.01519313E+06	0.02073203E+02	0.04369675E+02	3
0.08752245E-09	0.02980178E-12	0.01521703E+06	4
NA2B4O7(S)	81292B 4NA 2O 7	S 0300.00 2000.00 1000.00	1
0.02061542E+03	0.01728323E+00-0.04016503E-04-0.07600982E-08	0.05580242E-11	2
-0.04014288E+07-0.01006093E+04	0.01430907E+02	0.01167214E+01-0.02000861E-02	3
0.01698028E-05-0.05418888E-09-0.03982982E+07-0.01265829E+03			4
NA2B6O10(S)	81292B 6NA 2O 10	S 0300.00 2000.00 1000.00	1
0.02989617E+03	0.03053411E+00-0.02146684E-04-0.04458443E-07	0.09406424E-11	2
-0.05638429E+07-0.01571271E+04	0.09347958E+02	0.08948274E+00-0.01024848E-02	3
0.01015647E-05-0.04314482E-09-0.05570116E+07-0.04828430E+03			4
NA2C2N2	81292C 2N 2NA 2	G 0300.00 5000.00 1000.00	1
0.01253426E+03	0.03485206E-01-0.01426483E-04	0.02648455E-08-0.01838071E-12	2
-0.05033986E+05-0.03087649E+03	0.01092445E+03	0.09724206E-01-0.01190420E-03	3
0.08942515E-07-0.02847524E-10-0.04654688E+05-0.02294170E+03			4
NA2F2	80792F 2NA 2	G 0300.00 5000.00 1000.00	1
0.09265403E+02	0.09044011E-02-0.04233919E-05	0.08630666E-09-0.06408558E-13	2
-0.01047310E+07-0.01880290E+03	0.06422050E+02	0.09031559E-01-0.05593408E-04	3
-0.02581729E-07	0.02547837E-10-0.01040718E+07-0.04453081E+02		4
NA2H2O2	80792H 2NA 2O 2	G 0300.00 5000.00 1000.00	1
0.09347846E+02	0.05678318E-01-0.02077824E-04	0.03568716E-08-0.02342868E-12	2
-0.07634945E+06-0.01850110E+03	0.05441492E+02	0.01814821E+00-0.01733029E-03	3
0.09077551E-07-0.02055174E-10-0.07536770E+06	0.01240430E+02		4
NA2O(L)	81092NA 2O 1	L 0300.00 3000.00 1000.00	1
0.01258178E+03	0.00000000E+00	0.00000000E+00	2
-0.04859891E+06-0.06066678E+03	0.01258178E+03	0.00000000E+00	3
0.00000000E+00	0.00000000E+00-0.04859891E+06-0.06066677E+03		4
NA2O(S)	81092NA 2O 1	S 0300.00 2000.00 1000.00	1
0.08804423E+02	0.03253428E-01-0.03530522E-05-0.04324117E-08	0.01394574E-11	2
-0.05257507E+06-0.04209654E+03	0.04776964E+02	0.01483269E+00-0.01052247E-03	3
0.01278469E-07	0.01046187E-10-0.05155651E+06-0.02156737E+03		4
NA2O2	81092NA 2O 2	S 0300.00 2500.00 1000.00	1
0.01382402E+03-0.03556455E-02	0.02837263E-05-0.09701692E-09	0.01205762E-12	2
-0.06583802E+06-0.06789536E+03	0.08035418E+02	0.05983777E-01	3
-0.03410482E-06	0.01439706E-09-0.06395152E+06-0.03604480E+03		4
NA2SO4	80792NA 2O 4S 1	G 0300.00 5000.00 1000.00	1
0.01506456E+03	0.04508233E-01-0.02011474E-04	0.03963989E-08-0.02871466E-12	2
-0.01296053E+07-0.04683857E+03	0.05752581E+02	0.02964118E+00-0.02035211E-03	3
-0.01073243E-07	0.03960597E-10-0.01271767E+07	0.01016246E+02	4

NA2SO4 (D)	81092NA	2O	4S	1	S	0300.00	1500.00	1000.00	1
0.01062092E+03	0.01179912E+00	0.03608537E-04	-0.03424054E-09	-0.09650399E-11					2
-0.01684493E+07	-0.04191208E+03	0.01187237E+03	0.04287018E+00	-0.09072926E-03					3
0.09042235E-06	-0.02940634E-09	-0.01707163E+07	-0.05750085E+03						4
NA2SO4 (i)	81092NA	2O	4S	1	S	0300.00	1500.00	1000.00	1
0.01711668E+03	0.05878399E-01	0.01196697E-04	0.01676018E-08	-0.02640822E-11					2
-0.01714447E+07	-0.07997372E+03	0.01674756E+03	0.01133662E+00	-0.01526634E-03					3
0.01819548E-06	-0.06918027E-10	-0.01714932E+07	-0.07899648E+03						4
NA2SO4 (iii)	81092NA	2O	4S	1	S	0300.00	1000.00	1000.00	1
0.03701786E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-0.01854858E+07	-0.02084472E+04	0.01413394E+03	-0.01694491E+00	0.09403022E-03					3
-0.07815722E-06	0.02395583E-09	-0.01707247E+07	-0.06037737E+03						4
NA2SO4 (iv)	81092NA	2O	4S	1	S	0300.00	1000.00	1000.00	1
0.02590382E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-0.01779857E+07	-0.01365608E+04	0.05917499E+02	0.04507074E+00	-0.05672574E-03					3
0.04596655E-06	-0.01432523E-09	-0.01702527E+07	-0.02694892E+03						4
NA2SO4 (v)	81092NA	2O	4S	1	S	0300.00	1000.00	1000.00	1
0.02590382E+03	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-0.01780169E+07	-0.01366284E+04	0.05917499E+02	0.04507074E+00	-0.05672574E-03					3
0.04596655E-06	-0.01432523E-09	-0.01702840E+07	-0.02701654E+03						4
NA3CL6AL (S)	81292AL	1CL	6NA	3	S	0300.00	2000.00	1000.00	1
0.02863182E+03	0.08169580E-01	0.01787040E-05	-0.09984084E-08	0.01787581E-11					2
-0.02473307E+07	-0.01246570E+04	0.02610594E+03	0.09148861E-01	0.09743193E-04					3
0.01296166E-06	0.04124132E-10	-0.02462808E+07	-0.01099689E+04						4
NA3F6AL (S)	81292AL	1F	6NA	3	S	0300.00	1200.00	1000.00	1
0.01867366E+03	0.02426805E+00	0.01311169E-04	-0.01223061E-06	0.06326451E-10					2
-0.04056682E+07	-0.08492075E+03	0.01182130E+03	0.07831376E+00	-0.01387551E-02					3
0.01331742E-05	-0.04620547E-09	-0.04049948E+07	-0.05693419E+03						4
NABH4 (S)	81292B	1H	4NA	1	S	0300.00	2000.00	1000.00	1
0.08204329E+02	0.01008304E+00	-0.01032261E-04	-0.02815504E-07	0.09005147E-11					2
-0.02614390E+06	-0.03790153E+03	0.08076391E+02	0.05407829E-01	0.01208139E-03					3
-0.01450540E-06	0.04279918E-10	-0.02580298E+06	-0.03584760E+03						4
NABO2	81092B	1NA	1O	2	G	0300.00	5000.00	1000.00	1
0.07449052E+02	0.02730088E-01	-0.01165145E-04	0.02226924E-08	-0.01578063E-12					2
-0.08056425E+06	-0.09194809E+02	0.04413702E+02	0.01144045E+00	-0.01021892E-03					3
0.04340556E-07	-0.07548787E-11	-0.07974780E+06	0.06401325E+02						4
NABO2 (S)	81292B	1NA	1O	2	S	0300.00	2000.00	1000.00	1
0.07820448E+02	0.06702746E-01	-0.01488126E-04	-0.01033983E-07	0.04130615E-11					2
-0.01203511E+07	-0.03848530E+03	0.01695994E+02	0.03131723E+00	-0.04453876E-03					3
0.03572163E-06	-0.01178195E-09	-0.01189335E+07	-0.08471359E+02						4
NABR	81092BR	1NA	1	G	0300.00	5000.00	1000.00	1	
0.04424304E+02	0.01887477E-02	-0.04500799E-06	0.09226701E-10	-0.06871650E-14					2
-0.01865205E+06	0.03707466E+02	0.04097639E+02	0.01170972E-01	-0.07798224E-05					3
-0.01611608E-08	0.02489549E-11	-0.01857889E+06	0.05343556E+02						4
NABR (L)	81292BR	1NA	1	L	0300.00	2500.00	1000.00	1	
0.07498742E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-0.04305332E+06	-0.03017306E+03	0.07498742E+02	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-0.04305333E+06	-0.03017306E+03						4
NABR (S)	81292BR	1NA	1	S	0300.00	2000.00	1000.00	1	
0.05741811E+02	0.01766697E-01	-0.01899553E-05	0.01473021E-09	0.01715605E-12					2
-0.04526151E+06	-0.02279248E+03	0.04706446E+02	0.08010188E-01	-0.01346175E-03					3
0.01196933E-06	-0.03873765E-10	-0.04513442E+06	-0.01826015E+03						4
NACH	80792C	1N	1NA	1	G	0300.00	5000.00	1000.00	1
0.05791865E+02	0.01708993E-01	-0.06965832E-05	0.01288980E-08	-0.08921502E-13					2
0.09496355E+05	-0.04320624E+02	0.05123989E+02	0.04411283E-01	-0.05682223E-04					3
0.04664804E-07	-0.01593603E-10	0.09657925E+05	-0.01032367E+02						4
NACL	81092CL	1NA	1	G	0300.00	5000.00	1000.00	1	
0.04393820E+02	0.02153336E-02	-0.06198756E-06	0.01266879E-09	-0.09427806E-14					2
-0.02315864E+06	0.02486064E+02	0.03953003E+02	0.01514187E-01	-0.09819465E-05					3
-0.02807090E-08	0.03543574E-11	-0.02305831E+06	0.04701214E+02						4
NACL (S)	81092CL	1NA	1	S	0300.00	1500.00	1000.00	1	
0.07639640E+02	-0.03933726E-01	0.02071020E-04	0.04233998E-07	-0.02204761E-10					2
-0.05163684E+06	-0.03397957E+03	0.04982695E+02	0.05432908E-01	-0.07698454E-04					3
0.06300821E-07	-0.01211800E-10	-0.05112201E+06	-0.02104512E+03						4
NACL4AL (S)	81292AL	1CL	4NA	1	S	0300.00	2000.00	1000.00	1
0.02138498E+03	0.03252454E-01	-0.01769716E-05	-0.07072990E-08	0.01928080E-11					2

-0.01447874E+07-0.01021539E+04 0.01588411E+03 0.04527768E-01 0.02409928E-03	3
-0.03108224E-06 0.01051706E-09-0.01424874E+07-0.07002475E+03	4
NACN 81092C 1N 1NA 1 G 0300.00 5000.00 1000.00	1
0.05791865E+02 0.01708993E-01-0.06965832E-05 0.01288980E-08-0.08921502E-13	2
0.09496355E+05-0.04320624E+02 0.05123989E+02 0.04411283E-01-0.05682223E-04	3
0.04664804E-07-0.01593603E-10 0.09657925E+05-0.01032367E+02	4
NACN(S) 81292C 1N 1NA 1 S 0300.00 2000.00 1000.00	1
0.08137501E+02 0.03044670E-02-0.01811052E-05 0.08281245E-09-0.01435891E-12	2
-0.01334049E+06-0.03217693E+03 0.08239171E+02-0.05281579E-03 0.03829305E-05	3
-0.03800801E-08 0.01401136E-11-0.01336670E+06-0.03268830E+03	4
NAF 80792F 1NA 1 G 0300.00 5000.00 1000.00	1
0.04289078E+02 0.03377828E-02-0.01184403E-05 0.02398348E-09-0.01772778E-13	2
-0.03626513E+06 0.01538309E+02 0.03532346E+02 0.02495132E-01-0.01587195E-04	3
-0.04836335E-08 0.05739804E-11-0.03608573E+06 0.05367920E+02	4
NAF2- 81092F 2NA 1E 1 G 0300.00 5000.00 1000.00	1
0.07302279E+02 0.05655084E-02-0.02615340E-05 0.05285863E-09-0.03900402E-13	2
-0.08272088E+06-0.01028459E+03 0.05382830E+02 0.05231638E-01-0.03350411E-04	3
-0.01169983E-07 0.01291137E-10-0.08232816E+06-0.01928436E+02	4
NAF4AL 81092AL 1F 4NA 1 G 0300.00 5000.00 1000.00	1
0.01407161E+03 0.02285303E-01-0.01043457E-04 0.02090484E-08-0.01532874E-12	2
-0.02260449E+07-0.04013149E+03 0.08103421E+02 0.01881143E+00-0.01205279E-03	3
-0.03477927E-07 0.04123038E-10-0.02245760E+07-0.09731781E+02	4
NAH 80792H 1NA 1 G 0300.00 5000.00 1000.00	1
0.03818649E+02 0.08597439E-02-0.03202059E-05 0.06146711E-09-0.04364567E-13	2
0.01368120E+06 0.04367959E+01 0.02864363E+02 0.03308582E-01-0.02753919E-04	3
0.01399522E-07-0.04032581E-11 0.01396756E+06 0.05450493E+02	4
NAI(S) 81292I 1NA 1 S 0300.00 2000.00 1000.00	1
0.05987605E+02 0.01342139E-01-0.03807255E-06 0.01660138E-09-0.06066889E-13	2
-0.03648630E+06-0.02270427E+03 0.05407032E+02 0.04235908E-01-0.05679955E-04	3
0.04941357E-07-0.01602135E-10-0.03638396E+06-0.02000921E+03	4
NAO 80792NA 1O 1 G 0300.00 5000.00 1000.00	1
0.04349803E+02 0.02849959E-02-0.08615992E-06 0.01754054E-09-0.01301677E-13	2
0.08731694E+05 0.02618339E+02 0.03765728E+02 0.01980031E-01-0.01256303E-04	3
-0.03909831E-08 0.04664039E-11 0.08866889E+05 0.05562273E+02	4
NAO- 80792NA 1O 1E 1 G 0300.00 5000.00 1000.00	1
0.04343846E+02 0.02955424E-02-0.08923111E-06 0.01813572E-09-0.01343290E-13	2
-0.01592823E+06 0.01245911E+02 0.03740064E+02 0.02044313E-01-0.01291719E-04	3
-0.04080754E-08 0.04823669E-11-0.01578820E+06 0.04290303E+02	4
NAO2(S) 81092NA 1O 2 S 0300.00 2000.00 1000.00	1
0.07379480E+02 0.04377048E-01 0.06355202E-05-0.03238946E-08 0.06014399E-12	2
-0.03376432E+06-0.02946090E+03 0.07236605E+02 0.04751740E-01 0.03458707E-05	3
-0.02971627E-08 0.09124652E-12-0.03372514E+06-0.02872050E+03	4
NAO2AL(S) 81292AL 1NA 1O 2 S 0300.00 3000.00 1000.00	1
0.09963634E+02 0.02329677E-01-0.08188510E-07 0.02070425E-09-0.02306699E-12	2
-0.01394255E+07-0.04932653E+03 0.03669741E+02 0.02226343E+00-0.01558734E-03	3
-0.03446683E-07 0.05383614E-10-0.01381199E+07-0.01818990E+03	4
NAOH 80792H 1NA 1O 1 G 0300.00 5000.00 1000.00	1
0.05527852E+02 0.01420623E-01-0.04439615E-05 0.06635639E-09-0.03866820E-13	2
-0.02545869E+06-0.04374785E+02 0.04727895E+02 0.05001262E-01-0.04534391E-04	3
0.07051240E-08 0.06671123E-11-0.02537947E+06-0.07649678E+01	4
NAOH(L) 81092H 1NA 1O 1 L 0300.00 2500.00 1000.00	1
0.01061400E+03-0.03116447E-02-0.02964198E-05 0.05475463E-09 0.01021178E-12	2
-0.05327943E+06-0.05120959E+03 0.01079389E+03-0.08545728E-02 0.03780039E-05	3
-0.03848777E-08 0.01384542E-11-0.05332840E+06-0.05213201E+03	4
NAOH+ 80792H 1NA 1O 1E -1G 0300.00 5000.00 1000.00	1
0.05570452E+02 0.01387979E-01-0.04311444E-05 0.06372652E-09-0.03648954E-13	2
0.07985595E+06-0.02878876E+02 0.04974624E+02 0.04424591E-01-0.04296418E-04	3
0.01067747E-07 0.04168198E-11 0.07988680E+06-0.03068088E+01	4
NCN 103190C 1N 2 G 0300.00 4000.00 1500.00	1
0.06652121E+02 0.06108034E-02-0.01389727E-05 0.02695549E-10 0.01669944E-13	2
0.05172403E+06-0.01138517E+03 0.03101270E+02 0.09981674E-01-0.09920701E-04	3
0.04758919E-07-0.08968626E-11 0.05285757E+06 0.07317579E+02	4
NCO 110193C 1N 1O 1 G 0300.00 4000.00 1400.00	1
0.06072346E+02 0.09227829E-02-0.09845574E-06-0.04764123E-09 0.09090445E-13	2
0.01359820E+06-0.08507293E+02 0.03359593E+02 0.05393239E-01-0.08144585E-05	3
-0.01912868E-07 0.07836794E-11 0.01462809E+06 0.06549694E+02	4

NF	121286N	1F	1	G	0300.00	5000.00	1000.00	1
	0.03862177E+02	0.07551806E-02	-0.03044943E-05	0.05874447E-09	-0.04187479E-13			2
	0.02867243E+06	0.03457233E+02	0.02871947E+02	0.03312193E-01	-0.02691159E-04			3
	0.01121951E-07	-0.02475131E-11	0.02896257E+06	0.08640247E+02				4
NFO	121286N	1F	1O 1	G	0300.00	5000.00	1000.00	1
	0.05174520E+02	0.01938472E-01	-0.08222701E-05	0.01564291E-08	-0.01104497E-12			2
	-0.09670935E+05	-0.05352461E+01	0.03352307E+02	0.07229966E-01	-0.06951137E-04			3
	0.03828526E-07	-0.01023558E-10	-0.09167035E+05	0.08854189E+02				4
NFO2	121286N	1F	1O 2	G	0300.00	5000.00	1000.00	1
	0.06816857E+02	0.03462640E-01	-0.01492216E-04	0.02869665E-08	-0.02041857E-12			2
	-0.01560262E+06	-0.09320129E+02	0.02447529E+02	0.01544110E+00	-0.01300595E-03			3
	0.04856383E-07	-0.06852266E-11	-0.01439400E+06	0.01328360E+03				4
NH	31387H	1N	1	G	0300.00	5000.00	1000.00	1
	0.02760249E+02	0.01375346E-01	-0.04451914E-05	0.07692792E-09	-0.05017592E-13			2
	0.04207828E+06	0.05857199E+02	0.03339758E+02	0.01253009E-01	-0.03491646E-04			3
	0.04218812E-07	-0.01557618E-10	0.04185047E+06	0.02507181E+02				4
NH2	121686N	1H	2	G	0300.00	5000.00	1000.00	1
	0.02961311E+02	0.02932699E-01	-0.09063600E-05	0.01617257E-08	-0.01204200E-12			2
	0.02191977E+06	0.05777878E+02	0.03432493E+02	0.03299540E-01	-0.06613600E-04			3
	0.08590947E-07	-0.03572047E-10	0.02177228E+06	0.03090111E+02				4
NH3	121386N	1H	3	G	0300.00	5000.00	1000.00	1
	0.02461904E+02	0.06059166E-01	-0.02004977E-04	0.03136003E-08	-0.01938317E-12			2
	-0.06493270E+05	0.07472097E+02	0.02204352E+02	0.01011476E+00	-0.01465265E-03			3
	0.01447235E-06	-0.05328509E-10	-0.06525488E+05	0.08127138E+02				4
NNH	120186N	2H	1	G	0250.00	4000.00	1000.00	1
	0.04415342E+02	0.01614388E-01	-0.01632894E-05	-0.08559846E-09	0.01614791E-12			2
	0.02788029E+06	0.09042888E+01	0.03501344E+02	0.02053587E-01	0.07170410E-05			3
	0.04921348E-08	-0.09671170E-11	0.02833347E+06	0.06391837E+02				4
NO	121286N	1O	1	G	0300.00	5000.00	1000.00	1
	0.03245435E+02	0.01269138E-01	-0.05015890E-05	0.09169283E-09	-0.06275419E-13			2
	0.09800840E+05	0.06417294E+02	0.03376542E+02	0.01253063E-01	-0.03302751E-04			3
	0.05217810E-07	-0.02446263E-10	0.09817961E+05	0.05829590E+02				4
NO+	121286N	1O	1E -1	G	0300.00	5000.00	1000.00	1
	0.02914889E+02	0.01499335E-01	-0.05727972E-05	0.01017777E-08	-0.06825390E-13			2
	0.01181869E+07	0.06844346E+02	0.03297349E+02	0.01422890E-01	-0.04007441E-04			3
	0.05670551E-07	-0.02446972E-10	0.01180834E+07	0.04749948E+02				4
NO2	121286N	1O	2	G	0300.00	5000.00	1000.00	1
	0.04682859E+02	0.02462429E-01	-0.01042259E-04	0.01976902E-08	-0.01391717E-12			2
	0.02261292E+05	0.09885985E+01	0.02670600E+02	0.07838501E-01	-0.08063865E-04			3
	0.06161715E-07	-0.02320150E-10	0.02896291E+05	0.01161207E+03				4
NO2-	121286N	1O	2E 1	G	0300.00	5000.00	1000.00	1
	0.05043114E+02	0.02166428E-01	-0.09455454E-05	0.01816314E-08	-0.01238394E-12			2
	-0.02621554E+06	-0.01445905E+02	0.02448586E+02	0.08982507E-01	-0.07853431E-04			3
	0.03927277E-07	-0.01071694E-10	-0.02545097E+06	0.01213060E+03				4
NO3	121286N	1O	3	G	0300.00	5000.00	1000.00	1
	0.07120307E+02	0.03246228E-01	-0.01431613E-04	0.02797053E-08	-0.02013008E-12			2
	0.05864479E+05	0.01213730E+03	0.01221076E+02	0.01878797E+00	-0.01344321E-03			3
	0.01274601E-07	-0.01354060E-10	0.07473144E+05	0.01840203E+03				4
O	120186O	1		G	0300.00	5000.00	1000.00	1
	0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14			2
	0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04			3
	-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02				4
O+	121286O	1E	-1	G	0300.00	5000.00	1000.00	1
	0.02501869E+02	-0.06107262E-04	0.07324307E-07	-0.03438353E-10	0.05506408E-14			2
	0.01879553E+07	0.04372827E+02	0.02499273E+02	0.05820598E-04	-0.01120922E-06			3
	0.08232109E-10	-0.01916378E-13	0.01879557E+07	0.04384826E+02				4
O-	90589O	1E	1	G	0300.00	5000.00	1000.00	1
	0.02559581E+02	-0.07147888E-03	0.03301804E-06	-0.06660944E-10	0.04900727E-14			2
	0.01148935E+06	0.04426187E+02	0.02747263E+02	-0.05724860E-02	0.02712548E-05			3
	0.02691512E-08	-0.02002357E-11	0.01144395E+06	0.03469852E+02				4
O2	121386O	2		G	0300.00	5000.00	1000.00	1
	0.03697578E+02	0.06135197E-02	-0.01258842E-05	0.01775281E-09	-0.01136435E-13			2
	-0.01233930E+05	0.03189166E+02	0.03212936E+02	0.01127486E-01	-0.05756150E-05			3
	0.01313877E-07	-0.08768554E-11	-0.01005249E+05	0.06034738E+02				4
O2-	121286O	2E	1	G	0300.00	5000.00	1000.00	1
	0.03883013E+02	0.07407872E-02	-0.02961776E-05	0.05724305E-09	-0.04086548E-13			2



-0.07121644E+05	0.02658212E+02	0.02872292E+02	0.03359716E-01	-0.02664886E-04	3				
0.09807524E-08	-0.01670957E-11	-0.06829094E+05	0.07938373E+02		4				
O3	1212860	3	G	0300.00	5000.00	1000.00	1		
0.05429371E+02	0.01820380E-01	-0.07705607E-05	0.01499293E-08	-0.01075563E-12	2				
0.01523527E+06	-0.03266387E+02	0.02462609E+02	0.09582781E-01	-0.07087359E-04	3				
0.01363368E-07	0.02969647E-11	0.01606152E+06	0.01214187E+03		4				
OC(OH)2	103190C	1H	2O	3	G	0300.00	4000.00	1500.00	1
0.01124139E+03	0.02555103E-01	-0.04326538E-05	-0.05781341E-09	0.01545461E-12	2				
-0.07904865E+06	-0.03657201E+03	0.03540332E+01	0.03042528E+00	-0.02939616E-03	3				
0.01452934E-06	-0.02906245E-10	-0.07522630E+06	0.02250923E+03		4				
OCHCHO	103190C	2H	2O	2	G	0300.00	4000.00	1500.00	1
0.01056843E+03	0.02907353E-01	-0.03452401E-05	-0.01037593E-08	0.02042135E-12	2				
-0.02952623E+06	-0.03104084E+03	0.01863564E+02	0.02298297E+00	-0.01917997E-03	3				
0.08558604E-07	-0.01612346E-10	-0.02634847E+06	0.01601674E+03		4				
OCHNHO	103190C	1H	2N	2O	2G	0300.00	4000.00	1500.00	1
0.01124139E+03	0.04091551E-01	-0.04547841E-05	-0.01752324E-08	0.03271472E-12	2				
-0.06754774E+05	-0.04078722E+03	0.01405275E+02	0.02776281E+00	-0.02088466E-03	3				
0.08550259E-07	-0.01543486E-10	-0.02537631E+05	0.01937723E+03		4				
OH	1212860	1H	1	G	0300.00	5000.00	1000.00	1	
0.02882730E+02	0.01013974E-01	-0.02276877E-05	0.02174684E-09	-0.05126305E-14	2				
0.03886888E+05	0.05595712E+02	0.03637266E+02	0.01850910E-02	-0.01676165E-04	3				
0.02387203E-07	-0.08431442E-11	0.03606782E+05	0.01358860E+02		4				
OH+	1212860	1H	1E	-1	G	0300.00	5000.00	1000.00	1
0.02719059E+02	0.01508571E-01	-0.05029369E-05	0.08261952E-09	-0.04947453E-13	2				
0.01576341E+07	0.06234536E+02	0.03326979E+02	0.01345786E-01	-0.03777168E-04	3				
0.04687750E-07	-0.01780982E-10	0.01574029E+07	0.02744042E+02		4				
OH-	1212860	1H	1E	1	G	0300.00	5000.00	1000.00	1
0.02846205E+02	0.01041835E-01	-0.02416851E-05	0.02483215E-09	-0.07775605E-14	2				
-0.01807280E+06	0.04422712E+02	0.03390038E+02	0.07922381E-02	-0.01943430E-04	3				
0.02001770E-07	-0.05702087E-11	-0.01830494E+06	0.01249892E+02		4				
ONHNO	103190H	2N	2O	2	G	0300.00	4000.00	1500.00	1
0.01005510E+03	0.03525461E-01	-0.03868362E-05	-0.01298654E-08	0.02398500E-12	2				
0.07381692E+05	-0.02950581E+03	0.07815142E+01	0.02605711E+00	-0.02264714E-03	3				
0.01049925E-06	-0.02012847E-10	0.01062778E+06	0.02017946E+03		4				
ONHNOH	103190H	2N	2O	2	G	0300.00	4000.00	1500.00	1
0.01120874E+03	0.02650303E-01	-0.03760644E-05	-0.06355768E-09	0.01466251E-12	2				
-0.05721250E+05	-0.03476475E+03	0.01053271E+02	0.02809676E+00	-0.02637380E-03	3				
0.01270757E-06	-0.02478550E-10	-0.02244769E+05	0.01937011E+03		4				
S	121286S	1	G	0300.00	5000.00	1000.00	1		
0.02902148E+02	-0.05484546E-02	0.02764576E-05	-0.05017115E-09	0.03150685E-13	2				
0.03249423E+06	0.03838471E+02	0.03187329E+02	-0.01595776E-01	0.02005531E-04	3				
-0.01507081E-07	0.04931282E-11	0.03242259E+06	0.02414441E+02		4				
S(L)	120186S	1	L	0388.36	2000.00	1000.00	1		
0.03603667E+02	0.09903341E-02	-0.01011441E-04	0.04053633E-08	-0.05667914E-12	2				
-0.08453839E+04	-0.01634471E+03	-0.01270631E+03	0.09072521E+00	-0.01695179E-02	3				
0.01307064E-05	-0.03527615E-09	0.01234607E+05	0.05621016E+03		4				
S(S)	120186S	1	S	0300.00	0388.36	0388.36	1		
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2				
0.00000000E+00	0.00000000E+00	-0.05063703E+02	0.02881935E-01	-0.02133020E-03	3				
0.08478786E-05	-0.01734497E-07	0.07148263E+04	0.02871407E+03		4				
S+	121286S	1E	-1	G	0300.00	5000.00	1000.00	1	
0.02404600E+02	0.02410909E-02	-0.02041780E-05	0.06592945E-09	-0.05756939E-13	2				
0.01535223E+07	0.05924256E+02	0.02366101E+02	0.09130767E-02	-0.02140284E-04	3				
0.02076178E-07	-0.07133859E-11	0.01535091E+07	0.05993094E+02		4				
S-TRIAZINE	41687C	3N	3H	3	G	0300.00	4000.00	1000.00	1
0.01303617E+03	0.07711820E-01	-0.07724374E-05	-0.04385191E-08	0.08298992E-12	2				
0.02251663E+06	-0.04777676E+03	0.04493492E+01	0.02728306E+00	0.02309305E-04	3				
-0.01496844E-06	0.04546753E-10	0.02703032E+06	0.02178518E+03		4				
S2	121386S	2	G	0300.00	5000.00	1000.00	1		
0.03904443E+02	0.06925733E-02	-0.01233097E-05	0.08783809E-11	0.01374662E-13	2				
0.01425693E+06	0.04956834E+02	0.03157673E+02	0.03099480E-01	-0.01560746E-04	3				
-0.01357891E-07	0.01137444E-10	0.01439187E+06	0.08596062E+02		4				
SH	121286S	1H	1	G	0300.00	5000.00	1000.00	1	
0.03053810E+02	0.01258884E-01	-0.04249169E-05	0.06929591E-09	-0.04281691E-13	2				
0.01588225E+06	0.05973551E+02	0.04133327E+02	-0.03787893E-02	-0.02777854E-04	3				
0.05370112E-07	-0.02394006E-10	0.01555862E+06	0.01611535E+01		4				

SI	32989SI	1		G	0300.00	4000.00	1000.00	1
	0.02775846E+02	-0.06213257E-02	0.04843696E-05	-0.01275615E-08	0.01134482E-12			2
	0.05339791E+06	0.04543298E+02	0.03113515E+02	-0.02330991E-01	0.03518531E-04			3
	-0.02417573E-07	0.06391902E-11	0.05335062E+06	0.03009719E+02				4
SI(CH3)2	61991H	6C	2SI	1	G	0300.00	2500.00	1500.00
	0.01092572E+03	0.07986807E-01	-0.09096208E-06	-0.01014552E-07	0.02037989E-11			2
	0.01132561E+06	-0.02834187E+03	0.02308663E+02	0.02773810E+00	-0.01799333E-03			3
	0.06733023E-07	-0.01154743E-10	0.01442892E+06	0.01819319E+03				4
SI(CH3)3	61991H	9C	3SI	1	G	0300.00	2500.00	1500.00
	0.01536389E+03	0.01242119E+00	-0.01189769E-05	-0.01630302E-07	0.03308576E-11			2
	-0.05218398E+05	-0.05088962E+03	0.03907073E+02	0.03734813E+00	-0.02072025E-03			3
	0.06180575E-07	-0.08429605E-11	-0.01002462E+05	0.01138100E+03				4
SI(CH3)3CH2	61991H	11C	4SI	1	G	0300.00	2500.00	1500.00
	0.02061565E+03	0.01408136E+00	-0.01497876E-05	-0.01748111E-07	0.03468780E-11			2
	-0.01240235E+06	-0.07596671E+03	0.05258771E+02	0.04995369E+00	-0.03393958E-03			3
	0.01367592E-06	-0.02513506E-10	-0.06886708E+05	0.06814728E+02				4
SI(CH3)4	61991H	12C	4SI	1	G	0300.00	2500.00	1500.00
	0.02023461E+03	0.01648004E+00	-0.01486572E-05	-0.02161245E-07	0.04377236E-11			2
	-0.03702410E+06	-0.07661021E+03	0.05009315E+02	0.04952953E+00	-0.02745875E-03			3
	0.08231031E-07	-0.01137614E-10	-0.03140314E+06	0.06187860E+02				4
SI(L)	90589SI	1		L	0300.00	4500.00	1000.00	1
	0.03271263E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
	0.04855058E+05	-0.01329054E+03	0.03271263E+02	0.00000000E+00	0.00000000E+00			3
	0.00000000E+00	0.00000000E+00	0.04855059E+05	-0.01329054E+03				4
SI(NH2)3	42489SI	1N	3H	6	G	0300.00	3000.00	1000.00
	0.01406550E+03	0.07581744E-01	-0.05168510E-05	-0.06743626E-08	0.01397926E-11			2
	-0.01414403E+06	-0.04063874E+03	0.07598413E+02	0.02435266E+00	-0.04296202E-04			3
	-0.01756007E-06	0.01050102E-09	-0.01265343E+06	-0.07808647E+02				4
SI(NH2)4	22790SI	1N	4H	8	G	0300.00	4000.00	1000.00
	0.02032107E+03	0.08289798E-01	-0.07077612E-05	-0.04340724E-08	0.07747068E-12			2
	-0.05389855E+06	-0.07730464E+03	0.08454529E+02	0.03465772E+00	-0.04266782E-04			3
	-0.02495363E-06	0.01365466E-09	-0.05061518E+06	-0.01514301E+03				4
SI(S)	90589SI	1		S	0300.00	2500.00	1000.00	1
	0.02530275E+02	0.08522433E-02	-0.03223469E-05	0.01280821E-08	-0.01850849E-12			2
	-0.08395197E+04	-0.01251478E+03	0.05746418E+01	0.01026485E+00	-0.01775346E-03			3
	0.01457500E-06	-0.04491292E-10	-0.04969951E+04	-0.03400243E+02				4
SI2	111191SI	2		G	0300.00	4000.00	1500.00	1
	0.04402888E+02	0.01154530E-02	-0.06005177E-06	0.01469072E-09	-0.01357408E-13			2
	0.07199220E+06	0.02340066E+02	0.03439839E+02	0.03440171E-01	-0.04437681E-04			3
	0.02559961E-07	-0.05474618E-11	0.07222934E+06	0.07148545E+02				4
SI2C	112989C	1SI	2	G	0300.00	5000.00	1000.00	1
	0.06334110E+02	0.01210252E-01	-0.06798289E-05	0.02244433E-08	-0.02280178E-12			2
	0.06227189E+06	-0.07770097E+02	0.04157246E+02	0.07031825E-01	-0.07263033E-04			3
	0.04633583E-07	-0.01493448E-10	0.06292421E+06	0.03635126E+02				4
SI2CL5	40992SI	2CL	5	G	0300.00	4000.00	1500.00	1
	0.01800427E+03	0.05920529E-02	-0.03159743E-05	0.07962538E-09	-0.07553642E-13			2
	-0.08208587E+06	-0.04815622E+03	0.01218195E+03	0.02086930E+00	-0.02723261E-03			3
	0.01583266E-06	-0.03404617E-10	-0.08066122E+06	-0.01913372E+03				4
SI2CL5H	40992H	1SI	2CL	5	G	0300.00	4000.00	1500.00
	0.01977366E+03	0.01346980E-01	-0.04241463E-05	0.05994784E-09	-0.03079337E-13			2
	-0.01018307E+07	-0.05982624E+03	0.01104810E+03	0.02909474E+00	-0.03536307E-03			3
	0.01998957E-06	-0.04259074E-10	-0.09941194E+06	-0.01536396E+03				4
SI2CL6	40992SI	2CL	6	G	0300.00	4000.00	1500.00	1
	0.02095456E+03	0.06904584E-02	-0.03881968E-05	0.01014163E-08	-0.09844696E-13			2
	-0.01238540E+07	-0.06426893E+03	0.01372380E+03	0.02622361E+00	-0.03460508E-03			3
	0.02024950E-06	-0.04371480E-10	-0.01221143E+07	-0.02834094E+03				4
SI2F6	42489SI	2F	6	G	0300.00	3000.00	1000.00	1
	0.01830048E+03	0.02868753E-01	-0.04545577E-05	-0.02497900E-08	0.06630658E-12			2
	-0.02928185E+07	-0.05760425E+03	0.09998134E+02	0.02170314E+00	-0.03875092E-04			3
	-0.01670252E-06	0.09407529E-10	-0.02905483E+07	-0.01422886E+03				4
SI2H2	111191H	2SI	2	G	0300.00	4000.00	1500.00	1
	0.08099063E+02	0.01294220E-01	-0.02447198E-05	-0.01449512E-09	0.05867240E-13			2
	0.04476428E+06	-0.01877323E+03	0.09668390E+01	0.01932959E+00	-0.01825422E-03			3
	0.08404012E-07	-0.01537228E-10	0.04712241E+06	0.01907609E+03				4
SI2H3	90589SI	2H	3	G	0300.00	2000.00	1000.00	1
	0.07257627E+02	0.05123860E-01	-0.07633465E-05	-0.06662471E-08	0.02053053E-11			2

0.05062055E+06-0.01031413E+03	0.03335404E+02	0.02155615E+00-0.02933937E-03	3
0.02287785E-06-0.07272827E-10	0.05146157E+06	0.08656853E+02	4
SI2H5	90589SI 2H 5	G 0300.00 2000.00 1000.00	1
0.08451010E+02	0.09286371E-01-0.01091183E-04	0.01442367E-07 0.04250825E-11	2
0.02472719E+06-0.01710331E+03	0.01578848E+02	0.03549383E+00-0.04267511E-03	3
0.03059177E-06-0.09360425E-10	0.02630550E+06	0.01672073E+03	4
SI2H6	90589SI 2H 6	G 0300.00 2000.00 1000.00	1
0.08882090E+02	0.01151395E+00-0.01216216E-04	0.01905086E-07 0.05542379E-11	2
0.05967242E+05-0.02265611E+03	0.05301921E+01	0.04184056E+00-0.04685249E-03	3
0.03179525E-06-0.09484526E-10	0.07950598E+05	0.01880453E+03	4
SI3	32989SI 3	G 0300.00 4000.00 1000.00	1
0.07021585E+02	0.06981538E-02-0.04818729E-05	0.01720754E-08-0.01927025E-12	2
0.07429956E+06-0.08179233E+02	0.05312161E+02	0.05920181E-01-0.05075225E-04	3
0.05303866E-08	0.07031630E-11	0.07469502E+06	4
SI3H8	90589SI 3H 8	G 0300.00 2000.00 1000.00	1
0.01342277E+03	0.01563632E+00-0.01936565E-04	0.02388330E-07 0.07120030E-11	2
0.09165887E+05-0.04163000E+03	0.06319791E+01	0.06412995E+00-0.07772444E-03	3
0.05486969E-06-0.01646097E-09	0.01209258E+06	0.02133318E+03	4
SI3N4 (A)	42589N 4SI 3	S 0300.00 3000.00 1000.00	1
0.09667453E+02	0.01192721E+00-0.01709282E-04	0.01084607E-07 0.02713018E-11	2
-0.09324734E+06-0.04556492E+03	0.06631384E+02	0.02293929E+00-0.02152876E-03	3
0.01766237E-06-0.06632215E-10	0.09241684E+06	0.03021795E+03	4
SIC	112989C 1SI 1	G 0300.00 5000.00 1000.00	1
0.05024270E+02-0.04920894E-02	0.03109315E-05	0.06901344E-09 0.05215735E-13	2
0.08531026E+06-0.02478798E+02	0.02427812E+02	0.09551934E-01-0.02796633E-04	3
-0.01360012E-06	0.09196323E-10	0.08546512E+06	4
SIC (B)	112989C 1SI 1	S 0300.00 4000.00 1000.00	1
0.03548057E+02	0.03636817E-01-0.01734873E-04	0.03912869E-08-0.03337953E-12	2
-0.01018858E+06-0.01967253E+03	0.03551396E+01	0.01599881E+00-0.01393327E-03	3
0.03314914E-07	0.07825957E-11	0.09294352E+05	4
SIC2	112989C 2SI 1	G 0300.00 5000.00 1000.00	1
0.05753726E+02	0.02067546E-01-0.01132535E-04	0.03106456E-08-0.02799937E-12	2
0.07200461E+06-0.05294927E+02	0.03647725E+02	0.08765100E-01-0.01079869E-03	3
0.07974287E-07-0.02617042E-10	0.07258578E+06	0.05481050E+02	4
SICCH	61991H 1C 2SI 1	G 0300.00 2500.00 1500.00	1
0.08229114E+02	0.01220783E-01-0.01179375E-05	0.03293923E-09 0.02957217E-13	2
0.06029046E+06-0.01793033E+03	0.03946147E+02	0.01353938E+00-0.01476061E-03	3
0.08141935E-07-0.01743041E-10	0.06163490E+06	0.04400106E+02	4
SIC8	61991H 1C 1SI 1	G 0300.00 2500.00 1500.00	1
0.06212049E+02	0.05590981E-02-0.07015929E-06	0.03497540E-09-0.01203199E-12	2
0.06044180E+06-0.08520574E+02	0.03822068E+02	0.07938745E-01-0.09707239E-04	3
0.05877454E-07-0.01338338E-10	0.06118631E+06	0.03835953E+02	4
SIC82	61991H 2C 1SI 1	G 0300.00 2500.00 1500.00	1
0.06246250E+02	0.02147775E-01-0.06406396E-06	0.02067218E-08 0.03841890E-12	2
0.03490992E+06-0.08995611E+02	0.02794283E+02	0.01138805E+00-0.01041700E-03	3
0.05368052E-07-0.01132779E-10	0.03606279E+06	0.09246714E+02	4
SIC83	61991H 3C 1SI 1	G 0300.00 2500.00 1500.00	1
0.06681751E+02	0.03837387E-01-0.06162348E-06	0.04678285E-08 0.09346313E-12	2
0.03472013E+06-0.01022379E+03	0.02444652E+02	0.01367883E+00-0.09266249E-04	3
0.03704818E-07-0.06763833E-11	0.03624755E+06	0.01263619E+03	4
SICL	121986SI 1CL 1	G 0300.00 2000.00 1000.00	1
0.04258460E+02	0.04020317E-02-0.02888145E-05	0.01009777E-08-0.01411012E-12	2
0.01775614E+06	0.04134521E+02	0.03096406E+02	3
0.07643597E-07-0.02279179E-10	0.01796795E+06	0.09603212E+02	4
SICL2	121986SI 1CL 2	G 0300.00 2000.00 1000.00	1
0.06491205E+02	0.08242384E-02-0.05767737E-05	0.01972405E-08-0.02713757E-12	2
-0.02232408E+06-0.03570531E+02	0.03826666E+02	0.01308296E+00-0.02234087E-03	3
0.01760742E-06-0.05267404E-10	0.02183869E+06	0.08965448E+02	4
SICL2H2	121986SI 1H 2CL 2	G 0300.00 2000.00 1000.00	1
0.07727079E+02	0.05034189E-01-0.01095746E-04	0.04419587E-08 0.01631124E-11	2
-0.04028605E+06-0.01170816E+03	0.01100209E+02	0.03262362E+00-0.04691995E-03	3
0.03494565E-06-0.01036285E-09	0.03892087E+06	0.02022693E+03	4
SICL3	121986SI 1CL 3	G 0300.00 2000.00 1000.00	1
0.09098097E+02	0.01405353E-01-0.09317005E-05	0.02982296E-08-0.03822011E-12	2
-0.04140193E+06-0.01455012E+03	0.04485691E+02	0.02241754E+00-0.03794196E-03	3
0.02973183E-06-0.08861335E-10	0.04055264E+06	0.07198771E+02	4

SICL3CH2CH	10891C	2CL	3H	5SI	1G	0300.00	4000.00	1500.00	1
0.02087242E+03	0.05492755E-01	-0.06829558E-05	-0.01876697E-08	0.03787112E-12					2
-0.07972510E+06	-0.07741949E+03	0.04624781E+02	0.04378379E+00	-0.03850522E-03					3
0.01844376E-06	-0.03709272E-10	-0.07377043E+06	0.01029869E+03						4
SICL3H	121986SI	1H	1CL	3	G	0300.00	2000.00	1000.00	1
0.09663121E+02	0.03563368E-01	-0.01214911E-04	-0.01609009E-09	0.05641710E-12					2
-0.06295557E+06	-0.01894777E+03	0.02883770E+02	0.03308241E+00	-0.05169241E-03					3
0.03949918E-06	-0.01172104E-09	-0.06163323E+06	0.01337466E+03						4
SICL4	121986SI	1CL	4		G	0300.00	2000.00	1000.00	1
0.01170938E+03	0.01972092E-01	-0.01269077E-04	0.03900188E-08	-0.04756468E-12					2
-0.08347808E+06	-0.02791153E+03	0.05252110E+02	0.03122067E+00	-0.05254593E-03					3
0.04102707E-06	-0.01219907E-09	-0.08228177E+06	0.02575727E+02						4
SICLH3	121986SI	1H	3CL	1	G	0300.00	2000.00	1000.00	1
0.05964238E+02	0.06278087E-01	-0.08205635E-05	-0.09280558E-08	0.02796643E-11					2
-0.01854309E+06	-0.06395305E+02	0.05057173E+01	0.02703378E+00	-0.03301474E-03					3
0.02302732E-06	-0.06778703E-10	-0.01730819E+06	0.02043167E+03						4
SIF	42489SI	1F	1		G	0300.00	3000.00	1000.00	1
0.04120067E+02	0.03548821E-02	-0.07200222E-06	-0.02190434E-09	0.06764591E-13					2
-0.07561378E+05	0.02784246E+02	0.03144948E+02	0.02588557E-01	-0.05795912E-05					3
0.01807279E-07	0.01041172E-10	-0.07294439E+05	0.07876774E+02						4
SIF(NH2)2	22790SI	1F	1N	2H	4G	0300.00	4000.00	1000.00	1
0.01287944E+03	0.04598535E-01	-0.04004441E-05	-0.02374189E-08	0.04255211E-12					2
-0.05238279E+06	-0.03653418E+03	0.07210094E+02	0.01764698E+00	-0.02542060E-04					3
0.01242214E-06	0.06989787E-10	-0.05086706E+06	-0.07024622E+02						4
SIF(NH2)3	42489SI	1N	3H	6F	1G	0300.00	3000.00	1000.00	1
0.01611180E+03	0.08329222E-01	-0.06023787E-05	-0.07470125E-08	0.01570731E-11					2
-0.09137007E+06	-0.05098123E+03	0.08388268E+02	0.02746622E+00	-0.04455675E-04					3
-0.01955733E-06	0.01140721E-09	-0.08947806E+06	-0.01138178E+03						4
SIF2	42489SI	1F	2		G	0300.00	3000.00	1000.00	1
0.06142470E+02	0.07807974E-02	-0.01339312E-05	-0.06264839E-09	0.01725138E-12					2
-0.07744042E+06	-0.04712327E+02	0.03845345E+02	0.06038465E-01	-0.01167732E-04					3
-0.04579554E-07	0.02607414E-10	-0.07681634E+06	0.07272984E+02						4
SIF2(NH2)2	42489SI	1N	2H	4F	2G	0300.00	3000.00	1000.00	1
0.01441477E+03	0.06110646E-01	-0.04871145E-05	-0.05455935E-08	0.01172714E-11					2
-0.01292757E+07	-0.04308682E+03	0.07634268E+02	0.02315843E+00	-0.04193827E-04					3
-0.01715351E-06	0.01016462E-09	-0.01276410E+07	-0.08419031E+02						4
SIF2N	42489SI	1N	1F	2	G	0300.00	3000.00	1000.00	1
0.08687337E+02	0.01193488E-01	-0.01992661E-05	-0.09951334E-09	0.02704383E-12					2
-0.03463832E+06	-0.01494053E+03	0.05102583E+02	0.09456606E-01	-0.01819383E-04					3
-0.07309616E-07	0.04178902E-10	-0.03367294E+06	0.03734424E+02						4
SIF2NH2	42489SI	1N	1F	2H	2G	0300.00	3000.00	1000.00	1
0.09872415E+02	0.03722112E-01	-0.03271338E-05	-0.03321674E-08	0.07293692E-12					2
-0.08751628E+06	-0.01899096E+03	0.05890444E+02	0.01285128E+00	-0.01863556E-04					3
-0.08718963E-07	0.04848951E-10	-0.08644527E+06	0.01756163E+02						4
SIF3	42489SI	1F	3		G	0300.00	3000.00	1000.00	1
0.08524790E+02	0.01323792E-01	-0.02104279E-05	-0.01149504E-08	0.03055301E-12					2
-0.01223522E+07	-0.01550234E+03	0.04662868E+02	0.01008788E+00	-0.01805544E-04					3
-0.07769299E-07	0.04377852E-10	-0.01212965E+07	0.04672966E+02						4
SIF3NH	42489SI	1N	1F	3H	1G	0300.00	3000.00	1000.00	1
0.01163766E+03	0.02880769E-01	-0.03357310E-05	-0.02584594E-08	0.06162371E-12					2
-0.01295891E+07	-0.02590718E+03	0.06013822E+02	0.01597729E+00	-0.02791466E-04					3
-0.01214120E-06	0.06927415E-10	-0.01280974E+07	0.03316771E+02						4
SIF3NH2	42489SI	1N	1F	3H	2G	0300.00	3000.00	1000.00	1
0.01210964E+03	0.04383282E-01	-0.04142245E-05	-0.03989090E-08	0.08958954E-12					2
-0.01641768E+07	-0.03046928E+03	0.06229403E+02	0.01778015E+00	-0.02612304E-04					3
-0.01267243E-06	0.07044556E-10	-0.01625849E+07	0.02045441E+01						4
SIF3NHSIH3	42489SI	2N	1H	4F	3G	0300.00	3000.00	1000.00	1
0.01669941E+03	0.07789785E-01	-0.08110570E-05	-0.07650199E-08	0.01773956E-11					2
-0.01673412E+07	-0.05080007E+03	0.06216046E+02	0.02939330E+00	-0.02717745E-04					3
-0.01982878E-06	0.01002768E-09	-0.01642282E+07	0.04858261E+02						4
SIF3NSIH3	42489SI	2N	1H	3F	3G	0300.00	3000.00	1000.00	1
0.01599146E+03	0.06371086E-01	-0.07256824E-05	-0.06292690E-08	0.01495157E-11					2
-0.01331158E+07	-0.04495265E+03	0.06404372E+02	0.02601982E+00	-0.02491543E-04					3
-0.01769542E-06	0.08919883E-10	-0.01302520E+07	0.06002945E+02						4
SIF4	41389F	4SI	1		G	0300.00	2000.00	1000.00	1
0.09985301E+02	0.03532637E-01	-0.01197378E-04	-0.01036549E-08	0.08661585E-12					2

-0.01977200E+07-0.02472644E+03 0.02147416E+02 0.03402219E+00-0.04756874E-03 3  
 0.03252196E-06-0.08819304E-10-0.01960449E+07 0.01346315E+03 4  
 SIFH3 42489SI 1F 1H 3 G 0300.00 3000.00 1000.00 1  
 0.06799678E+02 0.04747086E-01-0.04767067E-05-0.04814665E-08 0.01107761E-11 2  
 -0.04577024E+06-0.01261433E+03 0.02032190E+02 0.01341363E+00-0.02806381E-05 3  
 -0.07803291E-07 0.03337474E-10-0.04421627E+06 0.01318768E+03 4  
 SIFNH 42489SI 1N 1F 1H 1G 0300.00 3000.00 1000.00 1  
 0.07163299E+02 0.01521325E-01-0.01536337E-05-0.01195933E-08 0.02684100E-12 2  
 -0.09065496E+05-0.06764144E+02 0.05390691E+02 0.06071319E-01-0.01359490E-04 3  
 -0.04267435E-07 0.02603154E-10-0.08644237E+05 0.02272065E+02 4  
 SIFNH2 22790F 1SI 1N 1H 2G 0300.00 4000.00 1000.00 1  
 0.08017582E+02 0.03209103E-01-0.03361364E-05-0.01796537E-08 0.03385552E-12 2  
 -0.04313426E+06-0.01487024E+03 0.04214050E+02 0.01105423E+00-0.01014725E-04 3  
 -0.07143728E-07 0.03634923E-10-0.04200629E+06 0.05318890E+02 4  
 SIH 121986SI 1H 1 G 0300.00 2000.00 1000.00 1  
 0.03110430E+02 0.01094946E-01 0.02898629E-06-0.02745104E-08 0.07051799E-12 2  
 0.04516898E+06 0.04193487E+02 0.03836010E+02-0.02702657E-01 0.06849070E-04 3  
 -0.05424184E-07 0.01472131E-10 0.04507593E+06 0.09350778E+01 4  
 SIH2 42489SI 1H 2 G 0300.00 3000.00 1000.00 1  
 0.04142390E+02 0.02150191E-01-0.02190730E-05-0.02073725E-08 0.04741018E-12 2  
 0.03110484E+06 0.02930745E+01 0.03475092E+02 0.02139338E-01 0.07672306E-05 3  
 0.05217668E-08-0.09898824E-11 0.03147397E+06 0.04436585E+02 4  
 SIH2CL 121986SI 1H 2CL 1 G 0300.00 2000.00 1000.00 1  
 0.05555902E+02 0.04046479E-01-0.06581751E-05-0.05027548E-08 0.01599110E-11 2  
 0.01912428E+05-0.01906890E+02 0.01699256E+02 0.01961407E+00-0.02622973E-03 3  
 0.01936417E-06-0.05846399E-10 0.02743662E+05 0.01683133E+03 4  
 SIH2F 42489SI 1F 1H 2 G 0300.00 3000.00 1000.00 1  
 0.06020399E+02 0.03074040E-01-0.03248887E-05-0.03052243E-08 0.07098090E-12 2  
 -0.02347670E+06-0.05919595E+02 0.02782566E+02 0.09148257E-01-0.04186788E-05 3  
 -0.05388971E-07 0.02412133E-10-0.02244201E+06 0.01152854E+03 4  
 SIH2F2 42489SI 1H 2F 2 G 0300.00 3000.00 1000.00 1  
 0.07997762E+02 0.03911538E-01-0.04222679E-05-0.03913812E-08 0.09171569E-12 2  
 -0.09682880E+06-0.01622400E+03 0.02701455E+02 0.01456545E+00-0.01163300E-04 3  
 -0.09685830E-07 0.04769591E-10-0.09522440E+06 0.01200689E+03 4  
 SIH3 42489SI 1H 3 G 0300.00 3000.00 1000.00 1  
 0.05015906E+02 0.03732750E-01-0.03609053E-05-0.03729193E-08 0.08468490E-12 2  
 0.02190233E+06-0.04291368E+02 0.02946733E+02 0.06466764E-01 0.05991653E-05 3  
 -0.02218413E-07 0.03052670E-11 0.02270173E+06 0.07347948E+02 4  
 SIH3NH2 42489SI 1N 1H 5 G 0300.00 3000.00 1000.00 1  
 0.08109945E+02 0.07215753E-01-0.06052251E-05-0.07086088E-08 0.01557864E-11 2  
 -0.08999782E+05-0.01651650E+03 0.02936348E+02 0.01674704E+00-0.03232859E-05 3  
 -0.09171970E-07 0.03979516E-10-0.07334716E+05 0.01141437E+03 4  
 SIH3NHSIH3 42489SI 2N 1H 7 G 0300.00 3000.00 1000.00 1  
 0.01265296E+03 0.01066748E+00-0.01007336E-04-0.01081222E-07 0.02452364E-11 2  
 -0.01249721E+06-0.03441428E+03 0.02468750E+02 0.02940255E+00-0.06248179E-05 3  
 -0.01731462E-06 0.07545261E-10-0.09209690E+05 0.02059560E+03 4  
 SIH3NSIH3 42489SI 2N 1H 6 G 0300.00 3000.00 1000.00 1  
 0.01201462E+03 0.09187517E-01-0.09159516E-05-0.09380967E-08 0.02156435E-11 2  
 0.01965066E+06-0.02978186E+03 0.02827574E+02 0.02580647E+00-0.04200478E-05 3  
 -0.01503859E-06 0.06388325E-10 0.02265351E+06 0.01997012E+03 4  
 SIH3SIH2CH3 111391H 8C 1SI 2 G 0300.00 4000.00 1500.00 1  
 0.01886736E+03 0.06449996E-01-0.06896411E-05-0.02584789E-08 0.04830521E-12 2  
 -0.06620909E+05-0.07374424E+03 0.02132164E+02 0.04348657E+00-0.03495608E-03 3  
 0.01588231E-06-0.03150773E-10-0.02040937E+04 0.01752930E+03 4  
 SIH4 121386SI 1H 4 G 0300.00 4000.00 1000.00 1  
 0.06893874E+02 0.04030501E-01-0.04183314E-05-0.02291395E-08 0.04384766E-12 2  
 0.01107037E+05-0.01749117E+03 0.02475167E+02 0.09003721E-01 0.02185394E-04 3  
 -0.02681423E-07-0.06621081E-11 0.02925488E+05 0.07751015E+02 4  
 SIHCL2 121986SI 1H 1CL 2 G 0300.00 2000.00 1000.00 1  
 0.07229734E+02 0.02869206E-01-0.08849876E-05-0.07495866E-09 0.05752338E-12 2  
 -0.01971399E+06-0.07052663E+02 0.02368353E+02 0.02401088E+00-0.03717220E-03 3  
 0.02851998E-06-0.08530494E-10-0.01875884E+06 0.01614587E+03 4  
 SIHF 42489SI 1F 1H 1 G 0300.00 3000.00 1000.00 1  
 0.05073509E+02 0.01533279E-01-0.01840659E-05-0.01440038E-08 0.03452517E-12 2  
 -0.01973880E+06-0.01079507E+02 0.03223728E+02 0.04981221E-01-0.03173051E-05 3  
 -0.02822231E-07 0.01247832E-10-0.01914168E+06 0.08906423E+02 4

```

SIHF2      42489SI  1H  1F  2    G  0300.00  3000.00  1000.00    1
  0.07216536E+02  0.02253240E-01-0.02737472E-05-0.02173460E-08  0.05255331E-12    2
-0.07280241E+06-0.09783487E+02  0.03377237E+02  0.01036607E+00-0.01239082E-04    3
-0.07267982E-07  0.03794989E-10-0.07168358E+06  0.01052189E+03    4
SIHF3      42489SI  1H  1F  3    G  0300.00  3000.00  1000.00    1
  0.09363567E+02  0.02947556E-01-0.03577633E-05-0.02858224E-08  0.06915729E-12    2
-0.01486074E+07-0.02169453E+03  0.03918053E+02  0.01463917E+00-0.01856070E-04    3
-0.01058200E-06  0.05617543E-10-0.01470439E+07  0.07024261E+02    4
SIN        42489SI  1N  1    G  0300.00  3000.00  1000.00    1
  0.04122909E+02  0.03521458E-02-0.07161081E-06-0.02154956E-09  0.06667571E-13    2
  0.05683927E+06  0.02389838E+02  0.03149182E+02  0.02584376E-01-0.05804625E-05    3
-0.01805627E-07  0.01041095E-10  0.05710564E+06  0.07474389E+02    4
SINH       42489SI  1N  1H  1    G  0300.00  3000.00  1000.00    1
  0.04928801E+02  0.01628624E-01-0.01367197E-05-0.01390460E-08  0.02998969E-12    2
  0.01767790E+06-0.02823472E+02  0.03166975E+02  0.05805823E-01-0.09524443E-05    3
-0.03991893E-07  0.02283188E-10  0.01813561E+06  0.06298440E+02    4
SINH2      42489SI  1N  1H  2    G  0300.00  3000.00  1000.00    1
  0.05186436E+02  0.03016656E-01-0.02165476E-05-0.02722658E-08  0.05706182E-12    2
  0.02270508E+06-0.01242140E+02  0.03362770E+02  0.07261176E-01-0.08721233E-05    3
-0.04400014E-07  0.02419532E-10  0.02318446E+06  0.08223867E+02    4
SN         121286S  1N  1    G  0300.00  5000.00  1000.00    1
  0.03888287E+02  0.06778427E-02-0.02725309E-05  0.05135927E-09-0.03593836E-13    2
  0.03044496E+06  0.04194291E+02  0.03407346E+02  0.01797887E-01-0.02018970E-04    3
  0.02107857E-07-0.09527592E-11  0.03062373E+06  0.06821481E+02    4
SO         121286S  1O  1    G  0300.00  5000.00  1000.00    1
  0.04021078E+02  0.02584856E-02  0.08948142E-06-0.03580145E-09  0.03228430E-13    2
-0.07119620E+04  0.03452523E+02  0.03080401E+02  0.01803106E-01  0.06705022E-05    3
-0.02069005E-07  0.08514657E-11-0.03986163E+04  0.08581028E+02    4
SO2        121286S  1O  2    G  0300.00  5000.00  1000.00    1
  0.05254498E+02  0.01978545E-01-0.08204226E-05  0.01576383E-08-0.01120451E-12    2
-0.03756886E+06-0.01146056E+02  0.02911439E+02  0.08103022E-01-0.06906710E-04    3
  0.03329016E-07-0.08777121E-11-0.03687882E+06  0.01111740E+03    4
SO3        121286S  1O  3    G  0300.00  5000.00  1000.00    1
  0.07050668E+02  0.03246560E-01-0.01408897E-04  0.02721535E-08-0.01942365E-12    2
-0.05020668E+06-0.01106443E+03  0.02575283E+02  0.01515092E+00-0.01229872E-03    3
  0.04240257E-07-0.05266812E-11-0.04894411E+06  0.01219512E+03    4
TI         41894TI  1    G  0300.00  5000.00  0800.00    1
  0.03136936E+02-0.01313357E-01  0.08940445E-05-0.01629410E-08  0.01015754E-12    2
  0.05609434E+06  0.04179979E+02  0.03768502E+02-0.03958362E-01  0.04286190E-04    3
-0.01178957E-07-0.03959347E-11  0.05598722E+06  0.01203708E+02    4
TI1CL     41894CL  1TI  1    G  0300.00  5000.00  1000.00    1
  0.05234878E+02-0.06804283E-03  0.01062016E-05-0.02729577E-09  0.02189332E-13    2
  0.01688888E+06-0.01482824E+01  0.03468008E+02  0.03799610E-01-0.01134367E-05    3
-0.04123500E-07  0.02217248E-10  0.01737617E+06  0.09110630E+02    4
TI1CL2    41894CL  2TI  1    G  0300.00  5000.00  0800.00    1
  0.07619173E+02-0.07106474E-02  0.06778838E-05-0.01629067E-08  0.01277916E-12    2
-0.03085448E+06-0.09947349E+02  0.06134803E+02  0.02576098E-01  0.02262539E-04    3
-0.07934520E-07  0.04455797E-10-0.03048455E+06-0.02290005E+02    4
TI1CL3    41894CL  3TI  1    G  0300.00  5000.00  0800.00    1
  0.09811998E+02  0.07343470E-02-0.03876140E-05  0.08435189E-09-0.06570051E-13    2
-0.06797809E+06-0.01840421E+03  0.05603371E+02  0.01296593E+00-0.05172034E-04    3
-0.01241024E-06  0.09472482E-10-0.06705052E+06  0.02636338E+02    4
TI1CL4    41894CL  4TI  1    G  0300.00  5000.00  0800.00    1
  0.01220230E+03  0.01003197E-01-0.04778859E-05  0.09877883E-09-0.07416465E-13    2
-0.09559289E+06-0.02743381E+03  0.09049202E+02  0.01030555E+00-0.05074092E-04    3
-0.07381952E-07  0.06054385E-10-0.09489398E+06-0.01167171E+03    4
END

```

## Transport parameters in CHEMKIN format

```
HE      0      10.200      2.576      0.000      0.000      0.000 !(*)
```

AR	0	136.500	3.330	0.000	0.000	0.000!
NE	0	32.800	2.820	0.000	0.000	0.000 !ReidApp
H	0	145.000	2.050	0.000	0.000	0.000!
H2	1	38.000	2.920	0.000	0.790	280.000!
C	0	71.400	3.298	0.000	0.000	0.000 ! (*)
CH	1	80.000	2.750	0.000	0.000	0.000!
CH2	1	144.000	3.800	0.000	0.000	0.000!
CH2SING	1	144.000	3.800	0.000	0.000	0.000!
CH2(S)	1	144.000	3.800	0.000	0.000	0.000 !
CH3	1	144.000	3.800	0.000	0.000	0.000!
CH4	2	141.400	3.746	0.000	2.600	13.000!
O	0	80.000	2.750	0.000	0.000	0.000!
OSING	0	80.000	2.750	0.000	0.000	0.000 !
OH	1	80.000	2.750	0.000	0.000	0.000!
H2O	2	572.400	2.605	1.844	0.000	4.000!
C2H	1	209.000	4.100	0.000	0.000	2.500!
C2H2	1	209.000	4.100	0.000	0.000	2.500!
C2H3	2	209.000	4.100	0.000	0.000	1.000 ! (*)
C2H4	2	280.800	3.971	0.000	0.000	1.500!
C2H5	2	252.300	4.302	0.000	0.000	1.500!
C2H6	2	252.300	4.302	0.000	0.000	1.500!
CO	1	98.100	3.650	0.000	1.950	1.800!
HCO	2	498.000	3.590	0.000	0.000	0.000!
CHO	2	498.000	3.590	0.000	0.000	0.000!
CH:O	2	498.000	3.590	0.000	0.000	0.000!
HCO+	1	498.000	3.590	0.000	0.000	0.000!
CH2O	2	498.000	3.590	0.000	0.000	2.000!
CH2:O	2	498.000	3.590	0.000	0.000	2.000!
CH3O	2	417.000	3.690	1.700	0.000	2.000!
CH2OH	2	417.000	3.690	1.700	0.000	2.000!
CH3OH	2	481.800	3.626	0.000	0.000	1.000 ! (SVE)
CH4O	2	417.000	3.690	1.700	0.000	2.000!
O2	1	107.400	3.458	0.000	1.600	3.800!
O3	1	107.400	3.458	0.000	1.600	3.800 !
HO2	2	107.400	3.458	0.000	0.000	1.000 ! (*)
H2O2	2	107.400	3.458	0.000	0.000	3.800!
C3H	1	252.000	4.760	0.000	0.000	1.000 !same as C3H3
C3H2	2	209.000	4.100	0.000	0.000	1.000 ! (*)
C3H3	2	252.000	4.760	0.000	0.000	1.000 ! (JAM)
H2CCCH	2	252.000	4.760	0.000	0.000	1.000 ! (JAM)
CH3CC	2	252.000	4.760	0.000	0.000	1.000 ! (JAM)
C3H4	1	252.000	4.760	0.000	0.000	1.000!
C3H4P	2	252.000	4.760	0.000	0.000	1.000 ! (JAM)
AC3H4	2	252.000	4.760	0.000	0.000	1.000
PC3H4	2	252.000	4.760	0.000	0.000	1.000
H2CCCH2	2	252.000	4.760	0.000	0.000	1.000
CH3CCH	2	252.000	4.760	0.000	0.000	1.000
cC3H4	2	252.000	4.760	0.000	0.000	1.000
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000
CH3CHCHE	2	260.000	4.850	0.000	0.000	1.000
CH3CHCHZ	2	260.000	4.850	0.000	0.000	1.000
C3H5	2	260.000	4.850	0.000	0.000	1.000 ! (JAM)
SC3H5	2	260.000	4.850	0.000	0.000	1.000 ! (JAM)
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000 ! (JAM)
TC3H5	2	260.000	4.850	0.000	0.000	1.000 ! (JAM)
AC3H5	2	260.000	4.850	0.000	0.000	1.000 ! (JAM)
C3H6	2	266.800	4.982	0.000	0.000	1.000!
C3H7	2	266.800	4.982	0.000	0.000	1.000!
I*C3H7	2	266.800	4.982	0.000	0.000	1.000!
nC3H7	2	266.800	4.982	0.000	0.000	1.000
NC3H7	2	266.800	4.982	0.000	0.000	1.000
iC3H7	2	266.800	4.982	0.000	0.000	1.000
IC3H7	2	266.800	4.982	0.000	0.000	1.000
C3H8	2	266.800	4.982	0.000	0.000	1.000!
HCCO	2	150.000	2.500	0.000	0.000	1.000 ! (*)
CH2CO	2	436.000	3.970	0.000	0.000	2.000!
HCCOH	2	436.000	3.970	0.000	0.000	2.000!

CH2CHO	2	436.000	3.970	0.000	0.000	2.000	!est.
CH2HCO	2	436.000	3.970	0.000	0.000	2.000	!est.
CH3CO	2	436.000	3.970	0.000	0.000	2.000	!
C2H3OO	2	556.000	4.610	0.000	0.000	0.000	!(Hennessy?)
C2H2OH	2	224.700	4.162	0.000	0.000	1.000	!(* )
CH3CHO	2	436.000	3.970	0.000	0.000	2.000	!
CH3HCO	2	436.000	3.970	0.000	0.000	2.000	!
CO2	1	244.000	3.763	0.000	2.650	2.100	!
C2H4O	2	436.000	3.970	0.000	0.000	2.000	!guess
C2H5O	2	436.000	3.970	0.000	0.000	2.000	!est
CH3OO	2	436.000	3.970	0.000	0.000	2.000	!est
CH3OOH	2	436.000	3.970	0.000	0.000	2.000	!est
CH3O2	2	436.000	3.970	0.000	0.000	2.000	!est
CH3O2H	2	436.000	3.970	0.000	0.000	2.000	!est
O3	2	180.000	4.100	0.000	0.000	2.000	!
C4H	1	357.000	5.180	0.000	0.000	1.000	!
C4H2	1	357.000	5.180	0.000	0.000	1.000	!
H2C4O	2	357.521	4.459	0.000	0.000	1.000	!LJcjp
nC4H3	2	357.000	5.180	0.000	0.000	1.000	!guess
iC4H3	2	357.000	5.180	0.000	0.000	1.000	!TC from Wang
C4H3	2	357.000	5.180	0.000	0.000	1.000	!guess
HCCCHCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
H2CCCHH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCHH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H4	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
H2CCCHH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H5	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCHH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000	!(JAM)
C4H6	2	357.000	5.176	0.000	0.000	1.000	
C4H6-13	2	357.000	5.176	0.000	0.000	1.000	
C4H6-1	2	357.000	5.176	0.000	0.000	1.000	!GEO added following two species
iiC4H6=1,2butadiene;iiiC4H6=1,3butadiene!done on 10/14/98							
iiC4H6	2	357.000	5.176	0.000	0.000	1.000	
iiiC4H6	2	357.000	5.176	0.000	0.000	1.000	
C2H5C2H	2	357.000	5.176	0.000	0.000	1.000	
C4H7	2	357.000	5.176	0.000	0.000	1.000	
C4H8	2	357.000	5.176	0.000	0.000	1.000	!
cC4H8	2	357.000	5.176	0.000	0.000	1.000	
tC4H8	2	357.000	5.176	0.000	0.000	1.000	
nC4H8-1	2	357.000	5.176	0.000	0.000	1.000	
IC4H8	2	357.000	5.176	0.000	0.000	1.000	
IIC4H8	2	357.000	5.176	0.000	0.000	1.000	
UC4H8	2	357.000	5.176	0.000	0.000	1.000	
nC4H9	2	357.000	5.176	0.000	0.000	1.000	!
S*C4H9	2	357.000	5.176	0.000	0.000	1.000	!
I*C4H9	2	357.000	5.176	0.000	0.000	1.000	!
C4H10	2	357.000	5.176	0.000	0.000	1.000	
NC4H10	2	357.000	5.176	0.000	0.000	1.000	
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	!(* )
HCCCHO	2	429.000	4.999	2.9	0.	1.	!est
CH2CCO	2	429.000	4.999	2.9	0.	1.	!est
HCCCH2O	2	429.000	4.999	2.9	0.	1.	!est
OCYCHCH	2	429.000	4.999	2.9	0.	1.	!est
CH2CHCO	2	429.000	4.999	2.9	0.	1.	!est
CH3CCO	2	429.000	4.999	2.9	0.	1.	!est
CH2CCHO	2	429.000	4.999	2.9	0.	1.	!est
CH3CHCO	2	429.000	4.999	2.9	0.	1.	!est
CH3CHOH	2	470.600	4.410	0.000	0.000	1.500	!From LLNL Marinov set
C2H4OH	2	470.600	4.410	0.000	0.000	1.500	!From LLNL Marinov set
CH3CH2O	2	470.600	4.410	0.000	0.000	1.500	!nmm !From LLNL Marinov set
C2H5OH	2	470.600	4.410	0.000	0.000	1.500	!nmm !From LLNL Marinov set
HOC2H4O2	2	470.600	4.410	0.000	0.000	1.500	!7/01 same as c2h5oh, wjp !From LLNL Marinov set
C2H3CO	2	429.000	4.999	2.9	0.	1.	!est
C2H3CHO	2	429.000	4.999	2.9	0.	1.	!PRW2/93
C2H3CH2O	2	429.000	4.999	2.9	0.	1.	!PRW5/93
CH3CHCHO	2	429.000	4.999	2.9	0.	1.	!est
cC3H5O	2	357.000	5.176	0.000	0.000	1.000	!est
CH2COCH3	2	357.000	5.176	0.000	0.000	1.000	
CH3COCH3	2	357.000	5.176	0.000	0.000	1.000	
C3H6O	2	357.000	5.176	0.000	0.000	1.000	



CH2CH2OCH2	2	357.000	5.176	0.000	0.000	1.000 !est
Propox	2	357.000	5.176	0.000	0.000	1.000
C3H6OH	2	576.7	4.549	0.000	0.000	1.000 !est.
nC3H7O	2	576.7	4.549	0.000	0.000	1.000 !est.
iC3H7O	2	576.7	4.549	0.000	0.000	1.000 !est.
CH3CO2	2	576.7	4.549	0.000	0.000	1.000 !est.
CH3CO2H	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H5OO	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H5O2	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H5OOH	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H5O2H	2	576.7	4.549	0.000	0.000	1.000 !est.
CH3OOCCH3	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H3CO2	2	576.7	4.549	0.000	0.000	1.000 !est.
C3H5OO	2	576.7	4.549	0.000	0.000	1.000 !est.
C3H5OOH	2	576.7	4.549	0.000	0.000	1.000 !est.
nC3H7OO	2	576.7	4.549	0.000	0.000	1.000 !est.
iC3H7OO	2	576.7	4.549	0.000	0.000	1.000 !est.
nC3H7OOH	2	576.7	4.549	0.000	0.000	1.000 !est.
iC3H7OOH	2	576.7	4.549	0.000	0.000	1.000 !est.
CH3CO3	2	576.7	4.549	0.000	0.000	1.000 !est.
CH3CO3H	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H3CO3	2	576.7	4.549	0.000	0.000	1.000 !est.
C2H3CO3H	2	576.7	4.549	0.000	0.000	1.000 !est.
O2C3H6OH	2	576.7	4.549	0.000	0.000	1.000 !est.
!C5H2	1	357.000	5.180	0.000	0.000	1.000!Deleted by Wenjun using Miller
!C5H3	1	357.000	5.180	0.000	0.000	1.000!Deleted by Wenjun using Miller
C5H4O	2	450.000	5.500	0.000	0.000	1.000!!
C5H4OH	2	450.000	5.500	0.000	0.000	1.000!!
pn2en4ynyl	1	357.000	5.180	0.000	0.000	1.000!same as C5H3
C5H5	1	357.000	5.180	0.000	0.000	1.000!same as C5H3!
C5H2	1	386.805	4.852	0.000	0.000	1.000!LJcjp
H2CCCCCH	2	389.341	5.055	0.000	0.000	1.000!LJcjp
HCCCCHCC	2	378.067	5.021	0.000	0.000	1.000!LJcjp
C5H4	1	357.000	5.180	0.000	0.000	1.000 !HR,10/00!
C5H5O	2	450.000	5.500	0.000	0.000	1.000!!
C5H5OH	2	450.000	5.500	0.000	0.000	1.000 !(JAM)
C5H6	2	354.700	5.13	0.000	0.000	1.000 !ab
C5H7	2	393.700	5.26	0.000	0.000	1.000 !ab
C5H8	2	393.700	5.26	0.000	0.000	1.000 !ab
C5H4	2	441.700	5.00	0.000	0.000	1.000 !ab
cypentenyl	2	354.700	5.13	0.000	0.000	1.000 !After ab C5H6
cypnt3enyl	2	354.700	5.13	0.000	0.000	1.000 !After ab C5H6
cypentene	2	354.700	5.13	0.000	0.000	1.000 !After ab C5H6
pentdienyl	2	393.700	5.26	0.000	0.000	1.000 !After ab C5H7
pentdienal	2	450.000	5.500	0.000	0.000	1.000 !After (JAM) C5H5OH
C5H4CH3	2	412.300	5.349	0.000	0.000	1.000 !like other C6H7's
C6H	1	412.300	5.349	0.000	0.000	1.000 !ab/97
C6H3	2	412.300	5.349	0.000	0.000	1.000 !ab/97
n-C6H5	2	412.300	5.349	0.000	0.000	1.000 !ab/97
i-C6H5	2	412.300	5.349	0.000	0.000	1.000 !ab/97
1-C6H6	2	412.300	5.349	0.000	0.000	1.000 !ab/97
C4H5C2H	2	412.3	5.349	0.00	0.00	1.00 !JAM(12/02)
n-C6H7	2	412.300	5.349	0.000	0.000	1.000 !ab/97
c-C6H7	2	412.300	5.349	0.000	0.000	1.000 !ab/97
i-C6H7	2	412.300	5.349	0.000	0.000	1.000 !ab/97
A1	2	412.300	5.349	0.000	0.000	1.000 !ab/97
A	2	412.300	5.349	0.000	0.000	1.000 !ab/97
1-C6H4	2	367.700	5.36	0.000	0.000	1.000 !ab/97
c-C6H4	2	367.700	5.36	0.000	0.000	1.000 !ab/97
C6H8	2	412.300	5.349	0.000	0.000	1.000 !ab/97
n-C4H5	2	357.000	5.180	0.000	0.000	1.000 !AB/97
i-C4H5	2	357.000	5.180	0.000	0.000	1.000 !AB/97
FC6H6	2	412.300	5.349	0.000	0.000	1.000 !ab/97
C6H2	1	357.000	5.180	0.000	0.000	1.000!
C6H5	2	412.300	5.349	0.000	0.000	1.000 !(JAM)
C6H5 (L)	2	412.300	5.349	0.000	0.000	1.000 !(JAM)
C6H6	2	412.300	5.349	0.000	0.000	1.000 !(SVE)
C6H7	2	412.300	5.349	0.000	0.000	1.000 !(JAM)
C6H10	2	399.3	5.949	0.000	0.000	1.000 !est
C6H14	2	399.3	5.949	0.000	0.000	1.000 !
C6H5O	2	450.000	5.500	0.000	0.000	1.000 !(JAM)
C6H5OH	2	450.000	5.500	0.000	0.000	1.000!!
CYC6H12	2	324.	6.093	0.000	0.000	1.000!BSL60
CYC6H11	2	324.	6.093	0.000	0.000	1.000!BSL60

C6H11	2	412.300	5.349	0.000	0.000	1.000 !mel/04 same as benzene
C6H11-13	2	412.300	5.349	0.000	0.000	1.000 !Wenjun/20080824 same as benzene
C6H11-12	2	399.3	5.949	0.000	0.000	1.000 !est from C6H10
C6H11-14	2	399.3	5.949	0.000	0.000	1.000 !est from C6H10
C6H11-15	2	399.3	5.949	0.000	0.000	1.000 !est from C6H10
CYC6H10	2	324.	6.093	0.000	0.000	1.000!BSL60
CYC6H9	2	324.	6.093	0.000	0.000	1.000!BSL60
C6H9	2	324.	6.093	0.000	0.000	1.000 !ab/97
CY13C6H8	2	412.300	5.349	0.000	0.000	1.000 !mel/04 same as benzene
CYC6H7	2	412.300	5.349	0.000	0.000	1.000 !mel/04 same as benzene
hexene1	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
hexene3	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
hex1yl	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
hex2yl	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
hex3yl	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
hex2enyl	2	413.	5.909	0.000	0.000	1.000!BSL60 for nC6H14
C4H6O	2	442.700	4.85	0.000	0.000	1.000 !ab
C4H8O	2	426.200	5.21	0.000	0.000	1.000 !ab
C6H4	2	367.700	5.36	0.000	0.000	1.000 !ab
C8H2	1	357.000	5.180	0.000	0.000	1.000!same as C6H2
N	0	71.400	3.298	0.000	0.000	0.000 !(*)
N2	1	97.530	3.621	0.000	1.760	4.000!
N2H2	2	71.400	3.798	0.000	0.000	1.000 !(*)
N2H3	2	200.000	3.900	0.000	0.000	1.000 !(*)
N2H4	2	205.000	4.230	0.000	4.260	1.500!
N2O	1	232.400	3.828	0.000	0.000	1.000 !(*)
NCN	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
NCO	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
NH	1	80.000	2.650	0.000	0.000	4.000!
NH2	2	80.000	2.650	0.000	2.260	4.000!
NH3	2	481.000	2.920	1.470	0.000	10.000!
NNH	2	71.400	3.798	0.000	0.000	1.000 !(*)
NO	1	97.530	3.621	0.000	1.760	4.000!
NCNO	2	232.400	3.828	0.000	0.000	1.000 !(OIS)
NO2	2	200.000	3.500	0.000	0.000	1.000 !(*)
NOO	2	200.000	3.500	0.000	0.000	1.000 !
NO3	2	200.000	3.500	0.000	0.000	1.000 !
HCN	1	569.000	3.630	0.000	0.000	1.000 !(OIS)
CN	1	75.000	3.856	0.000	0.000	1.000 !(OIS)
CNC	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
CNN	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
CN2	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
C2N	1	232.400	3.828	0.000	0.000	1.000 !(OIS)
C2N2	1	349.000	4.361	0.000	0.000	1.000 !(OIS)
H2CN	1	569.000	3.630	0.000	0.000	1.000 !(os/jm)
HC2N2	1	349.000	4.361	0.000	0.000	1.000 !(OIS)
HCNO	2	232.400	3.828	0.000	0.000	1.000 !(JAM)
HOCN	2	232.400	3.828	0.000	0.000	1.000 !(JAM)
HNCO	2	232.400	3.828	0.000	0.000	1.000 !(OIS)
HCOOH	2	232.400	3.828	0.000	0.000	1.000 !(TC,guess)
C2O	2	232.400	3.828	0.000	0.000	1.000 !(TC,no data)
HOCO	2	232.400	3.828	0.000	0.000	1.000 !
COOH	2	232.400	3.828	0.000	0.000	1.000 !dummy
HONO	2	232.400	3.828	0.000	0.000	1.000 !
HNO3	2	232.400	3.828	0.000	0.000	1.000 !
HOONO	2	232.400	3.828	0.000	0.000	1.000 !
HNO	2	116.700	3.492	0.000	0.000	1.000 !(*)
HNNO	2	232.400	3.828	0.000	0.000	1.000 !(*)
S	0	847.000	3.839	0.000	0.000	0.000 !(OIS)
S2	1	847.000	3.900	0.000	0.000	1.000 !(OIS)
SH	1	847.000	3.900	0.000	0.000	1.000 !(OIS)
H2S	2	301.000	3.600	0.000	0.000	1.000 !(OIS)
HSO2	2	252.000	4.290	0.000	0.000	1.000 !(OIS)
SO	1	301.000	3.993	0.000	0.000	1.000 !(OIS)
SO2	2	252.000	4.290	0.000	0.000	1.000 !(OIS)
SO3	2	378.400	4.175	0.000	0.000	1.000 !(OIS)
SIH4	2	207.6	4.084	0.000	0.000	1.000 !(mec)
SIH3	2	170.3	3.943	0.000	0.000	1.000 !(mec)
SIH2	2	133.1	3.803	0.000	0.000	1.000 !(mec)
SIH	1	95.8	3.662	0.000	0.000	1.000 !(mec)
SI	0	3036.	2.910	0.000	0.000	0.000 !(mec)
SI2H6	2	301.3	4.828	0.000	0.000	1.000 !(mec)

SI2H5	2	306.9	4.717	0.000	0.000	1.000	!(mec)
SI2H4	2	312.6	4.601	0.000	0.000	1.000	!(mec)
SI2H3	2	318.2	4.494	0.000	0.000	1.000	!(mec)
SI2H2	2	323.8	4.383	0.000	0.000	1.000	!(mec)
SI2	1	3036.	3.280	0.000	0.000	1.000	!(mec)
SI3	2	3036.	3.550	0.000	0.000	1.000	!(mec)
SIF4	2	171.9	4.880	0.000	0.000	1.000	!(sve)
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000	!(mec)
H3SISIH	2	312.6	4.601	0.000	0.000	1.000	!(mec)
SI3H8	2	331.2	5.562	0.000	0.000	1.000	!(mec)
ASH3	2	259.8	4.145	0.000	0.000	1.000	!(mec)
AS2	1	1045.5	5.510	0.000	0.000	1.000	!(mec)
GAME3	2	378.2	5.52	0.000	0.000	1.000	!(mec)
GAME2	2	675.8	5.22	0.000	0.000	1.000	!(mec)
GAME	2	972.7	4.92	0.000	0.000	1.000	!(mec)
GA	0	2961.8	4.62	0.000	0.000	0.000	!(mec)
K	0	850.	4.25	0.000	0.000	1.000	!(singh)
KOH	2	1213.	4.52	0.000	0.000	1.000	!(singh)
KO2	2	1213.	4.69	0.000	0.000	1.000	!(singh)
KO	1	383.0	3.812	0.000	0.000	1.000	!(singh)
KH	1	93.3	3.542	0.000	0.000	1.000	!(singh)
K+	0	850.	4.25	0.000	0.000	1.000	!(singh)
KCL	1	1989.	4.186	0.000	0.000	1.000	!(singh)
CL	0	130.8	3.613	0.000	0.000	1.000	!(singh)
CL-	0	130.8	3.613	0.000	0.000	1.000	!(singh)
HCL	1	344.7	3.339	1.084	0.000	1.000	!(singh)
CH2CL	2	858.000	3.400	0.000	0.000	0.000	!(*ois)
C2HCL3	2	280.000	3.971	0.000	0.000	0.000	!(*ois)
CCL	1	98.100	3.650	0.000	1.950	1.800	!(*ois)
CHOCL	2	498.000	3.590	0.000	0.000	0.000	!(*ois)
HOCL	2	107.400	3.458	0.000	0.000	0.000	!(*ois)
COCL	2	860.000	4.000	0.000	0.000	0.000	!(*ois)
CLO	2	110.000	3.590	0.000	0.000	0.000	!(*ois)
CL2O	2	356.000	2.649	0.000	0.000	0.000	!(*ois)
CLO2	2	107.400	3.458	0.000	0.000	0.000	!(*ois)
CH3CL	2	855.000	3.375	0.000	0.000	0.000	!(*ois)
F	0	80.000	2.750	0.000	0.000	0.000	!
F2	1	125.700	3.301	0.000	1.600	3.800	!
HF	1	330.000	3.148	1.920	2.460	1.000	!(sv/mec)
HF0	1	352.000	2.490	1.730	0.000	5.000	!
HF1	1	352.000	2.490	1.730	0.000	5.000	!
HF2	1	352.000	2.490	1.730	0.000	5.000	!
HF3	1	352.000	2.490	1.730	0.000	5.000	!
HF4	1	352.000	2.490	1.730	0.000	5.000	!
HF5	1	352.000	2.490	1.730	0.000	5.000	!
HF6	1	352.000	2.490	1.730	0.000	5.000	!
HF7	1	352.000	2.490	1.730	0.000	5.000	!
HF8	1	352.000	2.490	1.730	0.000	5.000	!
HOF	2	107.400	3.458	0.000	0.000	0.000	!(ois)
F2O	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO	1	109.600	3.412	0.000	0.000	0.000	!(ois)
HOOF	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
F2O2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
CH3F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CH2F2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF3	2	262.	4.123	1.8	0.000	0.000	!ReidPRW
CF4	2	134.0	4.662	0.000	0.000	0.000	!ReidPra
CH2F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF3	2	121.000	4.320	0.000	0.000	0.000	!(ois)
CHF	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF2	2	108.000	3.977	0.000	0.000	0.000	!(ois)
CF	1	94.200	3.635	0.000	0.000	0.000	!(Svehla)
CF3OH	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3OF	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CH2FO	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF2O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF:O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF2:O	2	350.500	4.906	0.000	0.000	0.000	!(ois)

CF:O	2	860.000	4.000	0.000	0.000	0.000	!(ois)
CH3-CH2F	2	312.2	4.583	2.0	0.000	0.000	!ReidPRW
CH3-CHF2	2	323.4	4.798	2.3	0.000	0.000	!ReidPRW
CH2F-CH2F	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF3	2	289.1	4.911	2.3	0.000	0.000	!ReidPRW
CH2F-CHF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF3	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CHF2-CHF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CHF2-CF3	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CF3-CF3	2	231.8	4.969	0.0	0.000	0.000	!PRW2/93
CH3-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH2F-CH2	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CHF2-CH2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CHF	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CF3-CH2	2	289.1	4.911	2.3	0.000	0.000	!PRW2/93
CF3-CHF	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CF3-CF2	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CH2:CHF	2	272.2	4.322	1.4	0.000	0.000	!ReidPRW
CH2:CF2	2	251.5	4.442	1.4	0.000	0.000	!ReidPRW
CHF:CHF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CHF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF2	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CF2	2	254.2	4.647	0.0	0.000	0.000	!ReidPRW
CH2:CF	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-E	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-Z	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CH	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CF	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
C2HF	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
C2F2	1	240.	4.4	0.	0.000	0.000	!PRW2/93
C2F	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
CHFCO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF2CO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
FCCO-E	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF2CL2	2	253.000	5.250	0.000	0.000	0.000	!(ois)
CF2CLBR	2	253.000	5.250	0.000	0.000	0.000	!(ois)
CF2CL	2	121.000	4.320	0.000	0.000	0.000	!(ois)
C6H5CH2	2	495.300	5.680	0.000	0.000	1.000	!NMM
C6H5CH3	2	495.300	5.680	0.430	12.30	1.000	!NMM
C6H5OCH3	2	495.300	5.680	0.430	12.30	1.000	!Est by Wenjun from C6H5CH3
C6H5OCH2	2	495.300	5.680	0.430	12.30	1.000	!Est by Wenjun from C6H5CH3
C6H4CH3	2	495.300	5.680	0.000	0.000	1.000	!NMM
C6H5CO	2	622.400	5.530	0.000	0.000	1.000	!NMM
C6H5CHO	2	622.400	5.530	0.000	0.000	1.000	!NMM
C6H5CH2OH	2	622.400	5.530	0.000	0.000	1.000	!Est from above
C6H5CH2O	2	622.400	5.530	0.000	0.000	1.000	!NMM
C6H5CH2O0	2	622.400	5.530	0.000	0.000	1.000	!EST by Wenjun as C6H5CH2OH
OC6H4CH3	2	621.100	5.640	0.000	0.000	1.000	!NMM
C6H4O2	2	621.100	5.640	0.000	0.000	1.000	!Est by Wenjun
HOC6H4CH3	2	621.100	5.640	0.000	0.000	1.000	!NMM
C6H5CH2CH3	2	523.600	5.960	0.000	0.000	1.000	!NMM
C6H5CH2CH2	2	523.600	5.960	0.000	0.000	1.000	!Est by Wenjun
C6H5CHCH2	2	546.200	6.000	0.130	15.00	1.000	!NMM
C6H5CHCH	2	546.200	6.000	0.000	0.000	1.000	!NMM
C6H5CCH2	2	546.200	6.000	0.000	0.000	1.000	!NMM
C6H5CCH	2	534.300	5.710	0.770	0.000	1.000	!NMM
C6H4CCH	2	534.300	5.710	0.000	0.000	1.000	!NMM
BiBenzyl	2	783.800	6.640	0.000	0.000	1.000	!NMM
C6H5C5H5	2	783.800	6.640	0.000	0.000	1.000	!NMM
C6H5C5H4	2	783.800	6.640	0.000	0.000	1.000	!NMM
C6H5C6H5	2	783.800	6.640	0.000	0.000	1.000	!Est by wenjun as above species!!
C3H2 isomers are From Miller 2008 email							
H2CCC(S)	1	290.616	4.368	0.000	0.000	1.000	!JAM 7/10/02
C3H2(S)	1	290.616	4.368	0.000	0.000	1.000	!JAM 7/10/02
C3H2C	1	290.616	4.368	0.000	0.000	1.000	!JAM 10/22/02
C3H	1	290.616	4.368	0.000	0.000	1.000	!LJcjp?

PC6H4O2	2	450.000	5.500	0.000	0.000	1.000!HR
OC6H4O2	2	450.000	5.500	0.000	0.000	1.000!HR
C6H3O2	2	450.000	5.500	0.000	0.000	1.000!HR
C6H3O3	2	450.000	5.500	0.000	0.000	1.000!
!						
!-----Added by Wenjun on 20091117-----						
A2	2	630.4	6.18	0.00	16.50	1.000 !naphthalene
A2-	2	630.4	6.18	0.00	16.50	1.000 !
P2	2	676.5	6.31	0.00	20.00	1.000 !biphe
!C6H5C6H5	2	783.800	6.640	0.000	0.000	1.000!Est by wenjun as above species
C6H5C6H5	2	676.5	6.31	0.00	20.00	1.000 !biphe!
P2-	2	676.5	6.31	0.00	20.00	1.000 !
INDENYL	2	402.9	6.744	0.000	0.000	1.000 !MIT2b
INDENE	2	402.9	6.744	0.000	0.000	1.000 !MIT2b
A2CH3	2	658.602	6.335	0.000	0.000	0.000 !from Marina, from Pitsch
A2CH2	2	655.890	6.320	0.000	0.000	0.000 !from Marina, from Pitsch
A2R5	2	693.1	6.47	0.00	18.00	1.000 !acena
A2R5-	2	693.1	6.47	0.00	18.00	1.000 !
A2C2H	2	693.1	6.47	0.00	18.00	1.000 !
A2C2H*	2	693.1	6.47	0.00	18.00	1.000 !
A3	2	772.0	6.96	0.00	38.80	1.000 !phenanthrene
A3-	2	837.500	7.275	0.000	0.000	0.000
A3C2H	2	879.600	7.561	0.000	0.000	0.000 !MIT2b
A3C2H*	2	879.600	7.561	0.000	0.000	0.000 !as A3C2H from MIT2b
A3CH3	2	879.600	7.561	0.000	0.000	0.000 !MIT2b
A3CH2	2	879.600	7.561	0.000	0.000	0.000 !as A3C2H MIT2b
A4	2	834.9	7.24	0.00	45.00	1.000 !pyrene
A4R5	2	879.600	7.561	0.000	0.000	0.000
A4-	2	834.9	7.24	0.00	45.00	1.000 !pyrene
A4C2H	2	776.2	7.407	0.000	0.000	1.000 !"PYRYNEP MIT2b
A4C2H*	2	776.2	7.407	0.000	0.000	1.000 !" PYRYNEP*S MIT2b
C18H12	2	879.600	7.561	0.000	0.000	0.000 !C18H10 from MIT2b
C18H11	2	879.600	7.561	0.000	0.000	0.000 !C18H10 from MIT2b
BAPYR	2	833.062	8.087	0.000	0.000	1.000 !MIT2b
BAPYR*S	2	833.062	8.087	0.000	0.000	1.000 !+MIT2b
BGHIF	2	870.7	7.559	0.000	0.000	1.000 !b[ghi] from MIT2b
C4H	1	357.000	5.180	0.000	0.000	1.000
C6H	1	357.000	5.180	0.000	0.000	1.000
C8H	1	357.000	5.180	0.000	0.000	1.000 !C6H
C8H2	1	357.000	5.180	0.000	0.000	1.000 !C6H2
C10H	1	357.000	5.180	0.000	0.000	1.000 !C6H
C10H2	1	357.000	5.180	0.000	0.000	1.000 !C6H2
C12H	1	357.000	5.180	0.000	0.000	1.000 !C6H
C12H2	1	357.000	5.180	0.000	0.000	1.000 !C6H2
C6H4CHCH2	2	546.2	6.00	0.13	15.00	1.000 !
H2CC	2	238.	4.07	0.0	0.0	2.5 !JAM(1/02)
c-C4H5	2	330.	5.09	0.0	0.0	1. !JAM 10/02
!						
! Below are from Detillex 09 JPCA						
!-----						
!C12H8	2	450.000	6.463	0.000	0.000	1.000!cp !
A2CH3-1	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH3-2	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-1	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-2	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-1f	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-2f	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-1f*	2	450.000	6.090	0.000	0.000	1.000!cp !
A2CH2-2f*	2	450.000	6.090	0.000	0.000	1.000!cp !
C9H7	2	402.900	6.744	0.000	0.000	1.000!A2 (HR)
C9H7a	2	402.900	6.744	0.000	0.000	1.000!A2 (HR)
C9H7b	2	402.900	6.744	0.000	0.000	1.000!A2 (HR)
C9H8	2	402.900	6.744	0.000	0.000	1.000!A2 (HR)
C10H7O-1	2	402.900	6.744	0.000	0.000	1.000!"
C10H7O-2	2	402.900	6.744	0.000	0.000	1.000!"
A1C2H*2	2	450.000	5.646	0.000	0.000	1.000!HR
C10H7	2	450.000	6.090	0.000	0.000	1.000!cp, HR
C10H7a	2	450.000	6.090	0.000	0.000	1.000!cp, HR
C10H7*2	2	450.000	6.090	0.000	0.000	1.000!cp, HR
C6H5C3H2	2	450.000	5.719	0.000	0.000	1.000!HR
!C12H9	2	450.000	6.463	0.000	0.000	1.000!cp !
!BICPD*	2	450.000	6.090	0.000	0.000	1.000!cp !

VALS0	2	450.000	6.090	0.000	0.000	1.000!cp !
VALC10H10	2	450.000	6.090	0.000	0.000	1.000!cp !
VALC10H9	2	450.000	6.090	0.000	0.000	1.000!cp !
VALS1	2	450.000	6.090	0.000	0.000	1.000!cp !
VALS2	2	450.000	6.090	0.000	0.000	1.000!cp !
VALS3	2	450.000	6.090	0.000	0.000	1.000!cp !
VALS4	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9a	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9b	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9c	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9d	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H9e	2	450.000	6.090	0.000	0.000	1.000!cp !
C10H8	2	450.000	6.090	0.000	0.000	1.000!cp !
C7H6f	2	357.000	5.176	0.000	0.000	1.000
C12H8	2	450.000	6.463	0.000	0.000	1.000!cp !
CH2CHCH2CCH	2	357.000	5.176	0.000	0.000	1.000
CH2CHCHCCH2	2	357.000	5.176	0.000	0.000	1.000
C6H5C3H2	2	450.000	5.719	0.000	0.000	1.000 !HR
C12H9	2	450.000	6.463	0.000	0.000	1.000!cp !
1-C5H5	1	357.000	5.180	0.000	0.000	1.000 !
!						
! Added transport data for Morpholine related species						
cyMorph	2	412.300	5.349	0.000	0.000	1.000 !same as benzene
cyOrthoMorphyl	2	412.300	5.349	0.000	0.000	1.000 !same as Benzenyl
cyMetaMorphyl	2	412.300	5.349	0.000	0.000	1.000 !same as Benzenyl
cyParaMorphyl	2	412.300	5.349	0.000	0.000	1.000 !same as Benzenyl
rNHCH2CH2OCHCH2	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rCH2CH2NHCH2CHO	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rOCH2CH2NHCHCH2	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rCH2CH2OCH2CHNH	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rCH2OCH2CH2NCH2	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rCH2OCHCH2	2	357.000	5.176	0.000	0.000	1.000 !same as CH2COCH3
rNHCH2CHO	2	429.000	4.999	2.9	0.	1. !same as CH3CHCHO
rCH2NHCHCH2	2	357.000	5.180	0.000	0.000	1.000 !same as CH2CHCHCH
rOCH2CHNH	2	429.000	4.999	2.9	0.	1. !same as C2H3CH2O
rCH2CH2NCH2	2	357.000	5.176	0.000	0.000	1.000 !same as C4H7
rCHNH	1	569.000	3.630	0.000	0.000	1.000 !same as HCN
CH2NH	1	569.000	3.630	0.000	0.000	1.000 !same as CH2N
!						
! added 1/4/10						
CH2CHOCH2CHNH	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
rCH2CHNH	2	436.000	3.970	0.000	0.000	2.000 !same as CH2CHO
CH2CNH	2	436.000	3.970	0.000	0.000	2.000 !same as CH2CO
OCHCH2NHCHCH2	2	399.3	5.949	0.000	0.000	1.000 !same as C6H10
cyOCHCHNHCH2CH2	2	324.	6.093	0.000	0.000	1.000 !same as CYC6H10
cyrNCH2CH2OCHCH	2	324.	6.093	0.000	0.000	1.000 !same as CYC6H9
rCH2CH2NCHCHO	2	324.	6.093	0.000	0.000	1.000 !same as C6H9
rCH2OCHCHNHCH2	2	324.	6.093	0.000	0.000	1.000 !same as C6H9
cyOCHCHNHCHCH2	2	412.300	5.349	0.000	0.000	1.000 !same as CY13C6H8
cyrCHOCHCHNHCH	2	412.300	5.349	0.000	0.000	1.000 !same as CYC6H7
cyOCH2CHNHCH2CH2	2	324.	6.093	0.000	0.000	1.000 !same as CYC6H10
CH2CHNHCH2	2	357.000	5.176	0.000	0.000	1.000 !same as iiiC4H6
rNCHCHO	2	429.000	4.999	2.9	0.	1. !same as CH3CHCHO
rCHCHNHCH2	2	357.000	5.176	0.000	0.000	1.000 !same as iiiC4H6
HNC	1	569.000	3.630	0.000	0.000	1.000!same as HCN (OIS)
HNO2	2	232.400	3.828	0.000	0.000	1.000!same as HONO
NH2O	2	116.700	3.492	0.000	0.000	1.000!same as HNO (*)
HNOH	2	116.700	3.492	0.000	0.000	1.000!JAM
!						
CH3ONO2	2	232.400	3.828	0.000	0.000	1.000!same as HOONO
CH3ONO	2	232.400	3.828	0.000	0.000	1.000!same as HOONO
CH3NO	2	436.000	3.970	0.000	0.000	2.000!same as CH3OO est
H2CNO2	2	576.7	4.549	0.000	0.000	1.000!Same as CH3CO2 est
CH3NO2	2	576.7	4.549	0.000	0.000	1.000!Same as CH3CO2 est
N2O4	2	232.400	3.828	0.000	0.000	1.000!same as HNO3
CH3NHNH2	2	266.800	4.982	0.000	0.000	1.000!same as C3H6
CH3NNH2	2	260.000	4.850	0.000	0.000	1.000!same as C3H5 (JAM)
CH3NH	1	569.000	3.630	0.000	0.000	1.000!same as H2CN (os/jm)
CH2NH	1	569.000	3.630	0.000	0.000	1.000!same as H2CN (os/jm)
CH3NNH	1	232.400	3.828	0.000	0.000	1.000!same as CNN (OIS)
CH3NN	1	232.400	3.828	0.000	0.000	1.000!same as CNN (OIS)
CH3NNCH3	2	357.000	5.180	0.000	0.000	1.000!same as CH3CCCH2 (JAM)
NO3	2	200.000	3.500	0.000	0.000	1.000 !
HNO3	2	232.400	3.828	0.000	0.000	1.000 !
N2O4	2	232.400	3.828	0.000	0.000	1.000!same as HNO3

CH3ONO	2	232.400	3.828	0.000	0.000	1.000!same as HOONO
CH3ONO2	2	232.400	3.828	0.000	0.000	1.000!same as HOONO
CH3NO	2	436.000	3.970	0.000	0.000	2.000!same as CH3OO est
CH3NO2	2	576.7	4.549	0.000	0.000	1.000!Same as CH3CO2 est
HCNN	2	232.400	3.828	0.000	0.000	1.000!Same as HCNO
CH2CN	2	436.000	3.970	0.000	0.000	2.000 !same as CH2CO
CH3CN	2	436.000	3.970	0.000	0.000	2.000 !same as CH3CO
CH3NH2	1	569.000	3.630	0.000	0.000	1.000!same as H2CN(os/jm)
CH2NH2	1	569.000	3.630	0.000	0.000	1.000!same as H2CN(os/jm)
!c7h16-2	2	546.85	5.99	0	13.61	1 !calc SMS 2010
TMEDA	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-1	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-3	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-2	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
!iC3H7	2	266.800	4.982	0.000	0.000	1
CH3NCH3	2	266.800	4.982	0.000	0.000	1 !same as iC3H7
!dc5h11	2	523.2	5.664	1.7	0.0	1!wjp
N(CH3)2CH2CH2	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
!ic4h10	2	295.8	5.392	0.1	0.0	1!!L-J from Mourits 1977 (Mani 2010)
N(CH3)2CH2	2	295.8	5.392	0.1	0.0	1 !same as ic4h10
!AC3H5	2	260.000	4.850	0.000	0.000	1 !(JAM)
CH3NCH2	2	260.000	4.850	0.000	0.000	1 !same as AC3H5
TMEDA-0-5	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
N(CH3)2CHCH2	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
TMEDA-0-4	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-0-3	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-1-3	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-1-4	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-1-5	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
TMEDA-3-5	2	546.85	5.99	0	0	1 !same as c7h16-2 with 0 polarizability
N(CH3)2CHCH	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
!C4H7	2	357.000	5.176	0.000	0.000	1
CH2CHNCH3	2	357.000	5.176	0.000	0.000	1 !same as C4H7
CH2CH2NCH2	2	357.000	5.176	0.000	0.000	1 !same as C4H7
!C3H5	2	260.000	4.850	0.000	0.000	1 !(JAM)
CH2NCH2	2	260.000	4.850	0.000	0.000	1 !same as AC3H5
N(CH3+CH2)CHCH2	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
N(CH3)2CCH2	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
!C4H6-13	2	357.000	5.176	0.000	0.000	1
CH2CHNCH2	2	357.000	5.176	0.000	0.000	1 !same as C4H6-13
N(CH3)2CCH	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
!CH2CHCHCH	2	357.000	5.180	0.000	0.000	1 !(JAM)
CHCHNCH2	2	357.000	5.180	0.000	0.000	1 !same as CH2CHCHCH
CH2CHNCH	2	357.000	5.180	0.000	0.000	1 !same as CH2CHCHCH
CH3NCH	2	260.000	4.850	0.000	0.000	1 !same as AC3H5
N(CH3+CH2)CH2CH3	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
!nC4H8-1	2	357.000	5.176	0.000	0.000	1
CH3CH2NCH2	2	357.000	5.176	0.000	0.000	1 !same as nC4H8-1
CH3CHNCH2	2	357.000	5.176	0.000	0.000	1 !same as C4H7
!PC3H4	1	252.000	4.760	0.000	0.000	1
CH2NCH	2	252.000	4.760	0.000	0.000	1 !same as PC3H4
CH3N(NH2)NO2	2	523.2	5.664	1.7	0.0	1 !same as dc5h11
CH3N(NH2)ONO	2	523.2	5.664	1.7	0.0	1 !same as dc5h11

## A.2.1 Full ARL Model

### Kinetic parameters in CHEMKIN format

```

REACTIONS
! the next reaction modified according to Tsang & Herron *****
NO2(+M)=NO+O(+M) 7.60E18 -1.27 73290.
!Tsang & Herron
LOW/ 2.47E28 -3.37 74800./

```

```

!keyed to N2=1.0
      !TSA/ 0.95 -1.0E-04 /
      N2O/1.5/ H2O/4.4/ N2/1.0/ CO2/2.3/
!EFFICIENCIES FROM Baulch et al,
! HE /0.54/ AR/0.71/ CH4/1.6/
!1973, for reverse reaction except CO2/N2
!from Tsang & Herron 91 (latter in forward dir)
!FC(N2)=0.95 - 1.0E-04 * T
!      K0(CO2)=2.16E26 -2.66 74300
! FC(CO2)=FC(N2)
!
N2O(+M)=N2+O(+M) 1.26E12 0.0 62620.
!Rohrig et al, 1996 preprint
      LOW/ 5.97E14 0.0 56640./
!to appear in IJCK; rekeyed to N2

!using N2/Ar = 1.5
!N2O(+M)=N2+O(+M) 7.91E10 0.0 56020.
!M. Allen et al, both HP and LP
!      LOW/ 9.13E14 0.0 57690./
!keyed to N2=1.0; per Baulch
! per Princeton group, Lindemann falloff is reasonable. Efficiencies
! kept as previous.
!
!N2O(+M)=N2+O(+M) 1.30E11 0.0 59610.
!T&H91 (HP and LP)
!      LOW/ 7.23E17 -0.73 62789./
!keyed to N2=1.0; per Baulch
!      T&H/ 1.167 -1.25E-04 /
!et al, N2/Ar=1.5 used here

!N2O/Ar also from Baulch et

!al.; H2,CO,NO estimated = N2

! N2O/5.0/ H2O/7.5/ N2/1.0/ CO2/3.2/ O2/0.82/
!H2O/AR,O2/AR from
! AR/0.67/
!Glarborg et al, C&F 99,523,1994

      N2O/5.0/ H2O/9.0/ N2/1.0/ CO2/3.2/ O2/0.82/
!O2/AR from
! NH3/5.0/
! AR/0.67/
!Glarborg et al, C&F 99,523,1994
! H2O/N2 efficiency is average of the values from Glarborg et al 94 and
! Venizelos & Sausa, C&F 115, 313 (1998). There is still a large uncertainty
! in this important efficiency factor. There may be some T dependence.
! NH3 is est.

!
!CO2/N2 from T&H91
!      N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/3.2/
!earlier choices
!      FC(N2)=1.167-1.25E-04*T
!
! the reaction throw out (incorp. in N2O+M) *****
! N2O(+CO2)=N2+O(+CO2)
!mod Bill,Ref 37d
!      LOW/ 1.20E18 -0.67 62190./
!LINDEMANN FALLOFF
!
!NEEDS ATTENTION
!
H+NO(+M)=HNO(+M) 1.52E15 -0.41 0.
!Fall-off, TH91

```



```

!          LOW/ 8.96E19   -1.32   735./
!TH91
!          T&H/ 0.82 /
!          LOW/ 4.00E20   -1.75     0./
!Glarborg et al, ISC 1998
!      used new LP limit with TH91 HP limit
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.3/
!CO2/N2 from TH91
!          FC(N2)=0.82
!
! HNO(+M)=H+NO(+M)  1.20E16   -0.43 49520.
!TH91
!          LOW/ 6.02E21   -1.61 50840./
!LINDEMANN FORM
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/3.2/
!NEEDS ATTENTION
!          FC(N2)=0.830

!SOME EFFS. FROM MB89
! this reaction eliminated (incluced in HNO + M) *****
! HNO(+CO2)=H+NO(+CO2)
!TH91
!          LOW/ 3.85E20   -1.24 50020./
!LINDEMANN FORM
!
!NEEDS ATTENTION
!
! new reaction : *****
NO+OH(+M)=HONO(+M) 1.988E12   -0.05 -721.
!Tsang & Herron
!          LOW/ 5.08E23   -2.51 -67.6/
!keyed to N2=1.0.
!          !TSA/ 0.62 0.0/
!          N2O/5.0/ H2O/8.3/ N2/1.0/ CO2/1.5/
!CO2/N2 from TH91;
!          AR/0.60/
!H2O from Overend et al; N2/AR ave from TH91 citations
!          FC(N2)=0.62
!          K(0,CO2)=1.705E23   -2.30 -246.
!          FC(CO2)=0.62
!
! HCN(+M)=H+CN(+M)  8.30E17   -0.93 123800.
!T&H91 [13,0]
!          LOW/ 3.57E26   -2.6 124900./      !
!          !TSA/ 0.95 -1.0E-04 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!N2/CO2 ratioed per Tsang;
!          FC(N2)=0.95-1.0E-04*T
!
!CN+H(+M)=HCN(+M)  1.80E15   -0.5   0.
!Tsang, 1992
!          LOW/ 8.71E23   -2.2 1130./      !
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!N2/CO2 ratioed per Tsang;
!          FC(N2)=0.95-1.0E-4*T
!
!CN+CN(+M)=C2N2(+M) 5.66E12    0.0   0.
!Tsang, 1992
!          LOW/ 3.43E25   -2.61   0./      !
!          !TSA/ 0.5 0.0 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/
!N2/CO2 ratioed per Tsang;
!          FC(N2)=0.5      !
!HNCO(+M)=NH+CO(+M) 6.00E13    0.0 99800.
!Tsang, 1992
!          LOW/ 2.17E28   -3.1 101900./

```

```

!
!TSA/ 0.9 -2.0E-04 /
N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/ ! N2/CO2 ratioed per Tsang;
! FC(N2)=0.9-2.0E-4*T !
HCN+H(+M)=H2CN(+M) 3.31E13 0.0 4844. ! TH91
LOW/ 1.60E24 -2.73 7660./ !
!TSA/ 0.95 -1.0E-04 /
N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/ ! N2/CO2 ratioed per Tsang;
! FC = 0.95-1.0E-04*T
CN+NO(+M)=NCNO(+M) 3.98E13 0.0 0. ! Tsang, 1992
LOW/ 1.56E36 -6.2 4878./ !
!TSA/ 0.65 0.0 /
N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/ ! N2/CO2 ratioed per Tsang;
! FC(N2)=FC(CO2)=0.65 ! others guessed
!C2N2+M=CN+CN+M 1.07E34 -4.3 123000. ! added
CN+M=C+N+M 2.50E14 0.0 141100. ! Tsang 92, keyed to Ar=1.0
N2/1.5/ CO2/2.4/ ! Tsang 92
NO+M=N+O+M 1.40E15 0.0 148430. ! TH91
! AR/0.75/ HE/0.35/
N2/1.0/ H2/2.2/ H2O/6.7/ CO2/3.0/ N2O/2.2/
! NO+M Efficiencies from Clyne & Thrush, as quoted in Baulch et al, 1973 for
! reverse reaction
N2+M=N+N+M 3.71E21 -1.6 225000. ! Baulch et al, 1973
!NCO+C=CO+CN 1.00E14 0.0 0. ! WRA, ul est.

! ***** N2O+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!N2O+N=N2+NO 1.00E13 0.0 19870. ! HS85, est.
! N2O+N removed per Fernandez & Fontijn ul measurement, ~2000.
! ***** End N2O+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****

! ***** NO2+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!NO2+N=N2O+O 5.01E12 0.0 0. ! HS85 (iffy; see Leeds)
!N+NO2=N2O+O 5.00E+12 0.00 0.000E+00
NO2+N=N2O+O 3.49E12 0.0 -437. ! DEM/SAN 97
!NO2+N=NO+NO 3.98E12 0.0 0. ! HS85 (iffy; see Leeds)
! Above removed per DEM/SAN 97
! ***** End NO2+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****

!NO2+NO=N2O+O2 1.0E12 0.0 60000. ! Thorne and Melius 89

! ***** NO2+NO2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
NO2+NO2=NO+NO3 9.64E09 0.73 20920. ! T&H91
!NO2+NO2=NO+NO+O2 1.63E12 0.0 26120. ! T&H91
NO2+NO2=NO+NO+O2 4.51E12 0.0 27600. ! PGML00
! ***** End NO2+NO2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

! ***** NO2+NO3 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
!NO2+NO3=NO+NO2+O2 1.40E11 0.0 3180. ! Baulch et al, 1973
NO2+NO3=NO+NO2+O2 2.71E10 0.0 2500. ! DEM/SAN 97
! ***** End NO2+NO3 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

!HNO+NO=N2O+OH 2.00E12 0.0 26000. ! Wilde, C&F, 1969
!HNO+NO=N2O+OH 4.00E12 0.0 26000. ! Wilde, C&F, 1969 x2 for test
!HNO+NO=N2O+OH 8.51E12 0.0 29590. ! Diau et al, IJCK 27,867(1995)
HNO+NO=N2O+OH 1.70E13 0.0 29590. ! comment follows
! WRA believes best value is 2 x Diau et al, IJCK 27,867(1995) because
! they had good result/review, but used wrong heat of formation of HNO,
! leading to x2 error in their final result.
!NO+NO=N2+O2 1.3E14 0.0 75630. !added Yetter
! previous reaction is a concern; products may be wrong
!NO+HO2=HNO+O2 2.0E11 0.0 2000. !added Yetter; traced to
! Thorne & Melius 89 jannaf
HNO+O2=HO2+NO 1.00E13 0.0 25000. ! MB91
!HNO+NO2=HONO+NO 6.0E11 0.0 1987. ! TH91, estimated

```

HNO+NO2=HONO+NO 4.42E4 2.64 4042. ! MLM98  
HONO+O=OH+NO2 1.2E13 0.0 5961. ! TH91  
HONO+OH=H2O+NO2 1.27E10 1.0 135. ! TH91  
!  
! WRA estimated HONO+NH2=NO2+NH3 k is similar to HONO+OH=H2O+NO2.  
! For HONO+OH, b~1 and Ea~0, so that was used for HONO+NH2. Then the  
! the A factor was reduced from original estimate of 1.0E10 so that the final  
! result passes through Bedford and Thomas' value at ~640 K. Note Bedford &  
! Thomas reduced their data with ancillary reactions now known to be wrong.  
! One would expect if anything their result for k(NO2+NH3) is too large because  
! they do not have NH2+NO=NNH+OH and their initial mixtures contained NO as  
! well as NH3 & NO2. Also, their T range, 615-660 K, was not large. That latter  
! observation is why it is best to assume b and Ea by reversing and just use  
! their data to set A factor. wra, 9/30/98  
!  
! Upon further examination of Bedford & Thomas' analysis, have decided they  
! have systematic analysis error, low by factor of ~2, due to mechanistic  
! errors. Therefore, have reverted to original estimate, which was ~ 1.3  
! higher (increasing by exactly that factor of 2 is not justified, is too  
! approximate without careful reanalysis B&T's data; not even sure that's  
! possible, don't know if they gave exacting details of how well equilibrated  
! was NO/NO2/O2 before introducing NH3 and result depends heavily on that).  
! Estimated error at 650K (B&T expts) x3, x5 at ends of recommended range =  
! 450 - 3000 K. wra, 10/1/98  
!HONO+NH2=NO2+NH3 7.7E09 1.0 0. ! wra, est fitted to B&T72  
HONO+NH2=NO2+NH3 1.0E10 1.0 0. ! wra, est, better analysis than B&T72  
!  
!HONO+HNO=H2O+2NO 1.0E12 0.0 40000. ! Thorne & Melius 89  
HNO+O=OH+NO 3.61E13 0.0 0. ! TH91  
!HNO+O=NO2+H 5.0E10 0.5 2000. ! Thorne & Melius 89  
NH+O=NO+H 5.50E13 0.0 0. ! MCHB91  
NH+O=N+OH 3.72E13 0.0 0. ! MCHB91  
NH+NH=N2+H+H 5.10E13 0.0 0. ! MCHB89  
NH+M=N+H+M 2.65E14 0.0 75510. ! MCHB91 keyed to Ar=1.0  
!  
!NH2+NO=N2O+H2 7.0E13 0.0 27820. ! RHK, 18th ISC, p 853  
!NH2+NO=N2O+H2 5.0E13 0.0 24640. ! Roose' thesis; per  
! ! discussion with Hanson, 4/7/95, this supercedes the 18th ISC result  
! WRA, 2/13/01.  
!  
! Per Miller & Klippenstein, JPC A104, 2061, 2000, the NH2+NO=N2O+H2  
! reaction has been removed. M&K conclude the reaction may be to HNNO+H,  
! or Roose et al may have been observing effects of 'contamination by  
! secondary reactions'. The endothermicity is ~40.5 kcal/mole to HNNO+H,  
! so the measured activation energy simply does not fit that interpretation.  
! So, I have decided to remove the reaction. It never played much of a  
! role in any process of which I know, anyway. WRA, 2/20/01  
!  
! See more on NH2+NO choices below. WRA, 5/22/03  
!  
!  
!  
CH+O2=HCO+O 3.30E13 0.0 0. ! MB89  
CH+O=CO+H 5.70E13 0.0 0. ! MB89  
CH+OH=HCO+H 3.00E13 0.0 0. ! MB89  
CH+CO2=HCO+CO 3.40E12 0.0 690. ! MB89  
CH+H=C+H2 1.50E14 0.0 0. ! MB89  
C+O2=CO+O 2.00E13 0.0 0. ! MB89  
C+OH=CO+H 5.00E13 0.0 0. ! MB89  
HCO+OH=H2O+CO 1.00E14 0.0 0. ! MB89  
HCO+M=H+CO+M 2.50E14 0.0 16802. ! MB89  
CO/1.9/ H2/1.9/ CO2/3.0/ H2O/5.0/  
HCO+H=CO+H2 1.19E13 0.25 0. ! MB89  
HCO+O=CO+OH 3.00E13 0.0 0. ! MB89  
HCO+O=CO2+H 3.00E13 0.0 0. ! MB89  
HCO+O2=HO2+CO 3.30E13 -0.4 0. ! MB89

```

!
CO+O(+M)=CO2(+M) 1.80E10 0.0 2380. ! Princeton preprint
      LOW/ 1.35E24 -2.79 4190./ ! Princeton preprint
      !TSA/ 1.0 0.0 / ! Princeton preprint
      H2O/12./ H2/2.5/ CO/1.9/ CO2/3.8/ N2O /5.0/ !
! All efficiencies above from Princeton preprint, except
! N2O is guessed.
!CO+O+M=CO2+M 2.36E15 0.0 4340.
! CO/1.77/ CO2/2.7/ H2O/5.0/ N2O/5.0/ ! N2,CO,CO2 per TH86,
! others guessed
CO+OH=CO2+H 1.51E07 1.3 -758. ! MB89
!CO+O2=CO2+O 1.60E13 0.0 41000. ! MB89
CO+O2=CO2+O 2.53E12 0.0 47688. ! TH86
HO2+CO=CO2+OH 5.80E13 0.0 22934. ! MB89
O+HCCO=H+2CO 1.00E14 0.0 0. ! MB89
HCCO+O2=2CO+OH 1.60E12 0.0 854. ! MB89
!H2+O2=2OH 1.70E13 0.0 47780. ! MB89
! for H2+O2=2OH, TH86 do not believe 2OH is a product (nor do
! most others, apparently). Main product is H+HO2. The reverse
! of this from TH86 is in below, and we use that and allow CHEMKIN
! to reverse using up to date thermo.
OH+H2=H2O+H 2.16E08 1.5 3430. ! Mich. & Suth. 88
O2+H=O+OH 3.52E16 -0.7 17070. ! MHB90
O+H2=OH+H 5.06E04 2.67 6290. ! SMPNK, ISC 88
H+O2+M=HO2+M 3.61E17 -0.72 0. ! MB89
      H2O/18.6/ CO2/4.2/ H2/2.9/ CO/2.1/ N2/1.3/
OH+HO2=H2O+O2 7.50E12 0.0 0. ! MB89
*****
! For H+HO2, switched from TH86 to BAU92. Yetter/Dryer, world
! experts on H2/O2 chem, use the TH86 expressions in much of their
! work. Note OH+OH is the main channel, followed by H2+O2. Also
! note, TH86 and BAU92 expressions are identical for OH+OH, and for
! H2+O2 channel agree very well at ~1000 K, which is the typical
! operating temperature for the Yetter/Dryer flow apparatus.
! Disagreement between TH86 and BAU92 for H2+O2 is only about a factor
! of two at low (300 K) and high (3000 K) temperature. This is
! similar to uncertainty limits each quotes.
!
! The O+H2O channel, as specified by BAU92, is newly included.
! It is unlikely to ever have much effect as its k is much smaller
! than the other 2 channels. BAU92 mention its error limit is
! much larger than for the other 2 channels.
!
!H+HO2=2OH 1.69E14 0.0 874. ! TH86
!H+HO2=H2+O2 6.63E13 0.0 2126. ! TH86
H+HO2=2OH 1.69E14 0.0 874. ! TH86/BAU92
H+HO2=H2+O2 4.28E13 0.0 1411. ! BAU92
H+HO2=O+H2O 3.01E13 0.0 1721. ! BAU92
*****
O+HO2=O2+OH 1.40E13 0.0 1073. ! MB89

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!2OH=O+H2O 6.00E08 1.3 0. ! MB89
OH+OH=H2O+O 3.57E04 2.40 2112. ! WHB94
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

2H+M=H2+M 1.00E18 -1.0 0. ! MB89
      H2/0.0/ H2O/0.0/ CO2/0.0/
2H+H2=2H2 9.20E16 -0.6 0. ! MB89
2H+H2O=H2+H2O 6.00E19 -1.25 0. ! MB89
2H+CO2=H2+CO2 5.49E20 -2.0 0. ! MB89
H+OH+M=H2O+M 1.60E22 -2.0 0. ! MB89
      H2O/5.0/
H+O+M=OH+M 6.20E16 -0.6 0. ! MB89
      H2O/5.0/
O+O+M=O2+M 1.89E13 0.0 -1788. ! MB89

```

```

2HO2=H2O2+O2      1.80E12   0.0   0.   ! TH86
!H2O2+M=2OH+M     1.30E17   0.0  45500. ! MB89
! H2O2+M removed because reverse, with P falloff, from GRI 3.0
! was inserted.

! The expressions for H2O2+H are from TH86, but there is
! much uncertainty in the HO2+H2 channel. (Main channel
! is known to be OH+H2O.) BAU92 is in fairly good
! agreement concerning the OH+H2O channel, but not for
! HO2+H2. Note BAU92 adopts WAR84; Warnatz was a coauthor
! of BAU92. Expressions for HO2+H2 from TH86 and BAU92
! cross near 1/T = 1.3e-3, or close to T = 773 K (500 C)
! which was used in many of the experiments by Baldwin,
! Walker et al in the 1970's (e.g. J.Chem.Soc.Far.Trans.I,
! v69, p352, 1973). Ranges are: TH86, 300-2500 K,
! BAU92 300-1000 K. TH86 state uncertainty for both
! reactions is high (factor of 5) above 1000 K, and
! since BAU92 don't even recommend using their expressions
! above 1000 K, they must generally agree with that
! assessment. But note the expressions of TH86 have the
! HO2+H2 channel nearly equal to the OH+H2O channel,
! whereas extrapolated BAU92 expressions don't do that.
! That is because the TH86 Ea is much larger than BAU92 for
! HO2+H2. If this is sensitive, more study than I have done
! is indicated. WRA, 12/20/00.
!
H2O2+H=HO2+H2     4.82E13   0.0  7948.   ! TH86
H2O2+H=OH+H2O     2.41E13   0.0  3975.   ! TH86
!H2O2+H=HO2+H2     1.69E12   0.0  3760.   ! BAU92
!H2O2+H=OH+H2O     1.02E13   0.0  3580.   ! BAU92
! inserted H2O2+O=HO2+OH from TH86. I had not used this before,
! never mattered much to anything I did. MB89 also did not use.
! probably doesn't matter much to MMH. WRA, 060503
H2O2+O=HO2+OH     9.63E6    2.0  3974.   ! TH86
H2O2+OH=H2O+HO2   1.75E12   0.0  318.    ! TH86
! ***** updated CH+N2 and NCN chemistry *****
!CH+N2=HCN+N       3.00E11   0.0  13600.  ! MB89
CH+N2=NCN+H        2.22E07   1.48 23367.  ! ML00
H+NCN=HCN+N        1.89E14   0.0  8425.   ! ML00
NCN+N=CN+N2        2.00E13   0.0   0.     ! WRA est.

! I do not expect NCN to matter much, but:
! if much NCN is formed in any system, the reaction NCN+OH
! probably should also be considered. Most likely products
! appear to be HOCN+N, based on structure. This is ~7kcal/mole
! exo, would likely have some barrier. Any estimate is likely
! to have appreciable error, so just left it out for now. (EP
! method to get Ea does not apply, this does not appear to
! be a simple abstraction. HNCO+N would be more exo products,
! but rearrangement to this appears to involve 4 center TS,
! seems likely to have large barrier. WRA, 052903

! ***** end updates to CH+N2 and NCN chemistry *****
CN+N=C+N2          1.04E15  -0.5   0.     ! MB89
!H2CN+M=HCN+H+M    3.00E14   0.0  22000.  ! MB89
C+NO=CN+O          6.60E13   0.0   0.     ! MB89
HCCO+NO=HCNO+CO    2.00E13   0.0   0.     ! MB89
!HCNO+H=HCN+OH     1.00E14   0.0  12000.  ! MB89
! replaced HCNO+H=HCN+OH by GRI 3.0 expression
CH+N=CN+H          1.30E13   0.0   0.     ! MB89
HCCO+N=HCN+CO      5.00E13   0.0   0.     ! MB89
!HCN+OH=CN+H2O     1.45E13   0.0  10929.  ! MB89
!CN+H2O=HCN+OH     7.83E12   0.0  7450.   !
! prev is from Jacobs et al (Wolfrum) 1988, per Baulch et al, 1992 crit rev.
! NOTE: k for HCN+OH direction if from thermo. Decided to use CN+H2O
! direction as this makes updates easy. Worry here regards controversy on

```

! Hf(CN), though this appears to be dying out recently due to Halpern's work  
! (1991); also see Bauchlicher et al, 1994 JCP.  
! I like Hf(CN,298)= 104.0 kcal, which current Sandia database uses. MB89  
! expression is from Hanson & coworkers, IJCK 1984. Reversing Jacobs  
! expression with my preferred Hf(CN), per Baulch et al, 1992, yields  
! (Hr = -19.2 kJ = -4.59 kcal @298; wra 3/3/95):

!HCN+OH=CN+H2O	9.04E12	0.0	10730.	! Baulch et al, 1992.
HCN+OH=CN+H2O	3.90E06	1.83	10290.	! WHB95
!OH+HCN=HOCN+H	5.85E04	2.4	12500.	! MB89
! OH+HCN=HOCN+H from MB89 replaced later by Miller&Melius, per DB00				
OH+HCN=HNCO+H	1.98E-03	4.0	1000.	! MB89
OH+HCN=NH2+CO	7.83E-04	4.0	4000.	! MB89
!HOCN+H=HNCO+H	1.00E13	0.0	0.	! MB89
HCN+O=NCO+H	1.38E04	2.64	4980.	! MB89;Perry&Melius 85 similar
HCN+O=NH+CO	3.45E03	2.64	4980.	! MB89;Perry&Melius 85 similar
HCN+O=CN+OH	2.70E09	1.58	26600.	! MB89; from Perry&Melius 85
!HCN+O=CN+OH	2.00E13	0.0	21800.	! wra ul est(Tsang on rev later)
!CN+H2=HCN+H	2.95E05	2.45	2237.	! MB89
CN+H2=HCN+H	3.61E08	1.55	3000.	! Tsang, 1992.; whb95 is similar
!CN+O=CO+N	1.80E13	0.0	0.	! MB89
CN+O=CO+N	2.05E13	0.0	417.	! Tsang, 1992.
!CN+O2=NCO+O	5.60E12	0.0	0.	! MB89
CN+O2=NCO+O	2.60E14	-0.5	0.	! S&S88
!CN+OH=NCO+H	6.00E13	0.0	0.	! MB89
CN+OH=NCO+H	4.00E13	0.0	0.	! Tsang,92; WHB95 confirm
!CN+OH=HCN+O	6.00E12	0.0	2000.	! Tsang,92
!CN+HCN=C2N2+H	2.00E13	0.0	0.	! MB89
CN+HCN=C2N2+H	1.51E07	1.71	1530.	!Tsang 92, from Yang et al 92;
! WHB 95 experiments support this result				
!CN+NO2=NCO+NO	3.00E13	0.0	0.	! MB89
!CN+NO2=NCO+NO	2.40E13	0.0	-370.	! Tsang,1992
! Note: previous versions had sign error for Ea in above rxn.				
CN+NO2=NCO+NO	6.16E15	-0.752	344.	! WMHB 25th ISC, 94
CN+CO2=NCO+CO	3.67E6	2.16	26900.	! WYL, IJCK 91
!CN+N2O=NCO+N2	1.00E13	0.0	0.	! MB89
CN+N2O=NCN+NO	2.40E13	0.0	13330.	! Williams etal1995, upp limb
!CN+N2O=NCN+NO	9.55E08	0.0	835.	! Williams etal1995, low limb
! NOTES: Wang,Yang,Lin&Melius1991 have similar expression (to sum of two ! previous terms), recommended by Tsang (all there was). Melius recommends ! same prods, Williams et al confirmed. Looks like first term alone will ! do well above ~600K. There is a pressure dependence that is not at all ! well-understood, and may indicate different prods, e.g. stabilizes, at ! lower T, higher P. So am leaving this out. This is something likely to ! require future attention. (WRA, 3.15.95).				
! Note: a further complication is that the NCO+N2 channel could open up at ! higher T.				
C2N2+O=NCO+CN	4.57E12	0.0	8880.	! MB89
!C2N2+OH=HOCN+CN	1.86E11	0.0	2900.	! MB89
! Above rxn has delta H = +18 kcal/mole, so products must be wrong.				
! Unlikely to matter to nitrate ester chem. Might for nitramines. WRA				
!NO2+OH=HO2+NO	1.80E13	0.0	6676.	! from CJ Howard, JACS 1980
NO+HO2=NO2+OH	2.11E12	0.0	-479.	! HS84 (from CJ Howard)
NO2+H=NO+OH	1.30E14	0.0	361.	! KF91
NO2+O=NO+O2	3.90E12	0.0	-238.	! ATK/BAU 89
NCO+H=NH+CO	5.40E13	0.0	0.	! Tsang 92
!NCO+O=NO+CO	2.00E13	0.0	0.	! MB89
NCO+O=NO+CO	4.52E13	0.0	0.	! Tsang,1992
NCO+O2=NO+CO2	2.0E12	0.0	20000.	! MB91
NCO+N=N2+CO	2.00E13	0.0	0.	! MB89
!				
! Tsang, 1992, thinks NCO+OH does not go to products NO+CO+H. He thinks ! the reaction NCO+OH=HNCO+O does. That reaction is in this mech in the ! reverse direction since its k is known best in that direction. Note ! Hf(NCO) is now believed quite different from what Tsang used. There is ! also a recombination channel to consider to HONCO, not used presently ! because of lack of thermo data that species. It is unlikely to be				

```

! important to DZ because of low concentrations these species, but should
! be included in a revised version.
!
! 4/20/95 NCO+OH=NO+CO+H appears to be a reasonable reaction.
! (WRA) An estimate is included below with a revised Ea vs MB89.
! This is consequence of a recent change in Hf(NCO) by ~+7.5 kcal.
! The HNCO+O channel is also still in (as the reverse). None
! of the possible channels seems to matter much for propellant
! DZ, major focus of the moment. A quick estimate of the reverse
! k for HNCO+O channel indicates it is main channel of NCO+OH,
! so the estimate for NO+CO+H is compatible with reverse k
! measurements.
!
NCO+OH=NO+CO+H 2.00E13 0.0 7500. ! WRA est
!NCO+OH=NO+CO+H 1.00E13 0.0 0. ! MB89(impossible w/revised Hr)
!NCO+M=N+CO+M 6.30E16 -0.5 48300. ! LH84
NCO+M=N+CO+M 1.14E23 -1.95 59930. ! Tsang,1992, N2
N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.5/ ! CO2/N2 per Tsang, others guessed
! NCO+NO=prods total is from MDHB92, 24th ISC, p702; branching based on
! 298 K work of Cooper and Hershberger, per Tsang,92. Prod ratio subject to
! revision pending higher T work.
!NCO+NO=N2O+CO 4.62E17 -1.73 763. !
!NCO+NO=CO2+N2 6.16E17 -1.73 763. !
!NCO+NO=CO+N2+O 3.22E17 -1.73 763. !
!
! New revision for above rxns follows.
! Revised per newer results of Cooper, Park & Hershberger for the branching
! ratio (298 J) and fit to data from 7 sources for total. Mertens et al
! recommendation was shortened to their T range studied for this fit as
! they did not give a fit to their data over that range only. RRKM result
! of Lin, He and Melius is pretty close. They do predict a modest branching
! ratio variation vs T, if reaction(s) is sensitive, this ratio should
! possibly be reconsidered.
!
! NCO+NO=products 2.01E18 -1.78 790. ! fit described above
!NCO+NO=N2O+CO 8.80E17 -1.78 790. ! 0.44 @ 298
!NCO+NO=CO2+N2 1.13E18 -1.78 790. ! 0.56 @ 298
NCO+NO=N2O+CO 3.98E19 -2.19 1743. ! ZL00, JPC A104, 10807, 2000
NCO+NO=CO2+N2 1.46E21 -2.74 1824. ! ZL00, JPC A104, 10807, 2000
NCO+H2=HNCO+H 2.07E06 2.0 6020. ! Tsang,1992
!NCO+NO2=CO+2NO 1.40E13 0.0 0. ! Tsang,1992,est
!NCO+NO2=CO2+N2O 0.40E13 0.0 0. ! Tsang,1992,est
!NCO+NO2=CO2+N2O 1.80E13 0.0 0. ! WRA, 1995, est
! 4/20/95 (WRA) CO+NO+NO doesn't seem to make sense as main channel of
! NCO+NO2.
!NCO+NO2=CO2+N2O 3.25E12 0.0 -707. ! WMHB, 25th ISC, 94
!NCO+NO2=CO2+N2O 2.98E12 0.0 -707. ! WMHB w/PH93 298 ratios
!NCO+NO2=CO+NO+NO 2.70E11 0.0 -707. ! WMHB w/PH93 298 ratios
!NCO+NO2=products 2.13E13 -0.258 -620. ! fit described below
NCO+NO2=CO2+N2O 1.95E13 -0.258 -620. ! see below
NCO+NO2=CO+NO+NO 1.77E12 -0.258 -620. ! see below

! NCO+NO2=products is taken from a fit to data from following 3 sources:
! WMHB94; 25th ISC, p983, 1994
! PH93; JPC 97, p13647, 1993
! JLW95; IJCK 27, p1111, 1995
! The branching ratio is taken from the room temperature measurement of PH93.
! Note WMHB95 recommendation above did not have the more recent data of
! PH93
!
! Effects of above branching need to be tested. Latter rxn could
! reverse (CO+NO+NO -> NCO+NO2) for DZ mixtures at high P. Have previously
! seen my predictions show this could matter. But that was using Tsang's
! (very large) estimate of the branching ratio to CO+NO+NO, which probably
! gives too high a k. No good measurements of the branching ratio for high T
! currently exist. - WRA, 2/2/96 -

```

```

!
NH+O2=HNO+O      4.61E05   2.0   6500.      ! M&M, 24th ISC, 92
NH+O2=NO+OH      1.28E06   1.5   100.       ! M&M, 24th ISC, 92
! the following reaction changed (slightly) ****
NH+NO=N2O+H      3.50E14   -0.46  16.1      ! B.Williams fit of MM calc
NH+NO=N2+OH      2.16E13   -0.23   0.       ! M&M, 24th ISC, 92

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!N2O+OH=N2+HO2   2.00E12   0.0  10000.    ! MB89 ; removed per
!
!           a number of studies, culminating with Glarborg's, C&F 95;
!           note these were around 1250 K studies.
N2O+OH=N2+HO2   1.29E-02   4.72  36561    ! Mebel et al 96, per DB00
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!N2O+H=N2+OH     2.53E10   0.0   4550.     ! MKF89
!   DUP
!N2O+H=N2+OH     2.23E14   0.0  16750.    ! MKF89
!   DUP
!
!   Following is WRA fit to selected experimental data for H+N2O=N2+OH.
!
!   Best for the range 714 - 2850 K. The expression is:

N2O+H=N2+OH     1.30E11   0.938  15210.    ! WRA01 (Fit#8, WRA, 3/16/01)

!   Recommended error limits are a factor of 1.3 from 714 to 1200 K,
!   increasing to a factor of 1.5 at 2850 K.
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

!N2O+H=NNH+O     5.00E-06   5.52  27420.    ! B&D93, July 1993 version
NNH+O=N2O+H      1.40E14   -0.40  477.      ! B&D95,QRRK,preprint on O+NNH
NNH+O=NO+NH      3.30E14   -0.23 -1013.    ! ditto
!N2O+O=N2+O2     1.00E14   0.0   28000.    ! HS85 (&TH91)
!N2O+O=N2+O2     1.40E12   0.0   10800.    ! DDCH92(Shock Waves,813,1992)
!N2O+O=NO+NO     6.92E13   0.0   26600.    ! HS85 (&TH91)
!N2O+O=N2+O2     3.654E12   0.0   15900.    ! M&A97
!N2O+O=NO+NO     9.985E13   0.0   28040.    ! M&A97
!N2O+O=N2+O2     3.691E12   0.0   15930.    ! M&A99
!N2O+O=NO+NO     9.172E13   0.0   27690.    ! M&A99
N2O+O=N2+O2     3.692E12   0.0   15940.    ! M&A00
N2O+O=NO+NO     9.155E13   0.0   27680.    ! M&A00
H+HNO=NH+OH     3.00E14   0.0   18000.    ! WRA, 1993 jannaf est
NH+OH=N+H2O     5.00E11   0.5   2000.     ! MB89
NH+N=N2+H       3.00E13   0.0    0.       ! MB89

! ***** N+H2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
!N+H2=NH+H       1.60E14   0.0  25140.    ! DH90
N+H2=NH+H       2.33E14   0.0  30830.    ! ZT00 (JCP 113, 6152, 2000)
! ***** End N+H2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH2+O=HNO+H     6.63E14   -0.5   0.       ! MB89
!HNO+H=NH2+O     3.50E15   -0.3  28200.    ! B&D July 93 preprint
!NH2+O=NH+OH     6.75E12   0.0   0.       ! MB89
NH2+O=HNO+H     4.60E+13   0.00  0        ! DB00
NH2+O=NH+OH     7.00E+12   0.00  0        ! DB00
DUPLICATE
NH2+O=NH+OH     3.33E+08   1.50  5077     ! DB00
DUPLICATE
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

NH2+OH=NH+H2O   4.00E06   2.0   1000.     ! MB89
NH2+H=NH+H2     4.00E13   0.0   3650.     ! DKCH90

```



NH2+NH=N2H2+H 1.50E15 -0.50 0. ! DKCH90  
 NH2+N=N2+H+H 7.20E13 0.0 0. ! MB89  
 NH2+O2=HNO+OH 4.50E12 0.0 25000. ! MB89

! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*  
 !NH2+NH2=N2H2+H2 5.00E11 0.0 0. ! MB89  
 ! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*

NH2+NH2=NH+NH3 5.00E13 0.0 10000. ! DKCH90  
 NH2+NH2=N2H3+H 1.79E13 -0.35 11320. ! B&D93, AMD, priv. comm.  
 NH2+NH2+M=N2H4+M 2.98E47 -9.44 9680. ! B&D93, AMD, priv. comm.

! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*  
 !NH2+NO2=N2O+H2O 2.84E18 -2.2 0. ! Baulch et al 84, per MB91  
 ! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*

! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*  
 !NH+NO2=N2O+OH 1.00E13 0.0 0. ! from Harrison et al  
 NH+NO2=N2O+OH 4.00E12 0.0 0. ! branching per QH95  
 NH+NO2=NO+HNO 5.70E12 0.0 0. ! branching per QH95  
 ! NH+NO2 total k=9.70E12 from HWP86, branching ratio from QH95  
 ! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*

! \*\*\*\*\*  
 ! Begin updates to DCS84 chem from ADN.051601. WRA, 5/22/03  
 ! \*\*\*\*\*

! You might think NxHy would matter a lot for MMH, but in fact the main  
 ! breakdown is likely scission of the N-N bond, rather than C-N.  
 ! I could have brought in lots of QRRK estimates I have for these  
 ! reactions, but it would seriously complicate things. I'm just  
 ! going to update the DCS84 reactions to DB00. WRA, 052203

!N2H4+H=N2H3+H2 1.00E12 0.50 2000. ! DCS84  
 !N2H4+OH=N2H3+H2O 3.00E10 0.68 1290. ! DCS84  
 !N2H4+O=N2H3+OH 2.00E13 0.00 1000. ! DCS84  
 !N2H3=N2H2+H 1.20E13 0.00 58000. ! DCS84  
 !N2H3+H=N2H2+H2 1.00E12 0.50 2000. ! DCS84  
 !N2H3+OH=N2H2+H2O 3.00E10 0.68 1290. ! DCS84  
 !N2H3+O=N2H2+OH 2.00E13 0.00 1000. ! DCS84

! NOTE, WRA has done QRRK on N2H3+M, but results are very complex to include, and  
 ! Ea is very large (> 50 kcal/mole) for all channels, so decided not to include  
 ! See ADN.051601 for QRRK results.

!N2H4+H=N2H3+H2 9.60E+08 1.50 4838 ! HTRAN EST. 12/22/95 (DB00)  
 N2H4+H=N2H3+H2 4.90E12 0.00 2130. ! fit to data from 6 sources in NIST (WRA)  
 N2H4+O=N2H3+OH 6.70E+08 1.50 2851 ! HTRAN EST. 12/22/95 (DB00)  
 N2H4+OH=N2H3+H2O 4.80E+06 2.00 -646 ! HTRAN EST. 12/22/95 (DB00)  
 N2H3+H=N2H2+H2 2.40E+08 1.50 -10 !ABSTRACTION 1/15/96 (DB00)  
 N2H3+O=NH2+HNO 3.00E+13 0.00 0 ! (DB00)  
 !N2H3+O=NH2NO+H 3.00E+13 0.00 0  
 N2H3+O=N2H2+OH 1.70E+08 1.50 -646 !ABSTRACTION 1/15/96 (DB00)  
 N2H3+OH=N2H2+H2O 1.20E+06 2.00 -1192 !ABSTRACTION 1/15/96 (DB00)  
 !N2H3+OH=H2NN+H2O 3.00E+13 0.00 0 ! 2/15/96 SAME AS ADDUCT FORMATION  
 (DB00)  
 N2H3+NH2=N2H2+NH3 9.20E+05 1.94 -1152 !ABSTRACTION 1/15/96 (DB00)  
 !N2H3+NH2=H2NN+NH3 3.00E+13 0.00 0 !SAME AS ADDUCT FORM. (2/20/96) (DB00)  
 !N2H3+HO2=H2NNHO+OH 3.00E+13 0.00 0 !RECOMBINATION(-5KCAL) (DB00)  
 N2H3+HO2=N2H2+H2O2 2.90E+04 2.69 -1600 ! UPDATE 10/18/97 (DB00)  
 N2H3+HO2=N2H4+O2 9.20E+05 1.94 2126 !NH2 WITH ADJUSTED THERMO (DB00)

```

! *****
! Begin updates to DCS84 chem from ADN.051601.   WRA, 5/22/03
! *****

```

```

N2H2+M=NNH+H+M   5.00E16   0.0  50000.   ! MB89
      H2O/15./ O2/2.0/ N2/2.0/ H2/2.0/
N2H2+H=NNH+H2    5.00E13   0.0   1000.   ! MB89
N2H2+O=NH2+NO    1.00E13   0.0    0.     ! MB89
N2H2+O=NNH+OH    2.00E13   0.0   1000.   ! MB89
N2H2+OH=NNH+H2O  1.00E13   0.0   1000.   ! MB89
N2H2+NH=NNH+NH2  1.00E13   0.0   1000.   ! MB89
N2H2+NH2=NH3+NNH 1.00E13   0.0   1000.   ! MB89

```

```

! *****
! Begin choices for NH2+NO taken from ADN.051601.   WRA, 5/22/03
!
! NOTE!!! ADN.051601 contains QRRK results for many other
! reactions and pressures on this PES. I'm just using the two
! channels for Nusca's MMH mech with low P expressions because
! that's all that will matter at low P. Ratio of the two
! channels can be very sensitive in a number of systems.
!
! *****

```

```

! *****
! Begin reactions on NH2NO surface (Note NH2+NO=N2O+H2 is commented out
! earlier for reasons discussed there.
! *****

```

```

! history of WRA choices and comments

```

```

!NH2+NO=NNH+OH    6.40E15   -1.25   0.     ! MB89
!NH2+NO=N2+H2O    6.20E15   -1.25   0.     ! MB89
!NH2+NO=N2+H+OH   9.30E11    0.0    0.     ! BVV mdl, C&Fv98,402(1994)
!NH2+NO=N2+H2O    2.00E20   -2.6    924.   ! BVV mdl, C&Fv98,402(1994)
! Note, BVV had prods for radical channel as shown, but they are
! actually NNH+OH (which equally well model their NH3/NO flame
! experiment because all NNH->N2+H under their conditions).
! BVV expressions good for high T.
!NH2+NO=NNH+OH    4.90E11   -0.03  -362.   ! DYWL94 (lin), JPC1994
!NH2+NO=N2+H2O    4.70E15   -1.09  186.   ! DYWL94 (lin), JPC1994
! Above two expressions ignore DYWL's recomb channels
!NH2+NO=NNH+OH    3.50E10    0.335  -765.   ! DB00
!NH2+NO=N2+H2O    4.70E12   -0.247 -1200.  ! DB00
!NH2+NO=NNH+OH    1.43E07    1.40  -1777.  ! PL99 corrected typo per ADN.051601.2
!NH2+NO=N2+H2O    1.20E17   -1.61   298.   ! PL99 corrected typo per ADN.051601.2
NH2+NO=NNH+OH    2.29E10    0.425  -815.   ! MG99
NH2+NO=N2+H2O    2.77E20   -2.65  1258.   ! MG99

```

```

!
!
! Regarding NH2+NO:
! I used the BVV expressions for several years as these have
! a good representation of the high T branching ratio.
! T > 1000 is very important for combustion applications,
! The BVV expressions at T < 500 K have NNH+OH too low vs expts
! for T < 500 K, but good at higher T; total is mildly high.
! DB00 has good total from 298 - 2500, but NNH+OH branching too
! low for T > 1000 K. The branching may be extremely important.
! Note the PL99 branching ratio is similar to MG99. However,
! the total of the two channels is larger than the other
! expressions at high T. There is a minimum in the total

```

! at about 2000 K for PL99 expressions and then increases  
! sharply towards higher T, which seems nonphysical.  
! PL99 say the PL97 expression for the total was retained  
! and just the branching ratio was changed. However, the  
! total of PL99 expressions deviates to significantly  
! higher values than the ktot expression given in PL97 for  
! T > 2000 K. (PL97 ktot expression does not have minimum and  
! then increase sharply towards higher T like PL99 does.)  
! MG99 has good branching representation over 298 - 3000.  
! MG99 maybe slightly low total (20%?) at high T (2500), but  
! not terrible; certainly within error limits of experiments.  
! Therefore these expressions were chosen. The branching ratio  
! is typically very sensitive when these reactions come into  
! play. WRA, 8/29 and 9/12/00  
!

! \*\*\*\*\*  
! End choices for NH2+NO taken from ADN.051601. WRA, 5/22/03  
! \*\*\*\*\*

NH3+OH=NH2+H2O	2.04E06	2.04	566.	! MB89
!NH3+H=NH2+H2	6.36E05	2.39	10171.	! MB89
NH3+H=NH2+H2	5.42E05	2.40	9917.	! KMF90 (Ko, Marshall...)
NH3+O=NH2+OH	9.40E06	1.94	6460.	! SUT/PAT/KLEMM90

! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*  
!NH3+M=NH2+H+M 2.20E16 0.0 93470. ! DKCH90; keyed for Ar=1.0  
NH3(+M)=NH2+H(+M) 5.50E15 0.00 107792.  
LOW/2.20E16 0.00 93470./  
! Low pressure limit is from reevaluation by DKCH90.  
! High pressure limit is from HW81 (assuming NH2+H products).  
! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*

!NNH+NO=N2+HNO	5.00E13	0.0	0.	! MB89
NNH+NO=N2+HNO	2.00E13	0.0	0.	! WRA, est, 040596
NNH+H=N2+H2	1.00E14	0.0	0.	! MB89
NNH+OH=N2+H2O	5.00E13	0.0	0.	! MB89
NNH+NH2=N2+NH3	5.00E13	0.0	0.	! MB89
NNH+NH=N2+NH2	5.00E13	0.0	0.	! MB89

! the next reaction rate changed \*\*\*\*\*  
HNO+OH=NO+H2O 1.295E07 1.884 -958. ! SPM91  
H+HNO=H2+NO 4.46E11 0.72 655. ! SP92  
HNO+NH2=NH3+NO 2.00E13 0.0 1000. ! MB89  
N+NO=N2+O 3.27E12 0.3 0. ! MB89  
O+NO=N+O2 3.80E09 1.0 41375. ! TH91  
NO+H=N+OH 1.70E14 0.0 48800. ! HS85  
HNO+HNO=N2O+H2O 3.63E-03 3.98 1190. ! LHM92  
HNC+O=NH+CO 5.44E12 0.0 0. ! TDLLM (Lin), 1994, preprint  
HNC+O=H+NCO 1.6E01 3.08 -224. ! TDLLM, 1994  
! note: 1st of two preceding k's from experiment, 2nd from TST by TDLLM  
! k's taken from the table (more digits than the abstract)  
HNC+OH=HNCO+H 2.80E13 0.0 3696. ! HLM, IJCK 24, 1103, (1992).  
!N2O+NO=N2+NO2 1.0E14 0.0 49675. !added Yetter,  
! traced source back to Smith and Thorne and then lost trail  
!N2O+NO=N2+NO2 2.75E14 0.0 50000. ! Borisov et al, 73, per NIST  
!N2O+NO=N2+NO2 2.71E14 0.0 50700. ! WRA, fit to selected (and  
! some of it corrected) data from four sources  
N2O+NO=N2+NO2 4.29E13 0.00 47130. ! WRA, 11/95; fit to reanalyzed  
! lit results. This is not as different as old recommendation as it at first  
! appears. Main difference is ~3 times smaller at high T. This has a strong  
! effect on the A-factor, a more modest (but impt.) effect on Ea.

```

NO+NO+NO=N2O+NO2 1.07E10 0.0 26800. ! GVO 79
HOCO+M=OH+CO+M 2.19E23 -1.89 35270. ! LSG88, LP LIMIT
HNC+OH=CN+H2O 1.5E12 0.00 7680. ! TST result from TDLLM, 1994
HNC+NO2=HNCO+NO 1.0E12 0.00 32000. ! TST result from TDLLM, 1994
!
! New reactions, added 3/8/95, hlwm92 ISC
!
!HNCO+M=NH+CO+M 3.26E35 -5.11 109900. ! MCHB89,IJCK measured;best
! except Tsang 92 (used Tsang's expression earlier; has falloff)
!HNCO+M=H+NCO+M 5.00E15 0.0 120000. ! MCHB89,IJCK est
! per Tsang, better watch last reaction at low T, high P conditions,
! might get into falloff - could matter if reversed.
HNCO+O=CO2+NH 9.80E07 1.41 8524. ! HLWM, 92 ISC, TST (Lin, p711)
HNCO+O=NCO+OH 2.20E06 2.11 11430. ! HLWM, 92 ISC, TST
! NOTE: modeled exp results in T range of exp are very similar
! for previous two rxns. Next rxn could not be measured.
! Just noted Tsang 92 recommends these. Another product channel of the reverse
! of 2nd rxn is discussed earlier in this file and eliminated, per Tsang.
HNCO+O=HNO+CO 1.49E08 1.57 44010. ! HLWM, 92 ISC, TST
!HNCO+OH=H2O+NCO 2.63E12 0.0 5544. ! Tully et al, 22nd ISC, 1989
!HNCO+OH=H2O+NCO 6.38E05 2.0 2560. ! Tsang,1992
HNCO+OH=H2O+NCO 4.79E05 2.0 2560. ! Tsang,1992/MB91
HNCO+OH=NH2+CO2 1.60E05 2.0 2560. ! Tsang,1992/MB91
! What's happening with HNCO+OH is Tsang's recommended total disappearance
! k for the rxn was used, but it was split into 2 channels 75:25 as
! recommended in MB91. This ratio is only established by the complex
! modeling work of MB91 (subject to error, especially the T dependence of
! the ratio), but seems reasonable. The total recommended by Tsang is
! close to that used by MB91, he just mentions having added a T**2
! dependence. -WRA-

! ***** Update to HNCO+HO2 from m-yet-wra.rdx.1.8.wNHx.wHC.5*****
! Miller & Bowman
!HNCO+HO2=NCO+H2O2 3.00E+11 0.00 2.900E+04
HNCO+HO2=NCO+H2O2 3.00E11 0.0 23700. !
! WRA revised MB91's estimate due to updates
! in thermo.
! *****End update from m-yet-wra.rdx.1.8.wNHx.wHC.5*****

!HNCO+NH=NH2+NCO 2.00E13 0.0 23840. ! per Lin et al, 1991 jannaf,v2,337
HNCO+NH=NH2+NCO 2.00E13 0.0 19300. ! WRA est, change due to new thermo
!HNCO+H=NH2+CO 2.10E14 0.0 16890. ! MK-HHB91 (Hanson)
HNCO+H=NH2+CO 2.25E07 1.7 3800. ! Miller&Melius IJCK92,TST,
! agrees well w/Hanson
!HNCO+H=H2+NCO 1.05E05 2.50 13300. ! M&M,IJCK92, rev appears earlier
! ! re prior reaction: am using Tsang's expression for the reverse
HNCO+NO2=HNNCO+CO2 2.50E12 0.0 26000. ! HLLM93
CH+NO=HCN+O 1.10E14 0.0 0. ! MB89
!
! added 3/10/95
!
!CN+NO=NCO+N 9.60E13 0.0 42100. ! Tsang 92
! see test estimates other channel at end
! Tsang's best est as of 1992 rev: remove cn+no -> n2+co
!
CN+NO=NCO+N 5.5E12 0.0 30620. ! HWLM95 (Lin); Shock Waves Symp.
CN+NO=N2+CO 3.9E11 0.0 27820. ! HWLM95, tst calc
CN+NO=NCN+O 1.8E13 0.0 38190. ! HWLM95, tst calc
CO+NO2=NO+CO2 9.04E13 0.0 33780. ! TH91
!CO+NO2=CO2+NO 1.26E14 0.0 27600. ! Zabarnick, C&F91
!
! Just noted: Zabarnick misquoted Thorne & Melius who had 1.26E12;27600.
! Thorne and Melius' choice appears to be an estimate.
!
! *****
! Watch Princeton group for new info on prior rxn, they are working

```

```

!           on it (see 1994 jannaf).
! *****
!
!CO+N2O=CO2+N2      left out per Princeton group and Lin recommendations.
!HO2+NO2=HONO+O2    4.64E11  0.0   -479. ! Zab, C&F91 cites Leeds, not there
CH+NO2=HCO+NO       1.01E14  0.0     0. ! WCF82
!HCO+NO2=CO+HONO    1.50E13  0.0   -430. ! T&M89, from TRG88 w/assumed prods
!HCO+NO2=CO2+H+NO   1.50E11  0.0   -430. ! T&M89, est?

! ***** H2+NO2 and HONO+ H revised per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!H2+NO2=HONO+H      3.21E12  0.0  28810. ! Yetter et al, 29th Jannaf;
! ~k(S&G)/7.5; Ea somewhat tentative, Yetter et al didn't cover wide range;
! extrapolation out of range ~694-944 should be done with caution pending
! further work. On the other hand, considering the reverse rxn thermo and
! with the expectation the reverse rxn might have a small barrier, 28-31
! kcal is probably about right.
!HONO+H=H2+NO2      1.205E13  0.0   7326.      ! TH91,est
!H2+NO2=HONO+H      2.40E13  0.0  29000. ! S&G78, as cited in nist
! Yetter et al criticised preceeding expression as S&G
! depended on using high conc mixtures of H2/air (no inert) which
! calculations show would not have (T,P) constant during experiment.
! Conditions used by Skinner and coworkers (data cited and reduced by
! S&G as well as their own) were similar. Therefore, Princeton group
! presently best expression. (NOTE: T ranges used by S&G, Skinner et al
! and Princeton group were very similar, a fact I'd forgotten until
! recently. WRA, 3/31/95)
H2+NO2=HONO+H      1.30E04      2.76  29770.      ! PGML98; see also MGYD00
HONO+H=HNO+OH       5.63E+10      0.86  4969.      ! HLMM97
HONO+H=H2O+NO       8.13E+06      1.89  3847.      ! HLMM97

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
2HONO=NO+NO2+H2O   0.349      3.64  12140.      ! MLM98
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

! **** End H2+NO2 and HONO+ H revised per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****

!*****
! Begin NNH+M
!*****
!
!           HEADS UP !!!!
!
! P dept rxns where I've used 3 param expressions; need attention in
! case of changing P.
!
! 12/22/00 NOTE: Don't worry about the above message anymore for NNH+M.
! I replaced old B&D95 limiting expressions with a Lindemann falloff form
! some time ago and forgot to clean the warning out. And JWB has gone
! over my Lindemann expression and tentatively approves. Above was an old
! note I forgot to clean out. I'm leaving it in to remind me what I did.
! Other P dept rxns in this section have been moved elsewhere and cleaned
! up to either falloff forms or specific P functions for which the user
! is instructed elsewhere what to do, i.e. chose from a list of
! functions. (see beginning of file in particular for a list of reactions
! thus affected). - WRA
!
!
!NNH=N2+H           1.00E04      0.0     0.      ! MB89
NNH(+M)=N2+H(+M)   4.10E09      1.13  5186.      ! B&D95; high P limit
      LOW/ 1.00E13      0.5     3060./      ! B&D95; low P limit
      N2O/5.0/ H2O/9.0/ N2/1.0/ O2/0.82/      ! like N2O+M
      HNO3/5.0/ NH3/5.0/ NO3/5.0/              !
! CO2/3.2/
NNH=N2+H           3.00E08      0.0     0.      ! tunneling term, B&D95
DUP
! NOTE: Low and high P limits taken from estimates of B&D in IJCK95

```

! paper. Simple Lindemann form assumed, uncertainty doesn't seem  
! to warrant better. Also, the reaction is not particularly  
! sensitive for most propellant conditions as virtually all NNH is  
! converted to N2+H. Finally, note B&D's low P expression  
! includes a constant nonradiative decay (tunneling) term.

! \*\*\*\*\*  
! End NNH+M  
! \*\*\*\*\*

! \*\*\*\*\*

!  
! HEADS UP !!!!  
!  
! P dept HCN=HNC rxn where I've used 3 param expressions; need attention in  
! case of changing P.  
!  
!

!HCN=HNC	1.95E24	-4.23	49572.	!	k(jwb, 1 atm;
!					rcd 2/8/95)
!HCN=HNC	1.06E26	-4.34	50194.	!	2 x k(jwb, 10 atm; i.e.for
!					! 20 atm; rcd 2/8/95)
!HCN=HNC	1.59E26	-4.34	50194.	!	3 x k(jwb, 10 atm; i.e.for
!					! 30 atm; rcd 2/8/95)
HCN+M=HNC+M	4.36E26	-3.34	50194.	!	2nd order form, easiest to use
!					! above is low P limit, appropriate if T > ~600K; rxn is not sensitive for DZ.
!					! Reason is it is strongly into partial equilibrium.
!					! The expression is not bad (factor of 2ish error) even for T < 600 K, 10 atm.
!					! Of more concern would be hof(HNC).
!					!

! *****					
HNO+NO+NO=HNNO+NO2	1.70E11	0.00	2100.	!	Diau et al, IJCK 27,867(1995)
HNNO+NO=NNH+NO2	3.2E12	0.00	270.	!	Diau et al, IJCK 27,867(1995)
HNNO+NO=N2+HONO	2.6E11	0.0	810.	!	Diau et al, IJCK 27,867(1995)
HNNO+M=H+N2O+M	2.2E15	0.0	21600.	!	Diau et al, IJCK 27,867(1995)
HNNO+M=N2+OH+M	1.0E15	0.0	25600.	!	Diau et al, IJCK 27,867(1995)
HNNO+OH=H2O+N2O	2.0E13	0.0	0.	!	wra est
HNNO+H=H2+N2O	2.0E13	0.0	0.	!	wra est
!NNH+M=N2+H+M	1.0E14	0.0	3000.	!	Diau et al, IJCK 27,867(1995)
HCO+NO=HNO+CO	7.23E12	0.0	0.	!	TH91; test

!  
! \*\*\*\*\* REACTIONS GLEANED FROM GRI 3.0 \*\*\*\*\*  
!

O+CH2<=>H+HCO	8.000E+13	.000	.00
O+CH2(S)<=>H2+CO	1.500E+13	.000	.00
O+CH2(S)<=>H+HCO	1.500E+13	.000	.00
O+CH3<=>H+CH2O	5.060E+13	.000	.00
O+CH4<=>OH+CH3	1.020E+09	1.500	8600.00
O+CH2O<=>OH+HCO	3.900E+13	.000	3540.00
O+CH2OH<=>OH+CH2O	1.000E+13	.000	.00
O+CH3O<=>OH+CH2O	1.000E+13	.000	.00
O+CH3OH<=>OH+CH2OH	3.880E+05	2.500	3100.00
O+CH3OH<=>OH+CH3O	1.300E+05	2.500	5000.00
O+C2H<=>CH+CO	5.000E+13	.000	.00
O+C2H2<=>H+HCCO	1.350E+07	2.000	1900.00
O+C2H2<=>OH+C2H	4.600E+19	-1.410	28950.00
O+C2H2<=>CO+CH2	6.940E+06	2.000	1900.00
O+C2H3<=>H+CH2CO	3.000E+13	.000	.00
O+C2H4<=>CH3+HCO	1.250E+07	1.830	220.00
O+C2H5<=>CH3+CH2O	2.240E+13	.000	.00
O+C2H6<=>OH+C2H5	8.980E+07	1.920	5690.00

O+CH2CO<=>OH+HCCO	1.000E+13	.000	8000.00
O+CH2CO<=>CH2+CO2	1.750E+12	.000	1350.00
O2+CH2O<=>HO2+HCO	1.000E+14	.000	40000.00
H+CH2 (+M) <=>CH3 (+M)	6.000E+14	.000	.00
LOW /	1.040E+26	-2.760	1600.00/
TROE/	.5620	91.00	5836.00 8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+CH2 (S) <=>CH+H2	3.000E+13	.000	.00
H+CH3 (+M) <=>CH4 (+M)	13.90E+15	-5.34	536.00
LOW /	2.620E+33	-4.760	2440.00/
TROE/	.7830	74.00	2941.00 6964.00 /
H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+CH4<=>CH3+H2	6.600E+08	1.620	10840.00
H+HCO (+M) <=>CH2O (+M)	1.090E+12	.480	-260.00
LOW /	2.470E+24	-2.570	425.00/
TROE/	.7824	271.00	2755.00 6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+CH2O (+M) <=>CH2OH (+M)	5.400E+11	.454	3600.00
LOW /	1.270E+32	-4.820	6530.00/
TROE/	.7187	103.00	1291.00 4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH2O<=>HCO+H2	5.740E+07	1.900	2742.00
H+CH2OH (+M) <=>CH3OH (+M)	1.055E+12	.500	86.00
LOW /	4.360E+31	-4.650	5080.00/
TROE/	.600	100.00	90000.0 10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH2OH<=>H2+CH2O	2.000E+13	.000	.00
H+CH2OH<=>OH+CH3	1.650E+11	.650	-284.00
H+CH2OH<=>CH2 (S) +H2O	3.280E+13	-.090	610.00
H+CH3O (+M) <=>CH3OH (+M)	2.430E+12	.515	50.00
LOW /	4.660E+41	-7.440	14080.0/
TROE/	.700	100.00	90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH3O<=>H+CH2OH	4.150E+07	1.630	1924.00
H+CH3O<=>H2+CH2O	2.000E+13	.000	.00
H+CH3O<=>OH+CH3	1.500E+12	.500	-110.00
H+CH3O<=>CH2 (S) +H2O	2.620E+14	-.230	1070.00
H+CH3OH<=>CH2OH+H2	1.700E+07	2.100	4870.00
H+CH3OH<=>CH3O+H2	4.200E+06	2.100	4870.00
H+C2H (+M) <=>C2H2 (+M)	1.000E+17	-1.000	.00
LOW /	3.750E+33	-4.800	1900.00/
TROE/	.6464	132.00	1315.00 5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+C2H2 (+M) <=>C2H3 (+M)	5.600E+12	.000	2400.00
LOW /	3.800E+40	-7.270	7220.00/
TROE/	.7507	98.50	1302.00 4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+C2H3 (+M) <=>C2H4 (+M)	6.080E+12	.270	280.00
LOW /	1.400E+30	-3.860	3320.00/
TROE/	.7820	207.50	2663.00 6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+C2H3<=>H2+C2H2	3.000E+13	.000	.00
H+C2H4 (+M) <=>C2H5 (+M)	0.540E+12	.454	1820.00
LOW /	0.600E+42	-7.620	6970.00/
TROE/	.9753	210.00	984.00 4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+C2H4<=>C2H3+H2	1.325E+06	2.530	12240.00
H+C2H5 (+M) <=>C2H6 (+M)	5.210E+17	-.990	1580.00
LOW /	1.990E+41	-7.080	6685.00/
TROE/	.8422	125.00	2219.00 6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
H+C2H5<=>H2+C2H4	2.000E+12	.000	.00
H+C2H6<=>C2H5+H2	1.150E+08	1.900	7530.00
H+HCCO<=>CH2 (S) +CO	1.000E+14	.000	.00
H+HCCOH<=>H+CH2CO	1.000E+13	.000	.00
H2+CO (+M) <=>CH2O (+M)	4.300E+07	1.500	79600.00

```

LOW / 5.070E+27 -3.420 84350.00/
TROE/ .9320 197.00 1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
2OH(+M)<=>H2O2(+M) 7.400E+13 -.370 .00
LOW / 2.300E+18 -.900 -1700.00/
TROE/ .7346 94.00 1756.00 5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
OH+CH2<=>H+CH2O 2.000E+13 .000 .00
OH+CH2<=>CH+H2O 1.130E+07 2.000 3000.00
OH+CH2(S)<=>H+CH2O 3.000E+13 .000 .00
OH+CH3(+M)<=>CH3OH(+M) 2.790E+18 -1.430 1330.00
LOW / 4.000E+36 -5.920 3140.00/
TROE/ .4120 195.0 5900.00 6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O 5.600E+07 1.600 5420.00
OH+CH3<=>CH2(S)+H2O 6.440E+17 -1.340 1417.00
OH+CH4<=>CH3+H2O 1.000E+08 1.600 3120.00
OH+CH2O<=>HCO+H2O 3.430E+09 1.180 -447.00
OH+CH2OH<=>H2O+CH2O 5.000E+12 .000 .00
OH+CH3O<=>H2O+CH2O 5.000E+12 .000 .00
OH+CH3OH<=>CH2OH+H2O 1.440E+06 2.000 -840.00
OH+CH3OH<=>CH3O+H2O 6.300E+06 2.000 1500.00
OH+C2H<=>H+HCCO 2.000E+13 .000 .00
OH+C2H2<=>H+CH2CO 2.180E-04 4.500 -1000.00
OH+C2H2<=>H+HCCOH 5.040E+05 2.300 13500.00
OH+C2H2<=>C2H+H2O 3.370E+07 2.000 14000.00
OH+C2H2<=>CH3+CO 4.830E-04 4.000 -2000.00
OH+C2H3<=>H2O+C2H2 5.000E+12 .000 .00
OH+C2H4<=>C2H3+H2O 3.600E+06 2.000 2500.00
OH+C2H6<=>C2H5+H2O 3.540E+06 2.120 870.00
OH+CH2CO<=>HCCO+H2O 7.500E+12 .000 2000.00
HO2+CH2<=>OH+CH2O 2.000E+13 .000 .00
HO2+CH3<=>O2+CH4 1.000E+12 .000 .00
HO2+CH3<=>OH+CH3O 2.000E+13 .000 .00
HO2+CH2O<=>HCO+H2O2 5.600E+06 2.000 12000.00
C+CH2<=>H+C2H 5.000E+13 .000 .00
C+CH3<=>H+C2H2 5.000E+13 .000 .00
CH+H2<=>H+CH2 1.080E+14 .000 3110.00
CH+H2O<=>H+CH2O 5.710E+12 .000 -755.00
CH+CH2<=>H+C2H2 4.000E+13 .000 .00
CH+CH3<=>H+C2H3 3.000E+13 .000 .00
CH+CH4<=>H+C2H4 6.000E+13 .000 .00
CH+CO(+M)<=>HCCO(+M) 5.000E+13 .000 .00
LOW / 2.690E+28 -3.740 1936.00/
TROE/ .5757 237.00 1652.00 5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
CH+CH2O<=>H+CH2CO 9.460E+13 .000 -515.00
CH+HCCO<=>CO+C2H2 5.000E+13 .000 .00
CH2+O2<=>OH+H+CO 5.000E+12 .000 1500.00
CH2+H2<=>H+CH3 5.000E+05 2.000 7230.00
2CH2<=>H2+C2H2 1.600E+15 .000 11944.00
CH2+CH3<=>H+C2H4 4.000E+13 .000 .00
CH2+CH4<=>2CH3 2.460E+06 2.000 8270.00
CH2+HCCO<=>C2H3+CO 3.000E+13 .000 .00
CH2(S)+N2<=>CH2+N2 1.500E+13 .000 600.00
!CH2(S)+AR<=>CH2+AR 9.000E+12 .000 600.00
CH2(S)+O2<=>H+OH+CO 2.800E+13 .000 .00
CH2(S)+O2<=>CO+H2O 1.200E+13 .000 .00
CH2(S)+H2<=>CH3+H 7.000E+13 .000 .00
CH2(S)+H2O(+M)<=>CH3OH(+M) 4.820E+17 -1.160 1145.00
LOW / 1.880E+38 -6.360 5040.00/
TROE/ .6027 208.00 3922.00 10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O 3.000E+13 .000 .00
CH2(S)+CH3<=>H+C2H4 1.200E+13 .000 -570.00
CH2(S)+CH4<=>2CH3 1.600E+13 .000 -570.00

```



```

CH2 (S) +CO<=>CH2+CO          9.000E+12      .000      .00
CH2 (S) +CO2<=>CH2+CO2        7.000E+12      .000      .00
CH2 (S) +CO2<=>CO+CH2O        1.400E+13      .000      .00
CH2 (S) +C2H6<=>CH3+C2H5      4.000E+13      .000     -550.00
CH3+O2<=>O+CH3O               3.560E+13      .000     30480.00
CH3+O2<=>OH+CH2O              2.310E+12      .000     20315.00
CH3+H2O2<=>HO2+CH4            2.450E+04      2.470     5180.00
2CH3 (+M) <=>C2H6 (+M)        6.770E+16     -1.180     654.00
    LOW / 3.400E+41   -7.030   2762.00/
    TROE/ .6190  73.20  1180.00  9999.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
2CH3<=>H+C2H5                  6.840E+12      .100     10600.00
CH3+HCO<=>CH4+CO              2.648E+13      .000      .00
CH3+CH2O<=>HCO+CH4            3.320E+03      2.810     5860.00
CH3+CH3OH<=>CH2OH+CH4         3.000E+07      1.500     9940.00
CH3+CH3OH<=>CH3O+CH4          1.000E+07      1.500     9940.00
CH3+C2H4<=>C2H3+CH4           2.270E+05      2.000     9200.00
CH3+C2H6<=>C2H5+CH4           6.140E+06      1.740     10450.00
CH2OH+O2<=>HO2+CH2O           1.800E+13      .000      900.00
CH3O+O2<=>HO2+CH2O            4.280E-13      7.600    -3530.00
C2H+O2<=>HCO+CO               1.000E+13      .000     -755.00
C2H+H2<=>H+C2H2               5.680E+10      0.900     1993.00
C2H3+O2<=>HCO+CH2O            4.580E+16     -1.390     1015.00
C2H4 (+M) <=>H2+C2H2 (+M)      8.000E+12      .440     86770.00
    LOW / 1.580E+51   -9.300  97800.00/
    TROE/ .7345  180.00  1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
C2H5+O2<=>HO2+C2H4            8.400E+11      .000     3875.00
2HCCO<=>2CO+C2H2              1.000E+13      .000      .00
NNH+CH3<=>CH4+N2              2.500E+13      .000      .00
NNH+O2<=>HO2+N2               5.000E+12      .000      .00
NNH+O<=>OH+N2                 2.500E+13      .000      .00
!NCO+O2<=>NO+CO2              2.000E+12      .000     20000.00
! NCO+O2 from MB89 w/same k appears above.
H2CN+N<=>N2+CH2               6.000E+13      .000     400.00
CH2+N2<=>HCN+NH               1.000E+13      .000     7400.00
CH2 (S) +N2<=>NH+HCN          1.000E+11      .000     65000.00
C+NO<=>CO+N                   2.900E+13      .000      .00
CH+NO<=>H+NCO                 1.620E+13      .000      .00
CH+NO<=>N+HCO                 2.460E+13      .000      .00
CH2+NO<=>H+HNCO              3.100E+17     -1.380     1270.00
CH2+NO<=>OH+HCN              2.900E+14     -.690      760.00
CH2+NO<=>H+HCNO              3.800E+13     -.360      580.00
CH2 (S) +NO<=>H+HNCO         3.100E+17     -1.380     1270.00
CH2 (S) +NO<=>OH+HCN         2.900E+14     -.690      760.00
CH2 (S) +NO<=>H+HCNO         3.800E+13     -.360      580.00
CH3+NO<=>HCN+H2O             9.600E+13      .000     28800.00
CH3+NO<=>H2CN+OH             1.000E+12      .000     21750.00
HCNO+H<=>H+HNCO              2.100E+15     -.690     2850.00
HCNO+H<=>OH+HCN              2.700E+11      .180     2120.00
HCNO+H<=>NH2+CO              1.700E+14     -.750     2890.00
CH3+N<=>H2CN+H               6.100E+14     -.310      290.00
CH3+N<=>HCN+H2               3.700E+12      .150     -90.00
!
! ***** END REACTIONS GLEANED FROM GRI 3.0 *****
!
!
! *****
! Following section from ketene2.020101.   WRA, 5/21/03
! *****
! *****

```

```

! Following reactions of HNO3 and NO3 taken from ADN.011701
! as of 1/25/01. WRA
! *****

!*****
! Reactions added by WRA for HNO3/NO3 chem; see notes of 8/23/00
!*****

! HNO3+M
OH+NO2 (+M)=HNO3 (+M) 2.41E13 0.0 0. ! TH91 keyed to N2
LOW/ 6.42E32 -5.49 2350./
!TSA/ 0.725 -2.5E-04 /
N2O/5.0/ H2O/9./ N2/1.0/ ! CO2/2.0/ ! CO2/N2 from TH91;
HNO3/5.0/ NH3/5.0/ NO3/5.0/

HNO3+H=NO3+H2 2.40E08 1.5 11600. ! WRA est following DB00 EP
HNO3+H=NO2+H2O 6.00E13 0.0 9800. ! WRA est following Laidler EP
HNO3+H=HNO2+OH 6.00E13 0.0 7000. ! WRA est following Laidler EP
HNO3+H=HONO+OH 2.00E13 0.0 8000. ! JWB est
! Above estimates agree with lower limit of Chapman & Wayne for H+HNO3
! of < 1.2e9 at 298 K. Seems reasonable the reactions should occur.
HNO3+O=NO3+OH 2.00E13 0.0 12000. ! WRA est following Laidler EP
!HNO3+O=NO2+HO2 2.00E13 0.0 6000. ! possible channel, JWB thinks
! unlikely
!HNO3+O=HNO2+O2 ! large exo would give
! fairly high k by EP method. But lit says no rxn at 298. Strange.
! DEM/SAN 97 has k(HNO3+O; 298) < 1.8E7. Above NO3+OH est works with this,
! but the other two estimates would not.

!*****
! HNO3+OH
!*****
HNO3+OH=H2O+NO3 4.34E09 0.0 -1560. ! DEM/SAN 97
!DUP
HNO3+OH (+M)=H2O+NO3 (+M) 2.47E08 0.0 -2860. ! DEM/SAN 97
LOW/ 6.89E14 0.00 -1440./ !
N2O/5.0/ H2O/9./ N2/1.0/ ! CO2/2.0/ ! est.
HNO3/5.0/ NH3/5.0/ NO3/5.0/
!DUP
!
! Note Connell & Howard, 1985, conclude H2O2+NO2 is unimportant channel.
! DEM/SAN 97 cite works that state [OH] removed = [NO3] formed.
! This rxn deserves further attention. Didn't look into P dependence,
! which DEM/SAN 97 briefly discusses, carefully at this time (9/28/00; WRA).
! Must involve some stabilized species which perhaps should be put into the
! mech. NOTE: Duplicate rxns for HNO3+OH, as shown, are intended. These
! apparently represent an abstraction and an association channel. The
! version of the CHEMKIN interpreter used will allow these without DUP
! keywords; if DUP keywords are used where falloff and 'normal' reactions
! are specified, the version used flagged an error, though it shouldn't have.
! Some versions may have this 'bug' fixed and require the DUP keywords be
! uncommented.
!*****
! END HNO3+OH
!*****

NO3+H2O2=HNO3+HO2 1.00E12 0.0 8500. ! WRA est following Laidler EP
! HNO3+NH=HNO+HNO2, WRA est will not go, spin forbidden.
HNO3+NH=HNOH+NO2 1.50E13 0.0 6000. ! WRA est, EP Laidler
HNO3+NH2=NO3+NH3 9.00E05 2.0 7300. ! WRA est following DB00 EP
HNO3+NH2=NH2O+HNO2 3.00E12 0.0 9000. ! WRA est, EP Laidler
HNO3+NH3=NH2O+H2O+NO 23.2 3.5 44930. ! ML98 + Liau et al 1999 JANNAF
! for HNO3+NH3, see notes at beginning of file. Apparently
! Liau et al (note Lin was a coauthor) assume NH2ONO rapidly breaks down

```

! to NH2O+NO, so putting the reaction in with these products circumvents  
! having to put in NH2ONO.  
HNO3+NO=HONO+NO2 8.00E06 2.0 11000. ! est Ea from Laidler EP, set  
! A to pass through 298K data  
HONO+NO3=HNO3+NO2 1.00E12 0.0 6000. ! WRA est, EP Laidler  
HNO2+NO3=HNO3+NO2 1.00E12 0.0 5000. ! WRA est, EP Laidler

! NO3+M  
O+NO2(+M)=NO3(+M) 1.33E13 0.0 0. ! TH91 keyed to N2  
LOW/ 1.49E28 -4.08 2470./  
!TSA/ 0.79 -1.8E-04/  
N2O/5.0/ H2O/9./ N2/1.0/ ! CO2/2.7/ ! CO2/N2 from TH91;  
HNO3/5.0/ NH3/5.0/ NO3/5.0/

NO3+H=NO2+OH 6.00E13 0.0 0. ! from refs in NIST database  
NO3+O=NO2+O2 1.00E13 0.0 0. ! ATK/BAU 92/99  
NO3+OH=HO2+NO2 1.20E13 0.0 0. ! ATK/BAU 99  
!NO3+HO2=HNO3+O2 2.00E12 0.0 0. ! from NIST, big error limits  
NO3+HO2=NO2+O2+OH 2.50E12 0.0 0. ! controversial reaction  
! For NO3+HO2 used recommendations from NIST for total, with C.J. Howard  
! (most recent word on the rxn) that NO2+O2+OH is only channel.  
! Some have the two channels of similar magnitudes at 298 K.  
! Also note above is 298 K value for total, T dependence is unknown.  
!

NO3+NH=HNO+NO2 1.50E13 0.0 0. ! WRA est, EP Laidler  
NO3+NH=HNO3+N 1.00E12 0.0 5000. ! WRA est, EP Laidler  
NO3+NH2=HNO3+NH 1.00E12 0.0 10000. ! WRA est, EP Laidler  
NO3+NH2=NH2O+NO2 9.00E05 0.0 100. ! WRA est, EP DB00  
NO3+NO3=2NO2+O2 5.12E11 0.0 4870. ! DEM/SAN 97

!NO2+HO2=OH+NO3 1.00E12 0.0 16000. ! est, JWB/WRA  
! Oops, this reaction already in as reverse above, with k established  
! by experiment.  
NO2+HO2=HONO+O2 1.00E12 0.0 5000. ! WRA est, EP Laidler  
! From CJ Howard, JCP 77, per NIST, k(298) < 2E9. This reaction  
! could be an important termination step in ADN model (if HO2 formed  
! in abundance by OH+NO3). Per NIST database, the k of NO2+HO2 is  
! very controversial. CJ Howard did excellent research on HO2+NO.  
! This is an open issue. For now, I'm using an EP based  
! estimate, which agrees with Howard's upper limit. The rxn is so  
! poorly known, we could easily revise the estimate downwards.  
! Presence of a much larger k for this rxn in Penn St mech may be  
! reason for (unpublished) low predicted burn rates of ADN by both  
! Penn St and ARL groups using that mech. WRA 9/1/00.  
!

! Obtained Howard paper. Arguments that HONO+O2 does not contribute look  
! pretty convincing, but it would be useful to obtain the other papers.  
! Note they state SH74 assumed HONO+O2 was the main channel (which  
! provides some confusion regarding limiting values in NIST), but no  
! clear evidence for this was presented, looks like an assumption. A  
! similar assumption clouds the interpretation of CD75. SH later (SH76)  
! restudied the reaction. Later: also checked Demore et al, Eval 12, 1997.  
! They cite k(300) < 3e8 from Tyndall et al 1995, must obtain that.  
! Sounds like they are convinced by Tyndall. Not much discussion, but  
! indication that the measurements included using FTIR to look for  
! products. Note above estimate (just) agrees with this upper limit.  
! WRA, 9/25/00  
! Obtained Tyndall et al, and it is properly quoted as k(298)<3e8, and  
! it does look pretty convincing. WRA, 10/17/00  
!

! NOTE: The reactions (HNO3+NO=HONO+NO2 followed by  
! HONO+M=OH+NO+M), NO2+HO2=HONO+O2, and NO3+NH3=HNO3+NH2 (put in as reverse  
! above) likely do have reasonably fast rate constants and are potentially  
! very important for ADN. Also, NO3+OH=HO2+NO2 followed by NO2+HO2=HONO+O2  
! (termination).

! Ancillary HNOH, NH2O, and HNO2 rxns necessitated by addition  
! of the HNO3 and NO3 rxns. Also obtained from ADN.011701.

HNOH+NO2=HONO+HNO	6.00E11	0.0	2000.		! MG99, est.
HNOH+H=NH2+OH	4.00E+13	0.00	0		!RECOMBINATION
HNOH+H=HNO+H2	4.80E+08	1.50	378		!ABSTRACTION
HNOH+O=HNO+OH	7.00E+13	0.00	0		!RECOMBINATION
DUPLICATE					
HNOH+O=HNO+OH	3.30E+08	1.50	-358		!ABSTRACTION
DUPLICATE					
HNOH+OH=HNO+H2O	2.40E+06	2.00	-1192		!ABSTRACTION
NH2O+H=NH2+OH	4.00E+13	0.00	0		!RECOMBINATION
NH2O+H=HNO+H2	4.80E+08	1.50	1560		!ABSTRACTION
NH2O+O=HNO+OH	3.30E+08	1.50	487		!ABSTRACTION
NH2O+OH=HNO+H2O	2.40E+06	2.00	-1192		!ABSTRACTION
NH2O+NH2=HNO+NH3	1.80E+06	1.94	-1152		!ABSTRACTION
HNO2+H=H2+NO2	2.40E+08	1.50	4163		! HTRAN EST. 12/22/95
HNO2+O=OH+NO2	1.70E+08	1.50	2365		! HTRAN EST. 12/22/95
HNO2+OH=H2O+NO2	1.20E+06	2.00	-795		! HTRAN EST. 12/22/95
HNO2+NH2=NO2+NH3	9.20E+05	1.94	874		! HTRAN EST. 12/22/95

! \*\*\*\*\*  
! End reactions of HNO3 and NO3 taken from ADN.011701  
! as of 1/25/01. WRA  
! \*\*\*\*\*

! \*\*\*\*\*  
! Reactions NO3 with carbon species brings in  
! \*\*\*\*\*

NO3+CH2O=HNO3+HCO 1.70E12 0.0 5000. ! WRA est.  
! NO3+CH2O: estimated A = 2x(8.4e11) from NO3+CH3CHO abstr,  
! then with 298 value of k = 3.5E8 from 92ATK/BAU we have  
! Ea~5 kcal/mole. The E-P estimate would normally be about  
! 9 kcal/mole for Ea from 12 - 0.25(delta H = -12.7), but  
! JWB points out the E/P factor for abstr by NO3 and ROO type  
! rads is about 1/3 or even 1/2, not 1/4, so an Ea est around  
! 5 or 6 kcal/mole is reasonable.

NO3+HCO=H+CO2+NO2 2.00E13 0.0 0. ! WRA est.  
! This is just a first estimate. Other prod channels (see  
! the following comments) could dominate at low T. Reaction  
! needs further work if sensitive. Likely goes mainly by  
! the activated complex H(C=O)-O-NO2. Complex could  
! stabilize at high P, low T. Main high T products are  
! likely HCO2+NO2, and HCO2 then mainly falls apart to  
! H+CO2 under combustion conditions. Other channels (see  
! following) could dominate at low T.  
! NOTE: NO3+HCO=HONO+CO2 or HNO3+CO are also possible via  
! the adduct with probably small or no barriers, but require  
! H transfer through 5 center TS, so would have low A-factors.  
! HCO2+NO2 is expected to have higher barrier (but below  
! reactants), so dominates at high T. HNO3+CO can also  
! result from H abstraction, but that's actually a  
! disproportionation, so likely has a barrier. At first  
! glance, this rxn looks like NO2+HCO, but it's not really  
! very similar. NO2+HCO would make N-C bond in adduct,  
! NO3+HCO would make O-C bond (ie, a nitro vs nitrate type  
! adduct).

NO3+C2H4=C2H4O+NO2 2.00E12 0.0 5720.  
! Above k from 99ATK/BAU with WRA est of high T prods.  
! NO3+C2H4 deserves more work, is more complex; a good one  
! for QRRK or other study. Complex could stabilize.  
! QM on PES surface, CNSTM, J.Org.Chem. 63, 6978, 1998, says

! C2H4O+NO2 is main channel.  
C2H4O=CH4+CO 1.21E13 0.0 57200. ! LB83  
C2H4O=CH3CHO 7.26E13 0.0 57200. ! LB83  
C2H4O=CH3+HCO 3.63E13 0.0 57200. ! LB83

! In some of following rxns, WRA has replaced oxiranyl  
! (cyclo c2h3o) with ch2cho because reaction to that species  
! should happen rapidly at high T, and it greatly simplifies.

C2H4O+CH3=CH4+CH2CHO 1.10E12 0.0 11800. ! BK84

!C2H4O+O=OH+CH2CHO results on this reaction are very  
! scattered. Am leaving it out because either H or OH or  
! both are always present in higher conc, and reactions  
! with each are rapid. Therefore, O+C2H4O will not  
! be imp.

C2H4O+OH=H2O+CH2CHO 1.40E13 0.0 3360.  
! C2H4O+OH from fit to 88WAL/LIU, 84BAL/KEE, and 84LOR/ZEL

C2H4O+H=H2+CH2CHO 3.80E13 0.0 9197.  
! C2H4O+H from fit to 84BAL/KEE and 83LIF/BEN. C2H4+OH and  
! H2O+C2H3 channels are much less significant and therefore  
! ignored.

!C2H4O+NO=HNO+CH2CHO delta H = +22 kcal/mole, ignore.

C2H4O+NO2=HONO+CH2CHO 1.30E12 0.0 3700.  
! C2H4O+NO2 k from Jaffe 71, WRA assigned products.

C2H4O+NO3=HNO3+CH2CHO 1.00E12 0.0 6000. ! WRA est. E/P  
! ignore CH2CHO+M for now

CH2CHO+H=CH3+HCO 1.00E14 0.0 0. ! WRA est.

CH2CHO+H=H2+CH2CO 1.00E13 0.0 0. ! WRA est.  
! CH2CHO+H=CH3+HCO est. is so large because this is add/diss,  
! and the A-factor is large due to low H entropy compared to  
! typical complex entropy (compare to H+C2H4 and H+N2O).

CH2CHO+OH=CH2OH+HCO 2.00E13 0.0 0. ! WRA est.

CH2CHO+OH=CH2CO+H2O 1.20E06 2.0 0.  
! last rxn est. by WRA using Ea = 0 and E/P method of DB00

! CH2CHO+OH=H2O+HCOOH is exothermic and possibly even fast  
! (addition of OH at C of C=O), but left out at present  
! because of lack of thermo and chem for HCOOH and need to  
! finish mech rapidly.

CH2CHO+NO=HNO+CH2CO 1.00E12 0.0 8600. ! WRA est. E/P  
! per Gutman, ON-CH2CHO can stabilize at low T. This seems  
! unlikely at high T, and I don't have time to work up  
! chemistry on that species. Possible future topic.  
! WRA 1/30/01

CH2CHO+NO2=HONO+CH2CO 8.90E12 0.0 -160.  
! C2H4O+NO2 k is from Barnhard et al, WRA estimated prods.  
! O2N-CH2CHO could stabilize at low T.  
!

CH2CHO+NO3=HNO3+CH2CO 1.00E12 0.0 0. ! WRA est., E/P  
! adduct formation is also possible, not considered

!CH3+NO2=CH3O+NO 1.40E13 0.0 0. ! ave GT74, YSG81,

!! and BC93. Williams & Fleming, C&F 97 is close.  
!Identical reaction appears in HC/NO2 block below.

CH3+NO3=CH3O+NO2 2.00E13 0.0 0. ! WRA est.

!  
! \*\*\*\*\*  
! pertinent CH3CHO and CH2CHO chem from GRImech3.0:  
! \*\*\*\*\*

!  
O+C2H5<=>H+CH3CHO 1.096E+14 .000 .00  
O+CH3CHO<=>OH+CH2CHO 2.920E+12 .000 1808.00  
O+CH3CHO=>OH+CH3+CO 2.920E+12 .000 1808.00  
O2+CH3CHO=>HO2+CH3+CO 3.010E+13 .000 39150.00  
H+CH3CHO<=>CH2CHO+H2 2.050E+09 1.160 2405.00  
H+CH3CHO=>CH3+H2+CO 2.050E+09 1.160 2405.00  
OH+CH3CHO=>CH3+H2O+CO 2.343E+10 0.730 -1113.00  
HO2+CH3CHO=>CH3+H2O2+CO 3.010E+12 .000 11923.00  
CH3+CH3CHO=>CH3+CH4+CO 2.720E+06 1.770 5920.00  
O+C2H4<=>H+CH2CHO 6.700E+06 1.830 220.00  
C2H3+O2<=>O+CH2CHO 3.030E+11 .290 11.00  
C2H3+O2<=>HO2+C2H2 1.337E+06 1.610 -384.00  
H+CH2CO (+M) <=>CH2CHO (+M) 4.865E+11 0.422 -1755.00

LOW/ 1.012E+42 -7.63 3854.0/  
TROE/ 0.465 201.0 1773.0 5333.0 /

H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/

!CH4/2.00/ C2H6/3.00/ AR/ .70/

O+CH2CHO=>H+CH2+CO2 1.500E+14 .000 .00

O2+CH2CHO=>OH+CO+CH2O 1.810E+10 .000 .00

!O2+CH2CHO=>OH+2HCO 2.350E+10 .000 .00

! WRA on O2+CH2CHO: GRI uses above two channels, but the first has a  
! 5c TS with likely only a small barrier and low A factor; second has  
! a 4c TS and it seems this would have a much more significant  
! barrier. JWB and student(s) have considered this rxn by QRRK. They  
! do not consider the second channel to be significant, and it does  
! not appear in NIST database. QRRK results indicate O2CH2CHO will  
! significantly stabilize at temperatures even as high as 1000 K at  
! modest P (1 atm); not important at very low P. At very low P, the  
! first channel is T independent, and the k value obtained is close  
! to that given above (traced to BAU/COB92). At modest P and low to  
! intermediate T, the first channel falls off. It seems unlikely  
! this reaction (to any products) can matter much to propellant  
! combustion because conditions are rich, and there is little O2.  
! I was originally going to leave the reaction out, but decided to  
! keep it in for test purposes. It will be necessary to examine  
! modeling results to watch for unexpected influence of this reaction.  
! If it matters, further thought and a more elaborate treatment, and  
! possibly also addition of reactions with O2CH2CHO, will be  
! necessary. WRA, 2/1/01

! \*\*\*\*\*  
! end pertinent CH3CHO and CH2CHO chem from GRImech3.0:  
! \*\*\*\*\*  
! \*\*\*\*\*  
! End reactions for NO3 with carbon species brings in  
! \*\*\*\*\*

! \*\*\*\*\*  
! End section from ketene2.020101. WRA, 5/21/03  
! \*\*\*\*\*

! \*\*\*\*\*  
! Begin section of updates from ketene2.020101 to  
! ketene2.051601 and other key rxns from 051601. WRA, 5/22/03  
! NOTE: some of these overlap reactions in ketene2.020101.

```

! (Went carefully over all reactions towards the end of
! those files, prior sections are from DZ mech core of
! small molecule reactions I started with above. Chose
! not to include CHOCHO or CH2CO.)
! *****
CH3+NH=H2CN+H2      3.50E13   0.0   290. ! WF97
! Above was an estimate by W&F, C&F 110, 1, 1997, used in modeling
! CH4/O2 flames doped with NH3, CH3NH2 or CH3CN. Reasonable estimate
! explained some of their results.

!
! ***** Thess reactions could be very impnt for CH2O/NO2 mixtures.
! k's taken from th91. CH2O+NO is obtained by reversing Tsang's estimate
! for HCO+HNO = CH2O+NO. Should be better than his forward k, as that is
! obtained from Keq, and he didn't have best thermo at time of his review.
!
HCO+HNO=CH2O+NO     6.00E11   0.0   2000. ! TH91 - estimated
!
! Following 3 reactions are potentially very important in DB modeling.
! They are recommended by Tsang (TH91). There are a few studies, but the
! most complete work includes RRKM modeling of HCO+NO2 by the Emory group.
! Note the reaction involves activated intermediate complexes which could
! stabilize at high P, low T, a factor which may need future study. Note
! NIST database contains a couple bad typos re these rxns. Note the 2nd
! of these was included in earlier reactions previously, is commented out
! now.
!
CH2O+NO2=HCO+HONO   8.02E02    2.77  13730. ! Lin et al; TH91
HCO+NO2=CO+HONO     1.24E23   -3.29  2355. ! Lin et al; TH91
HCO+NO2=H+CO2+NO    8.39E15   -0.75  1930. ! Lin et al; TH91

! HCO+HCO only measured at 298
HCO+HCO=CH2O+CO     3.00E13   0.0     0. ! Bau 92
HCO+HCO=H2+CO+CO    5.20E12   0.0     0. ! ratioed to CH2O per TH86

! *****
! Begin hydrocarbon - NO2 reactions.
! *****

CH4+NO2=CH3+HONO     1.20E13   0.0  30000. ! SG81
! Note, other workers, e.g. Yetter/Dryer group, have pointed out
! possible systematic errors in temperatures in the similar
! experiments of S&G on the H2+NO2=H+HONO reaction.

CH3+NO2=CH3O+NO      1.40E13   0.0     0. ! ave GT74, YSG81,
! and BC93. Williams & Fleming, C&F 100, 571, 1995 uses
! a very close value (1.5E13) in modeling of CH4/O2/NO2/N2 flames,
! and states the results are sensitive.

CH2+NO2=CH2O+NO      5.00E13   0.0     0. ! ave STWW89 & DM95
! Study of CH2+NO2 at 298 K indicates that it is fast, as shown,
! but products have not been measured. (No measurements at other
! than 298 K.) CH2O+NO is highly exothermic and would appear to
! be the most likely, but HCO+H+NO is mildly exothermic and could
! easily and justifiably be tried in modeling. The stabilized
! radical adducts H2C-ONO or H2C-NO2 would also be formed
! exothermally. However, the experiments were performed at
! pressures of only a few torr, so it seems unlikely that those
! products were formed in the experiments.

! CH+NO2 is included in an earlier section.

! The reaction CH3+N2O=CH3O+N2 may eventually deserve some
! thought. However, it is beyond the scope of the present work.
! There is only one measurement and one upper limit in NIST

```

```

! database.
! *****
! End hydrocarbon - NO2 reactions.
! *****

! *****
! End section of updates from ketene2.020101 to
! ketene2.051601 and other key rxns from 051601. WRA, 5/22/03
! *****

!*****
! Following H2CN rxns taken from m-yet-wra.rdx.1.8.wNHx.wHC.5.
!
! WRA added three reactions of H2CN.
! First two k's taken from Marston & Stief, 1989 NASA tech note.
! Need to get their open lit paper. k for H2CN+H is lower limit.
! Measurements were at low T, long extrapolation necessary for
! combustion.
! Last k estimated.
!*****
H2CN+N=HCN+NH      7.20E+13   0.00   4.000E+02
H2CN+H=HCN+H2      4.00E+13   0.00   0.0          ! lower limit
! see H2CN+OH=HCN+H2O from Catoire et al 98 below.
!H2CN+OH=HCN+H2O   2.00E+13   0.00   0.0          ! WRA est
!*****
! end addition of H2CN reactions from m-yet-wra.rdx.1.8.wNHx.wHC.5.
!*****

!*****
! Following HOCN+H rxns taken from m-yet-wra.rdx.1.8.wNHx.wHC.5.
!
! Begin WRA mods to HOCN+H; also note one rev rxn commented out
! earlier.
!*****
! 17.5, 4
! Glarborg and Miller, Combust. Flame, 1994.
!HOCN+H=HNCO+H     2.00E+07   2.00   2.000E+03
! following lines from B&D 97 preprint and private communication
!H+HOCN=HCN+OH     2.00E+13   -0.04  2136   ! REV. OF 41B2
! WRA comment: B&D switched to and recommend reverse expression:
OH+HCN=HOCN+H     1.10E+06   2.03   13373   !MILLER/MELIUS
HOCN+H=HNCO+H     3.10E+08   0.84   1917
HOCN+H=NH2+CO     1.20E+08   0.61   2076
HOCN+H=H2+NCO     2.40E+08   1.50   6617   ! HTRAN EST. 12/22/95
! end B&D 97 preprint and private communication lines
!*****
! End WRA mods to HOCN+H
!*****

!*****
! Begin section on MMH and large fragment reactions.
!*****

! Rxns 1 - 16 of Catoire et al, 96 (Shock Waves, v6, 139, 1996):
CH3NHNH2+M=CH3NH+NH2+M   2.5E14   0.0   40940. ! Catoire et al, 96
CH3NHNH2+H=CH3NNH2+H2    1.3E13   0.0   2500. ! Catoire et al, 96
CH3NHNH2+H=CH3NH+NH3     4.46E09  0.0   3100. ! Catoire et al, 96
CH3NHNH2+CH3=CH4+CH3NNH2 1.0E13   0.0   6990. ! Catoire et al, 96
CH3NHNH2+NH2=NH3+CH3NNH2 1.0E11   0.5   1990. ! Catoire et al, 96
CH3NNH2+M=CH3NNH+H+M     1.0E17   0.0   35770. ! Catoire et al, 96
CH3NH+M=CH3+NH+M         1.0E14   0.0   18000. ! Catoire et al, 96
CH3NH+M=CH2NH+H+M       1.0E16   0.0   23800. ! Catoire et al, 96
CH3NH+H=CH2NH+H2        1.0E08   2.0    0. ! Catoire et al, 96

```



CH3NH+H=CH3+NH2	6.0E13	0.0	0.	! Catoire et al, 96
CH3NNH+CH3=CH4+CH3NN	4.6E13	0.0	4850.	! Catoire et al, 96
CH3NNH+NH2=NH3+CH3NN	4.6E13	0.0	4850.	! Catoire et al, 96
CH3NN=CH3+N2	3.0E06	0.0	0.	! Catoire et al, 96
CH3NNCH3=CH3NN+CH3	6.9E15	0.0	50880.	! Catoire et al, 96
CH3NNCH3=C2H6+N2	2.0E11	0.0	33000.	! Catoire et al, 96
CH2NH+M=HCN+H2+M	1.0E14	0.0	10000.	! Catoire et al, 96

! Rxns 1 - 30 of Catoire et al, 98 (Proc. Instn. Mech. Engrs., v212, ! 393, 1998):

CH3NHNH2=CH3NNH+H2	3.16E13	0.0	57000.	! Golden et al, 72
CH3NHNH2=CH2NH+NH3	1.58E13	0.0	54000.	! Golden et al, 72
CH3NNH2+HO2=CH3NHNH2+O2	1.0E06	2.0	0.	! Catoire et al, 98
CH3NN+HO2=CH3NNH+O2	1.0E06	2.0	0.	! Catoire et al, 98
CH3NHNH2+O=CH3NNH+H2O	9.6E12	0.0	0.	! Catoire et al, 98
CH3NNH2+OH=CH3NNH+H2O	1.0E08	2.0	0.	! Catoire et al, 98
CH3NNH2+O=CH3NNH+OH	1.0E08	2.0	0.	! Catoire et al, 98
CH3NNH2+HO2=CH3NNH+H2O2	1.0E08	2.0	0.	! Catoire et al, 98
CH3NNH2+O2=CH3NNH+HO2	4.0E12	0.0	0.	! Catoire et al, 98
CH3NHNH2+HO2=CH3NNH2+H2O2	2.7E11	0.0	1987.	! Catoire et al, 98
CH3NNH+HO2=CH3NN+H2O2	1.0E11	0.0	1987.	! Catoire et al, 98
CH3NHNH2+OH=CH3NNH2+H2O	3.92E13	0.0	0.	! Catoire et al, 98
CH3NNH+OH=CH3NN+H2O	3.92E13	0.0	0.	! Catoire et al, 98
CH3NHNH2+O=CH3NNH2+OH	9.6E12	0.0	0.	! Catoire et al, 98
CH3NNH+O=CH3NN+OH	9.6E12	0.0	0.	! Catoire et al, 98
CH3NH+OH=CH2NH+H2O	1.0E08	2.0	0.	! Catoire et al, 98
CH3NH+O=CH2NH+OH	1.0E08	2.0	0.	! Catoire et al, 98
CH3NH+O2=CH2NH+HO2	1.0E07	2.0	6300.	! Catoire et al, 98
CH3NH+O=CH3O+NH	6.0E13	0.0	0.	! Catoire et al, 98
CH3NH+OH=CH4+HNO	6.0E12	0.0	0.	! Catoire et al, 98
CH3NH+O2=CH3O+HNO	6.0E12	0.0	4000.	! Catoire et al, 98
CH2NH+O=CH2O+NH	1.0E07	2.0	2800.	! Catoire et al, 98
CH2NH+OH=CH2O+NH2	1.8E05	2.0	14800.	! Catoire et al, 98
CH2NH+O=H2CN+OH	3.16E08	2.0	6100.	! Catoire et al, 98
H2CN+HO2=CH2NH+O2	7.87E04	2.0	21700.	! Catoire et al, 98
CH2NH+OH=H2CN+H2O	1.0E07	2.0	4000.	! Catoire et al, 98
H2CN+O=HCN+OH	1.0E07	2.0	6100.	! Catoire et al, 98
H2CN+OH=HCN+H2O	1.0E07	2.0	3700.	! Catoire et al, 98
H2CN+O2=HCN+HO2	2.7E04	2.0	17300.	! Catoire et al, 98
H2CN+NO=HCN+HNO	1.0E07	2.0	4400.	! Catoire et al, 98

! Reactions taken from Catoire et al, JPP 20, 87, 2004, these matter ! mainly at low T, and they are mostly quite rough estimates:

CH3NNH2+NO2 (+M)=CH3N(NH2)NO2 (+M)	1.0E13	0.0	0.	! Catoire et al, 04
LOW/	1.0E17	0.0	0. / !	
CH3NNH2+NO2 (+M)=CH3N(NH2)ONO (+M)	1.0E13	0.0	0.	! Catoire et al, 04
LOW/	1.0E17	0.0	0. / !	
CH3NHNH2+NO2=CH3NNH2+HONO	2.2E11	0.0	5900.	! Catoire et al, 04
CH3NNH+NO2=CH3NN+HONO	2.2E11	0.0	5900.	! Catoire et al, 04
CH3NNH2+NO2=CH3NNH+HONO	1.0E08	2.0	0.	! Catoire et al, 04
!CH3NN=CH3+N2	3.0E06	0.0	0.	! Catoire et al, 04 THIS RXN ALREADY IN ABOVE

! \*\*\*\*\*  
! End section on MMH and large fragment reactions.  
! \*\*\*\*\*

! \*\*\*\*\*  
! Section on further small molecule reactions mentioned by  
! Catoire et al and of interest WRA, 060203  
! \*\*\*\*\*

```

! *****
! NH2+HO2=NH3+O2
! *****
! following rxn, not used previously by WRA, cited as sensitive in
! Catoire et al, 27th ISC, 1998 (ignition delay in MMH/O2/AR
! mixtures):

NH2+HO2=NH3+O2          2.0E13    0.0      0. ! DEM/SAN 97, 298 K
!NH2+HO2=NH3+O2        4.52E13   0.0      0. ! Catoire et al, 98
! Looking at NIST database (and my expectations), the Catoire
! cited value seems a bit large.

! *****
! HO2+HO2=H2O2+O2
! *****
! See 2HO2=H2O2+O2 used previously by WRA above.
! Catoire et al cite HO2+HO2=H2O2+O2 k = 4.2E14exp(-11980/RT), this
! traces to 94 BAU/COB, 850- 1250 K per NIST. But the Ea is WIERD!!
! Extrap to 298 = BAD agreement with expt. (per NIST). And that Ea
! seems way too big to me. MB89 used 2E12, and TH86 recommended
! 1.8E12. I've kept TH86, which I've been using for a long time.
! I don't think anything I ever did was sensitive to this rxn.
! Catoire et al state this rxn is sensitive for MMH, better keep an
! eye on it.

! Further comments on some small moc rxns Catoire et al say are
! sensitive:
! For H2O2+M=OH+OH+M, I use reverse from GRI, with falloff.
! For CH3+CH3(+M)=C2H6(+M), I use GRI. Both GRI and Catoire had
! falloff. Expressions are slightly different.
! For CH4+HO2=CH3+H2O2, I have reverse from GRI.
! For CH3+NO2=CH4+O2, I use same expression as Catoire.
! My expression for O2+H=O+OH from MHB90, slightly different from
! Catoire, I'm sure is excellent.

! *****
! End section on further small molecule reactions mentioned by
! Catoire et al and of interest      WRA, 060203
! *****

! *****
! Catoire et al 2004 recommend using NO2=N2O4      WRA, 062104
! *****

! *****
! NO2 = N2O4
! *****
! Atkinson et al, JPCRD 1997, as cited by Catoire et al,
! JPP 20, 87, 2004.

N2O4(+M)=NO2+NO2(+M)  4.05E18   -1.1   12840.
                    LOW/ 1.96E28   -3.8   12800. /

! *****
! End NO2=N2O4                      WRA, 062104
! *****

! Initially inserted NAMMH complex formation at high P limit only,
! for testing.
!CH3NHNH2+HNO3=NAMMH  7.83E21   -3.46  -276. ! WRA EMAIL 1/18/2005

```

```

!CH3NHNH2+HNO3=NAMMH 2.00E13 0.0 0. ! WRA est, hi P lim.
!CH3NHNH2+HNO3=CH3NHNH2-HNO3 2.00E13 0.0 0. ! WRA est, hi P lim.

```

```

! *****
! Block of reactions for CH3NO2
! *****

```

```

! Reactions are taken from: Glarborg, Bendtsen, and Miller, IJCK 31,
! 591, 1999, Appendix A.

```

```

! NOTES:

```

- ! 1. These authors considered CH3+NO2(+M)=CH2ONO(+M) to be negligible.
- ! 2. Species CH3NO2 CH3NO H2CNO2 CH3ONO CH3ONO2 had to be added.  
! Thermo from Sandia database used.
- ! 3. CH3+NO2=CH3+NO is already in above. I kept the k(T) I have  
! been using for years, it is only slightly different (about  
! 20-60 % larger) than that of GBD99 commented out below.  
! at combustion T.
- ! 4. CH4+NO2=CH3+HONO is already in above with k(T) identical to  
! that of GBD99 commented out below.

```

CH3NO2 (+M) =CH3+NO2 (+M) 1.80E16 0.00 58500. !GBD99
LOW/ 1.30E17 0.00 42000. / !GBD99
!TSA/ 0.183 0.0 /
CH3NO2+H=CH3+HONO 3.30E12 0.00 3730. !GBD99
CH3NO2+H=CH3NO+OH 1.40E12 0.00 3730. !GBD99
CH3NO2+H=H2CNO2+H2 5.40E02 3.50 5200. !GBD99
CH3NO2+O=H2CNO2+OH 1.50E13 0.00 5350. !GBD99
CH3NO2+OH=H2CNO2+H2O 5.00E05 2.00 1000. !GBD99
CH3NO2+OH=CH3OH+NO2 2.00E10 0.00 -1000. !GBD99
CH3NO2+CH3=H2CNO2+CH4 5.50E-01 4.00 8300. !GBD99
CH3NO2+CH2 (S) =H2CNO2+CH3 1.20E14 0.00 0. !GBD99
CH3NO2+CH2=H2CNO2+CH3 6.50E12 0.00 7900. !GBD99
H2CNO2=CH2O+NO 1.00E13 0.00 36000. !GBD99
CH3+NO (+M) =CH3NO (+M) 9.00E12 0.00 119. !GBD99
LOW/ 3.20E23 -1.87 0. / !GBD99
!CH3+NO2=CH3O+NO 4.00E13 -0.20 0. !GBD99
!CH4+NO2=CH3+HONO 1.20E13 0.00 30000. !GBD99
CH3O+NO=CH2O+HNO 1.30E14 -0.70 0. !GBD99
CH3O+NO (+M) =CH3ONO (+M) 6.60E14 -0.60 0. !GBD99
LOW/ 2.70E27 -3.50 0. / !GBD99
CH3O+NO2=CH2O+HONO 6.00E12 0.00 2285. !GBD99
CH3O+NO2 (+M) =CH3ONO2 (+M) 1.20E13 0.00 0. !GBD99
LOW/ 1.40E30 -4.50 0. / !GBD99

```

```

! *****
! End block of reactions for CH3NO2 WRA, 122305
! *****

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!! ADDED FROM GRI MECH AND MORPHOLINE BY NJL !!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!N+NO<=>N2+O 2.700E+13 .000 355.00
!N+O2<=>NO+O 9.000E+09 1.000 6500.00
!N+OH<=>NO+H 3.360E+13 .000 385.00
!N2O+O<=>N2+O2 1.400E+12 .000 10810.00
!N2O+O<=>2NO 2.900E+13 .000 23150.00
!N2O+H<=>N2+OH 3.870E+14 .000 18880.00
!N2O+OH<=>N2+HO2 2.000E+12 .000 21060.00
!N2O (+M) <=>N2+O (+M) 7.910E+10 .000 56020.00
! LOW / 6.370E+14 .000 56640.00/

```

```

!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .625/
!HO2+NO<=>NO2+OH          2.110E+12    .000   -480.00
!NO+O+M<=>NO2+M            1.060E+20   -1.410    .00
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!NO2+O<=>NO+O2             3.900E+12    .000   -240.00
!NO2+H<=>NO+OH             1.320E+14    .000    360.00
!NH+O<=>NO+H                4.000E+13    .000    .00
!NH+H<=>N+H2                3.200E+13    .000    330.00
!NH+OH<=>HNO+H              2.000E+13    .000    .00
!NH+OH<=>N+H2O              2.000E+09    1.200    .00
!NH+O2<=>HNO+O              4.610E+05    2.000   6500.00
!NH+O2<=>NO+OH              1.280E+06    1.500    100.00
!NH+N<=>N2+H                 1.500E+13    .000    .00
NH+H2O<=>HNO+H2             2.000E+13    .000  13850.00
!NH+NO<=>N2+OH              2.160E+13   -.230    .00
!NH+NO<=>N2O+H               3.650E+14   -.450    .00
!NH2+O<=>OH+NH               3.000E+12    .000    .00
!NH2+O<=>H+HNO               3.900E+13    .000    .00
!NH2+H<=>NH+H2              4.000E+13    .000   3650.00
!NH2+OH<=>NH+H2O            9.000E+07    1.500  -460.00
NNH<=>N2+H                   3.300E+08    .000    .00
DUP
!NNH+M<=>N2+H+M              1.300E+14   -.110   4980.00
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!NNH+O2<=>HO2+N2            5.000E+12    .000    .00
!NNH+O<=>OH+N2               2.500E+13    .000    .00
!NNH+O<=>NH+NO               7.000E+13    .000    .00
!NNH+H<=>H2+N2               5.000E+13    .000    .00
!NNH+OH<=>H2O+N2            2.000E+13    .000    .00
!NNH+CH3<=>CH4+N2           2.500E+13    .000    .00
!H+NO+M<=>HNO+M              4.480E+19   -1.320   740.00
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!HNO+O<=>NO+OH              2.500E+13    .000    .00
!HNO+H<=>H2+NO               9.000E+11    .720   660.00
!HNO+OH<=>NO+H2O            1.300E+07    1.900  -950.00
!HNO+O2<=>HO2+NO            1.000E+13    .000  13000.00
!CN+O<=>CO+N                  7.700E+13    .000    .00
!CN+OH<=>NCO+H                4.000E+13    .000    .00
!CN+H2O<=>HCN+OH             8.000E+12    .000   7460.00
!CN+O2<=>NCO+O               6.140E+12    .000  -440.00
!CN+H2<=>HCN+H               2.950E+05    2.450   2240.00
!NCO+O<=>NO+CO               2.350E+13    .000    .00
!NCO+H<=>NH+CO               5.400E+13    .000    .00
!NCO+OH<=>NO+H+CO           0.250E+13    .000    .00
!NCO+N<=>N2+CO               2.000E+13    .000    .00
!NCO+O2<=>NO+CO2            2.000E+12    .000  20000.00
!NCO+M<=>N+CO+M              3.100E+14    .000  54050.00
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!NCO+NO<=>N2O+CO            1.900E+17   -1.520   740.00
!NCO+NO<=>N2+CO2             3.800E+18   -2.000   800.00
!HCN+M<=>H+CN+M              1.040E+29   -3.300 126600.00
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!HCN+O<=>NCO+H               2.030E+04    2.640   4980.00
!HCN+O<=>NH+CO                5.070E+03    2.640   4980.00
!HCN+O<=>CN+OH                3.910E+09    1.580  26600.00
!HCN+OH<=>HOCN+H             1.100E+06    2.030  13370.00
!HCN+OH<=>HNCO+H              4.400E+03    2.260   6400.00
!HCN+OH<=>NH2+CO              1.600E+02    2.560   9000.00
!H2CN+N<=>N2+CH2              6.000E+13    .000   400.00
!C+N2<=>CN+N                  6.300E+13    .000  46020.00
CH+N2<=>HCN+N                 3.120E+09    0.880  20130.00
!CH+N2 (+M) <=>HCNN (+M)      3.100E+12    .150    .00
!      LOW / 1.300E+25   -3.160   740.00/
!      TROE/ .6670  235.00 2117.00 4536.00 /~H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/
CO2/2.00/ C2H6/3.00/ AR/ 1.0/
!CH2+N2<=>HCN+NH              1.000E+13    .000  74000.00

```

!CH2 (S) +N2<=>NH+HCN	1.000E+11	.000	65000.00	
!C+NO<=>CN+O	1.900E+13	.000	.00	
!C+NO<=>CO+N	2.900E+13	.000	.00	
!CH+NO<=>HCN+O	4.100E+13	.000	.00	
!CH+NO<=>H+NCO	1.620E+13	.000	.00	
!CH+NO<=>N+HCO	2.460E+13	.000	.00	
!CH2+NO<=>H+HNCO	3.100E+17	-1.380	1270.00	
!CH2+NO<=>OH+HCN	2.900E+14	-.690	760.00	
!CH2+NO<=>H+HCNO	3.800E+13	-.360	580.0	
!CH2 (S) +NO<=>H+HNCO	3.100E+17	-1.380	1270.00	
!CH2 (S) +NO<=>OH+HCN	2.900E+14	-.690	760.00	
!CH2 (S) +NO<=>H+HCNO	3.800E+13	-.360	580.00	
!CH3+NO<=>HCN+H2O	9.600E+13	.000	28800.00	
!CH3+NO<=>H2CN+OH	1.000E+12	.000	21750.00	
!HCNN+O<=>CO+H+N2	2.200E+13	.000	.00	
!HCNN+O<=>HCN+NO	2.000E+12	.000	.00	
!HCNN+O2<=>O+HCO+N2	1.200E+13	.000	.00	
!HCNN+OH<=>H+HCO+N2	1.200E+13	.000	.00	
!HCNN+H<=>CH2+N2	1.000E+14	.000	.00	
!HNCO+O<=>NH+CO2	9.800E+07	1.410	8500.00	
!HNCO+O<=>HNO+CO	1.500E+08	1.570	44000.00	
!HNCO+O<=>NCO+OH	2.200E+06	2.110	11400.00	
!HNCO+H<=>NH2+CO	2.250E+07	1.700	3800.00	
!HNCO+H<=>H2+NCO	1.050E+05	2.500	13300.00	
!HNCO+OH<=>NCO+H2O	3.300E+07	1.500	3600.00	
!HNCO+OH<=>NH2+CO2	3.300E+06	1.500	3600.00	
!HNCO+M<=>NH+CO+M	1.180E+16	.000	84720.00	
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/				
!HCNO+H<=>H+HNCO	2.100E+15	-.690	2850.00	
!HCNO+H<=>OH+HCN	2.700E+11	.180	2120.00	
!HCNO+H<=>NH2+CO	1.700E+14	-.750	2890.00	
!HOCN+H<=>H+HNCO	2.000E+07	2.000	2000.00	
!HCCO+NO<=>HCNO+CO	0.900E+13	.000	.00	
!NH3+H<=>NH2+H2	5.400E+05	2.400	9915.00	
!NH3+OH<=>NH2+H2O	5.000E+07	1.600	955.00	
!NH3+O<=>NH2+OH	9.400E+06	1.940	6460.00	
!NH+CO2<=>HNO+CO	1.000E+13	.000	14350.00	
!CN+NO2<=>NCO+NO	6.160E+15	-0.752	345.00	
!NCO+NO2<=>N2O+CO2	3.250E+12	.000	-705.00	
N+CO2<=>NO+CO	3.000E+12	.000	11300.00	
!CH2NH + H = rCHNH + H2	0.56E+07	2.12	13366.0	! Based on H + C2H4 by
Bhargava; RPD =2 vs 4				
!CH2NH + OH = rCHNH + H2O	2.77E+05	2.31	2900.0	! Based on OH+C2H4 by
Bhargava; RPD =2 vs 4				
!CH2NH + O = rCHNH + OH	1.08E+06	2.55	11900.0	! Based on
C2H4+O=C2H3+OH; RPD =2 vs 4				
CH2NH + H = H2CN + H2	0.28E+07	2.12	13366.0	! Based on H + C2H4 by
Bhargava; RPD =1 vs 4				
!CH2NH + OH = H2CN + H2O	1.39E+05	2.31	2900.0	! Based on OH+C2H4 by
Bhargava; RPD =1 vs 4				
!CH2NH + O = H2CN + OH	0.54E+06	2.55	11900.0	! Based on
C2H4+O=C2H3+OH; RPD =1 vs 4				
CH2NH + O = NH2 + HCO	0.57E+08	1.60	1020.0	! Based on
C2H4+O=CH3+HCO; RPD =1 vs 2				
CH2NH + O = CH3 + NO	0.57E+08	1.60	1020.0	! Based on
C2H4+O=CH3+HCO; RPD =1 vs 2				
!				
!rCHNH(+M)=HCN+H(+M)	1.93E+08	1.62	37058.0	! Based
on C2H3 decomposition; RPD =1				
!LOW /1.28E27	-3.40	35789.7/		
!TROE /0.2134	36.643	7794.56	4007.66 /	
!H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/				
!H2CN(+M)=HCN+H(+M)	3.86E+08	1.62	37058.0	! Based
on C2H3 decomposition; RPD =2				
!LOW /2.56E27	-3.40	35789.7/		

```

!TROE /0.2134      36.643 7794.56      4007.66 /
!H2/2.0/  H2O/6.0/  CH4/2.0/  CO/1.5/  CO2/2.0/  C2H6/3.0/  AR/0.7/
!CH3+NH2 (+M)=CH3NH2 (+M)      6.77E+16      -1.18  654.0
ABOVE BY ANALOGY
!LOW /3.40E+41      -7.03 2763.0/
!TROE /0.619 73.2 1180 9999 /
!H2/2.0/  H2O/6.0/  CH4/2.0/  CO/1.5/  CO2/2.0/  C2H6/3.0/  AR/0.7/

```

!SAME AS

## A.2.2 Red ARL Model

### Kinetic parameters in CHEMKIN format

```

REACTIONS
! the next reaction modified according to Tsang & Herron *****
NO2(+M)=NO+O(+M) 7.60E18 -1.27 73290. ! Tsang & Herron
          LOW/ 2.47E28 -3.37 74800./ ! keyed to N2=1.0
          !TSA/ 0.95 -1.0E-04 /
          H2O/4.4/ N2/1.0/ CO2/2.3/ !N2O/1.5/ ! EFFICIENCIES FROM Baulch et al,
! HE /0.54/ AR/0.71/ ! CH4/1.6/ 1973, for reverse reaction except CO2/N2
! ! from Tsang & Herron 91 (latter in forward dir)
! FC(N2)=0.95 - 1.0E-04 * T
! K0(CO2)=2.16E26 -2.66 74300
! FC(CO2)=FC(N2)
!
!N2O(+M)=N2+O(+M) 1.26E12 0.0 62620. ! Rohrig et al, 1996 preprint
! LOW/ 5.97E14 0.0 56640./ ! to appear in IJCK; rekeyed to N2
! ! using N2/Ar = 1.5
!N2O(+M)=N2+O(+M) 7.91E10 0.0 56020. ! M. Allen et al, both HP and LP
! LOW/ 9.13E14 0.0 57690./ ! keyed to N2=1.0; per Baulch
! per Princeton group, Lindemann falloff is reasonable. Efficiencies
! kept as previous.
!
!N2O(+M)=N2+O(+M) 1.30E11 0.0 59610. ! T&H91 (HP and LP)
! LOW/ 7.23E17 -0.73 62789./ ! keyed to N2=1.0; per Baulch
! T&H/ 1.167 -1.25E-04 / ! et al, N2/Ar=1.5 used here
! ! N2O/Ar also from Baulch et
! ! al.; H2,CO,NO estimated = N2

! N2O/5.0/ H2O/7.5/ N2/1.0/ CO2/3.2/ O2/0.82/ ! H2O/AR,O2/AR from
! AR/0.67/ ! Glarborg et al, C&F 99,523,1994

! N2O/5.0/ H2O/9.0/ N2/1.0/ CO2/3.2/ O2/0.82/ ! O2/AR from
! NH3/5.0/
! AR/0.67/ ! Glarborg et al, C&F 99,523,1994
! H2O/N2 efficiency is average of the values from Glarborg et al 94 and
! Venizelos & Sausa, C&F 115, 313 (1998). There is still a large uncertainty
! in this important efficiency factor. There may be some T dependence.
! NH3 is est.

! ! CO2/N2 from T&H91
! N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/3.2/ ! earlier choices
! FC(N2)=1.167-1.25E-04*T
!
! the reaction throw out (incorp. in N2O+M) *****
! N2O(+CO2)=N2+O(+CO2) ! mod Bill, Ref 37d
! LOW/ 1.20E18 -0.67 62190./ ! LINDEMANN FALLOFF
! ! NEEDS ATTENTION
!
H+NO(+M)=HNO(+M) 1.52E15 -0.41 0. ! Fall-off, TH91

```

```

!          LOW/ 8.96E19   -1.32   735./          ! TH91
!          T&H/ 0.82 /
!          LOW/ 4.00E20   -1.75   0./          ! Glarborg et al, ISC 1998
!      used new LP limit with TH91 HP limit
!          H2O/5.0/ N2/1.0/ CO2/1.3/   ! N2O/5.0/   ! CO2/N2 from TH91
!          FC(N2)=0.82
!
! HNO(+M)=H+NO(+M) 1.20E16  -0.43 49520.      ! TH91
!          LOW/ 6.02E21  -1.61 50840./        ! LINDEMANN FORM
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/3.2/ ! NEEDS ATTENTION
!          FC(N2)=0.830
!
!                                     ! SOME EFFS. FROM MB89
! this reaction eliminated (incluced in HNO + M) *****
! HNO(+CO2)=H+NO(+CO2)
!          LOW/ 3.85E20  -1.24 50020./        ! LINDEMANN FORM
!                                     ! NEEDS ATTENTION
!
! new reaction : *****
NO+OH(+M)=HONO(+M) 1.988E12  -0.05 -721.      ! Tsang & Herron
!          LOW/ 5.08E23  -2.51 -67.6/        ! keyed to N2=1.0.
!          !TSA/ 0.62 0.0/
!          H2O/8.3/ N2/1.0/ CO2/1.5/ !N2O/5.0/   ! CO2/N2 from TH91;
!          AR/0.60/   ! H2O from Overend et al; N2/AR ave from TH91 citations
!          FC(N2)=0.62
!          K(0,CO2)=1.705E23  -2.30 -246.
!          FC(CO2)=0.62
!
! HCN(+M)=H+CN(+M) 8.30E17  -0.93 123800.     ! T&H91 [13,0]
!          LOW/ 3.57E26  -2.6 124900./       !
!          !TSA/ 0.95 -1.0E-04 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/   ! N2/CO2 ratioed per Tsang;
!          FC(N2)=0.95-1.0E-04*T             !
! CN+H(+M)=HCN(+M) 1.80E15  -0.5 0.          ! Tsang, 1992
!          LOW/ 8.71E23  -2.2 1130./         !
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/   ! N2/CO2 ratioed per Tsang;
!          FC(N2)=0.95-1.0E-4*T             !
! CN+CN(+M)=C2N2(+M) 5.66E12  0.0 0.         ! Tsang, 1992
!          LOW/ 3.43E25  -2.61 0./           !
!          !TSA/ 0.5 0.0 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/   ! N2/CO2 ratioed per Tsang;
!          FC(N2)=0.5                       !
! HNCO(+M)=NH+CO(+M) 6.00E13  0.0 99800.     ! Tsang, 1992
!          LOW/ 2.17E28  -3.1 101900./       !
!          !TSA/ 0.9 -2.0E-04 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.6/   ! N2/CO2 ratioed per Tsang;
!          FC(N2)=0.9-2.0E-4*T             !
! HCN+H(+M)=H2CN(+M) 3.31E13  0.0 4844.      ! TH91
!          LOW/ 1.60E24  -2.73 7660./        !
!          !TSA/ 0.95 -1.0E-04 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/   ! N2/CO2 ratioed per Tsang;
!          FC = 0.95-1.0E-04*T             !
! CN+NO(+M)=NCNO(+M) 3.98E13  0.0 0.         ! Tsang, 1992
!          LOW/ 1.56E36  -6.2 4878./         !
!          !TSA/ 0.65 0.0 /
!          N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/2.0/   ! N2/CO2 ratioed per Tsang;
!          FC(N2)=FC(CO2)=0.65             ! others guessed
! C2N2+M=CN+CN+M 1.07E34  -4.3 123000.      ! added
! CN+M=C+N+M 2.50E14  0.0 141100.           ! Tsang 92, keyed to Ar=1.0
!          N2/1.5/ CO2/2.4/                   ! Tsang 92
! NO+M=N+O+M 1.40E15  0.0 148430.           ! TH91
!          AR/0.75/ HE/0.35/
!          N2/1.0/ H2/2.2/ H2O/6.7/ CO2/3.0/ N2O/2.2/
! NO+M Efficiencies from Clyne & Thrush, as quoted in Baulch et al, 1973 for
! reverse reaction
! N2+M=N+N+M 3.71E21  -1.6 225000.          ! Baulch et al, 1973
! NCO+C=CO+CN 1.00E14  0.0 0.              ! WRA, ul est.

```

```

! ***** N2O+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!N2O+N=N2+NO      1.00E13      0.0 19870.      ! HS85, est.
! N2O+N removed per Fernandez & Fontijn ul measurement, ~2000.
! ***** End N2O+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****

! ***** NO2+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!NO2+N=N2O+O      5.01E12      0.0 0.      ! HS85 (iffy; see Leeds)
!N+N2O=N2O+O      5.00E+12      0.00 0.000E+00
!NO2+N=N2O+O      3.49E12      0.0 -437.      ! DEM/SAN 97
!NO2+N=NO+NO      3.98E12      0.0 0.      ! HS85 (iffy; see Leeds)
! Above removed per DEM/SAN 97
! ***** End NO2+N revisions per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****

!NO2+NO=N2O+O2    1.0E12      0.0 60000.      ! Thorne and Melius 89

! ***** NO2+NO2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
!NO2+NO2=NO+NO3   9.64E09      0.73 20920.      ! T&H91
!NO2+NO2=NO+NO+O2 1.63E12      0.0 26120.      ! T&H91
NO2+NO2=NO+NO+O2 4.51E12      0.0 27600.      ! PGML00
! ***** End NO2+NO2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

! ***** NO2+NO3 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
!NO2+NO3=NO+NO2+O2 1.40E11      0.0 3180.      ! Baulch et al, 1973
!NO2+NO3=NO+NO2+O2 2.71E10      0.0 2500.      ! DEM/SAN 97
! ***** End NO2+NO3 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

!HNO+NO=N2O+OH    2.00E12      0.0 26000.      ! Wilde, C&F, 1969
!HNO+NO=N2O+OH    4.00E12      0.0 26000.      ! Wilde, C&F, 1969 x2 for test
!HNO+NO=N2O+OH    8.51E12      0.0 29590.      ! Diau et al, IJCK 27,867(1995)
!HNO+NO=N2O+OH    1.70E13      0.0 29590.      ! comment follows
! WRA believes best value is 2 x Diau et al, IJCK 27,867(1995) because
! they had good result/review, but used wrong heat of formation of HNO,
! leading to x2 error in their final result.
!NO+NO=N2+O2      1.3E14      0.0 75630.      !added Yetter
! previous reaction is a concern; products may be wrong
!NO+HO2=HNO+O2    2.0E11      0.0 2000.      !added Yetter; traced to
!
! HNO+O2=HO2+NO    1.00E13      0.0 25000.      ! MB91
!HNO+NO2=HONO+NO  6.0E11      0.0 1987.      ! TH91, estimated
HNO+NO2=HONO+NO  4.42E4      2.64 4042.      ! MLM98
HONO+O=OH+NO2    1.2E13      0.0 5961.      ! TH91
HONO+OH=H2O+NO2  1.27E10      1.0 135.      ! TH91
!
! WRA estimated HONO+NH2=NO2+NH3 k is similar to HONO+OH=H2O+NO2.
! For HONO+OH, b~1 and Ea~0, so that was used for HONO+NH2. Then the
! the A factor was reduced from original estimate of 1.0E10 so that the final
! result passes through Bedford and Thomas' value at ~640 K. Note Bedford &
! Thomas reduced their data with ancillary reactions now known to be wrong.
! One would expect if anything their result for k(NO2+NH3) is too large because
! they do not have NH2+NO=NNH+OH and their initial mixtures contained NO as
! well as NH3 & NO2. Also, their T range, 615-660 K, was not large. That latter
! observation is why it is best to assume b and Ea by reversing and just use
! their data to set A factor. wra, 9/30/98
!
! Upon further examination of Bedford & Thomas' analysis, have decided they
! have systematic analysis error, low by factor of ~2, due to mechanistic
! errors. Therefore, have reverted to original estimate, which was ~ 1.3
! higher (increasing by exactly that factor of 2 is not justified, is too
! approximate without careful reanalysis B&T's data; not even sure that's
! possible, don't know if they gave exacting details of how well equilibrated
! was NO/NO2/O2 before introducing NH3 and result depends heavily on that).
! Estimated error at 650K (B&T exps) x3, x5 at ends of recommended range =
! 450 - 3000 K. wra, 10/1/98

```



```

!HONO+NH2=NO2+NH3 7.7E09 1.0 0. ! wra, est fitted to B&T72
!HONO+NH2=NO2+NH3 1.0E10 1.0 0. ! wra, est, better analysis than B&T72
!
!HONO+HNO=H2O+2NO 1.0E12 0.0 40000. ! Thorne & Melius 89
HNO+O=OH+NO 3.61E13 0.0 0. ! TH91
!HNO+O=NO2+H 5.0E10 0.5 2000. ! Thorne & Melius 89
!NH+O=NO+H 5.50E13 0.0 0. ! MCHB91
!NH+O=N+OH 3.72E13 0.0 0. ! MCHB91
!NH+NH=N2+H+H 5.10E13 0.0 0. ! MCHB89
!NH+M=N+H+M 2.65E14 0.0 75510. ! MCHB91 keyed to Ar=1.0
!
!NH2+NO=N2O+H2 7.0E13 0.0 27820. ! RHK, 18th ISC, p 853
!NH2+NO=N2O+H2 5.0E13 0.0 24640. ! Roose' thesis; per
! ! discussion with Hanson, 4/7/95, this supercedes the 18th ISC result
! WRA, 2/13/01.
!
! Per Miller & Klippenstein, JPC A104, 2061, 2000, the NH2+NO=N2O+H2
! reaction has been removed. M&K conclude the reaction may be to HNNO+H,
! or Roose et al may have been observing effects of 'contamination by
! secondary reactions'. The endothermicity is ~40.5 kcal/mole to HNNO+H,
! so the measured activation energy simply does not fit that interpretation.
! So, I have decided to remove the reaction. It never played much of a
! role in any process of which I know, anyway. WRA, 2/20/01
!
! See more on NH2+NO choices below. WRA, 5/22/03
!
!
!CH+O2=HCO+O 3.30E13 0.0 0. ! MB89
!CH+O=CO+H 5.70E13 0.0 0. ! MB89
!CH+OH=HCO+H 3.00E13 0.0 0. ! MB89
!CH+CO2=HCO+CO 3.40E12 0.0 690. ! MB89
!CH+H=C+H2 1.50E14 0.0 0. ! MB89
!C+O2=CO+O 2.00E13 0.0 0. ! MB89
!C+OH=CO+H 5.00E13 0.0 0. ! MB89
HCO+OH=H2O+CO 1.00E14 0.0 0. ! MB89
HCO+M=H+CO+M 2.50E14 0.0 16802. ! MB89
CO/1.9/ H2/1.9/ CO2/3.0/ H2O/5.0/
HCO+H=CO+H2 1.19E13 0.25 0. ! MB89
HCO+O=CO+OH 3.00E13 0.0 0. ! MB89
HCO+O=CO2+H 3.00E13 0.0 0. ! MB89
HCO+O2=HO2+CO 3.30E13 -0.4 0. ! MB89
!
CO+O(+M)=CO2(+M) 1.80E10 0.0 2380. ! Princeton preprint
LOW/ 1.35E24 -2.79 4190./ ! Princeton preprint
!TSA/ 1.0 0.0 / ! Princeton preprint
H2O/12./ H2/2.5/ CO/1.9/ CO2/3.8/ !N2O /5.0/ !
! All efficiencies above from Princeton preprint, except
! N2O is guessed.
!CO+O+M=CO2+M 2.36E15 0.0 4340.
! CO/1.77/ CO2/2.7/ H2O/5.0/ N2O/5.0/ ! N2,CO,CO2 per TH86,
! others guessed
CO+OH=CO2+H 1.51E07 1.3 -758. ! MB89
!CO+O2=CO2+O 1.60E13 0.0 41000. ! MB89
CO+O2=CO2+O 2.53E12 0.0 47688. ! TH86
HO2+CO=CO2+OH 5.80E13 0.0 22934. ! MB89
!O+HCCO=H+2CO 1.00E14 0.0 0. ! MB89
!HCCO+O2=2CO+OH 1.60E12 0.0 854. ! MB89
!H2+O2=2OH 1.70E13 0.0 47780. ! MB89
! for H2+O2=2OH, TH86 do not believe 2OH is a product (nor do
! most others, apparently). Main product is H+HO2. The reverse
! of this from TH86 is in below, and we use that and allow CHEMKIN
! to reverse using up to date thermo.
OH+H2=H2O+H 2.16E08 1.5 3430. ! Mich. & Suth. 88
O2+H=O+OH 3.52E16 -0.7 17070. ! MHB90
O+H2=OH+H 5.06E04 2.67 6290. ! SMPNK, ISC 88

```

```

H+O2+M=HO2+M      3.61E17  -0.72    0.      ! MB89
  H2O/18.6/ CO2/4.2/ H2/2.9/ CO/2.1/ N2/1.3/
OH+HO2=H2O+O2     7.50E12   0.0    0.      ! MB89
!*****
! For H+HO2, switched from TH86 to BAU92. Yetter/Dryer, world
! experts on H2/O2 chem, use the TH86 expressions in much of their
! work. Note OH+OH is the main channel, followed by H2+O2. Also
! note, TH86 and BAU92 expressions are identical for OH+OH, and for
! H2+O2 channel agree very well at ~1000 K, which is the typical
! operating temperature for the Yetter/Dryer flow apparatus.
! Disagreement between TH86 and BAU92 for H2+O2 is only about a factor
! of two at low (300 K) and high (3000 K) temperature. This is
! similar to uncertainty limits each quotes.
!
! The O+H2O channel, as specified by BAU92, is newly included.
! It is unlikely to ever have much effect as its k is much smaller
! than the other 2 channels. BAU92 mention its error limit is
! much larger than for the other 2 channels.
!
!H+HO2=2OH        1.69E14   0.0    874.    ! TH86
!H+HO2=H2+O2      6.63E13   0.0   2126.   ! TH86
H+HO2=2OH         1.69E14   0.0    874.    ! TH86/BAU92
H+HO2=H2+O2      4.28E13   0.0   1411.   ! BAU92
H+HO2=O+H2O      3.01E13   0.0   1721.   ! BAU92
!*****
O+HO2=O2+OH      1.40E13   0.0   1073.   ! MB89

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!2OH=O+H2O        6.00E08   1.3    0.      ! MB89
OH+OH=H2O+O      3.57E04   2.40  2112.   ! WHB94
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

2H+M=H2+M        1.00E18  -1.0    0.      ! MB89
  H2/0.0/ H2O/0.0/ CO2/0.0/
2H+H2=2H2        9.20E16  -0.6    0.      ! MB89
2H+H2O=H2+H2O    6.00E19  -1.25   0.      ! MB89
2H+CO2=H2+CO2    5.49E20  -2.0    0.      ! MB89
H+OH+M=H2O+M     1.60E22  -2.0    0.      ! MB89
  H2O/5.0/
H+O+M=OH+M       6.20E16  -0.6    0.      ! MB89
  H2O/5.0/
O+O+M=O2+M       1.89E13   0.0  -1788.   ! MB89
!2HO2=H2O2+O2    1.80E12   0.0    0.      ! TH86
!H2O2+M=2OH+M    1.30E17   0.0  45500.   ! MB89
! H2O2+M removed because reverse, with P falloff, from GRI 3.0
! was inserted.

! The expressions for H2O2+H are from TH86, but there is
! much uncertainty in the HO2+H2 channel. (Main channel
! is known to be OH+H2O.) BAU92 is in fairly good
! agreement concerning the OH+H2O channel, but not for
! HO2+H2. Note BAU92 adopts WAR84; Warnatz was a coauthor
! of BAU92. Expressions for HO2+H2 from TH86 and BAU92
! cross near 1/T = 1.3e-3, or close to T = 773 K (500 C)
! which was used in many of the experiments by Baldwin,
! Walker et al in the 1970's (e.g. J.Chem.Soc.Far.Trans.I,
! v69, p352, 1973). Ranges are: TH86, 300-2500 K,
! BAU92 300-1000 K. TH86 state uncertainty for both
! reactions is high (factor of 5) above 1000 K, and
! since BAU92 don't even recommend using their expressions
! above 1000 K, they must generally agree with that
! assessment. But note the expressions of TH86 have the
! HO2+H2 channel nearly equal to the OH+H2O channel,
! whereas extrapolated BAU92 expressions don't do that.
! That is because the TH86 Ea is much larger than BAU92 for
! HO2+H2. If this is sensitive, more study than I have done

```

```

! is indicated.      WRA, 12/20/00.
!
!H2O2+H=HO2+H2      4.82E13   0.0   7948.      ! TH86
!H2O2+H=OH+H2O      2.41E13   0.0   3975.      ! TH86
!H2O2+H=HO2+H2      1.69E12   0.0   3760.      ! BAU92
!H2O2+H=OH+H2O      1.02E13   0.0   3580.      ! BAU92
! inserted H2O2+O=HO2+OH from TH86. I had not used this before,
! never mattered much to anything I did. MB89 also did not use.
! probably doesn't matter much to MMH.      WRA, 060503
!H2O2+O=HO2+OH      9.63E6    2.0   3974.      ! TH86
!H2O2+OH=H2O+HO2    1.75E12   0.0   318.       ! TH86
! ***** updated CH+N2 and CN chemistry *****
!CH+N2=HCN+N        3.00E11   0.0   13600.     ! MB89
!CH+N2=NCN+H        2.22E07   1.48  23367.    ! ML00
!H+NCN=HCN+N        1.89E14   0.0   8425.     ! ML00
!NCN+N=CN+N2        2.00E13   0.0    0.         ! WRA est.

! I do not expect CN to matter much, but:
! if much CN is formed in any system, the reaction CN+OH
! probably should also be considered. Most likely products
! appear to be HOCN+N, based on structure. This is ~7kcal/mole
! exo, would likely have some barrier. Any estimate is likely
! to have appreciable error, so just left it out for now. (EP
! method to get Ea does not apply, this does not appear to
! be a simple abstraction. HNCO+N would be more exo products,
! but rearrangement to this appears to involve 4 center TS,
! seems likely to have large barrier.      WRA, 052903

! ***** end updates to CH+N2 and CN chemistry *****!!!
!CN+N=C+N2          1.04E15  -0.5   0.         ! MB89
!H2CN+M=HCN+H+M    3.00E14   0.0  22000.     ! MB89
!C+NO=CN+O         6.60E13   0.0   0.         ! MB89
!HCCO+NO=HCNO+CO   2.00E13   0.0   0.         ! MB89
!HCNO+H=HCN+OH     1.00E14   0.0  12000.     ! MB89
! replaced HCNO+H=HCN+OH by GRI 3.0 expression
!CH+N=CN+H         1.30E13   0.0   0.         ! MB89
!HCCO+N=HCN+CO     5.00E13   0.0   0.         ! MB89
!HCN+OH=CN+H2O     1.45E13   0.0  10929.     ! MB89
!CN+H2O=HCN+OH     7.83E12   0.0   7450.     !
! prev is from Jacobs et al (Wolfrum) 1988, per Baulch et al, 1992 crit rev.
! NOTE: k for HCN+OH direction if from thermo. Decided to use CN+H2O
! direction as this makes updates easy. Worry here regards controversy on
! Hf(CN), though this appears to be dying out recently due to Halpern's work
! (1991); also see Bauchlicher et al, 1994 JCP.
! I like Hf(CN,298)= 104.0 kcal, which current Sandia database uses. MB89
! expression is from Hanson & coworkers, IJCK 1984. Reversing Jacobs
! expression with my preferred Hf(CN), per Baulch et al, 1992, yields
! (Hr = -19.2 kJ = -4.59 kcal @298; wra 3/3/95):
!HCN+OH=CN+H2O     9.04E12   0.0  10730.     ! Baulch et al, 1992.
!HCN+OH=CN+H2O     3.90E06   1.83  10290.     ! WHB95
!OH+HCN=HOCN+H     5.85E04   2.4  12500.     ! MB89
! OH+HCN=HOCN+H from MB89 replaced later by Miller&Melius, per DB00
!OH+HCN=HNCO+H     1.98E-03   4.0  1000.     ! MB89
!OH+HCN=NH2+CO     7.83E-04   4.0  4000.     ! MB89
!HOCN+H=HNCO+H     1.00E13   0.0   0.         ! MB89
!HCN+O=NCO+H       1.38E04   2.64  4980.     ! MB89;Perry&Melius 85 similar
!HCN+O=NH+CO       3.45E03   2.64  4980.     ! MB89;Perry&Melius 85 similar
!HCN+O=CN+OH       2.70E09   1.58  26600.    ! MB89; from Perry&Melius 85
!HCN+O=CN+OH       2.00E13   0.0  21800.    ! wra ul est(Tsang on rev later)
!CN+H2=HCN+H       2.95E05   2.45  2237.     ! MB89
!CN+H2=HCN+H       3.61E08   1.55  3000.     ! Tsang, 1992.; whb95 is similar
!CN+O=CO+N         1.80E13   0.0   0.         ! MB89
!CN+O=CO+N         2.05E13   0.0   417.      ! Tsang, 1992.
!CN+O2=NCO+O       5.60E12   0.0   0.         ! MB89
!CN+O2=NCO+O       2.60E14  -0.5   0.         ! S&S88
!CN+OH=NCO+H       6.00E13   0.0   0.         ! MB89

```

```

!CN+OH=NCO+H      4.00E13   0.0   0.      ! Tsang,92; WHB95 confirm
!CN+OH=HCN+O      6.00E12   0.0  2000.   ! Tsang,92
!CN+HCN=C2N2+H    2.00E13   0.0   0.      ! MB89
!CN+HCN=C2N2+H    1.51E07   1.71  1530.   !Tsang 92, from Yang et al 92;
!                                     WHB 95 experiments support this result
!CN+NO2=NCO+NO    3.00E13   0.0   0.      ! MB89
!CN+NO2=NCO+NO    2.40E13   0.0  -370.   ! Tsang,1992
! Note: previous versions had sign error for Ea in above rxn.
!CN+NO2=NCO+NO    6.16E15  -0.752  344.   ! WMHB 25th ISC, 94
!CN+CO2=NCO+CO    3.67E6    2.16  26900.  ! WYL, IJCK 91
!CN+N2O=NCO+N2    1.00E13   0.0   0.      ! MB89
!CN+N2O=NCN+NO    2.40E13   0.0  13330.  ! Williams etal1995, upp limb
!CN+N2O=NCN+NO    9.55E08   0.0   835.   ! Williams etal1995, low limb
! NOTES: Wang,Yang,Lin&Melius1991 have similar expression (to sum of two
! previous terms), recommended by Tsang (all there was). Melius recommends
! same prods, Williams et al confirmed. Looks like first term alone will
! do well above ~600K. There is a pressure dependence that is not at all
! well-understood, and may indicate different prods, e.g. stabilizes, at
! lower T, higher P. So am leaving this out. This is something likely to
! require future attention. (WRA, 3.15.95).
! Note: a further complication is that the NCO+N2 channel could open up at
! higher T.
!C2N2+O=NCO+CN    4.57E12   0.0  8880.   ! MB89
!C2N2+OH=HOCN+CN  1.86E11   0.0  2900.   ! MB89
! Above rxn has delta H = +18 kcal/mole, so products must be wrong.
! Unlikely to matter to nitrate ester chem. Might for nitramines. WRA
!NO2+OH=HO2+NO    1.80E13   0.0  6676.   ! from CJ Howard, JACS 1980
NO+HO2=NO2+OH    2.11E12   0.0  -479.   ! HS84 (from CJ Howard)
NO2+H=NO+OH      1.30E14   0.0  361.    ! KF91
NO2+O=NO+O2      3.90E12   0.0  -238.   ! ATK/BAU 89
!NCO+H=NH+CO     5.40E13   0.0   0.      ! Tsang 92
!NCO+O=NO+CO     2.00E13   0.0   0.      ! MB89
!NCO+O=NO+CO     4.52E13   0.0   0.      ! Tsang,1992
!NCO+O2=NO+CO2   2.0E12    0.0  20000.  ! MB91
!NCO+N=N2+CO     2.00E13   0.0   0.      ! MB89
!
! Tsang, 1992, thinks NCO+OH does not go to products NO+CO+H. He thinks
! the reaction NCO+OH=HNCO+O does. That reaction is in this mech in the
! reverse direction since its k is known best in that direction. Note
! Hf(NCO) is now believed quite different from what Tsang used. There is
! also a recombination channel to consider to HONCO, not used presently
! because of lack of thermo data that species. It is unlikely to be
! important to DZ because of low concentrations these species, but should
! be included in a revised version.
!
! 4/20/95 NCO+OH=NO+CO+H appears to be a reasonable reaction.
! (WRA) An estimate is included below with a revised Ea vs MB89.
! This is consequence of a recent change in Hf(NCO) by ~+7.5 kcal.
! The HNCO+O channel is also still in (as the reverse). None
! of the possible channels seems to matter much for propellant
! DZ, major focus of the moment. A quick estimate of the reverse
! k for HNCO+O channel indicates it is main channel of NCO+OH,
! so the estimate for NO+CO+H is compatible with reverse k
! measurements.
!
!NCO+OH=NO+CO+H   2.00E13   0.0  7500.   ! WRA est
!NCO+OH=NO+CO+H   1.00E13   0.0   0.      ! MB89(impossible w/revised Hr)
!NCO+M=N+CO+M     6.30E16  -0.5  48300.  ! LH84
!NCO+M=N+CO+M     1.14E23  -1.95  59930.  ! Tsang,1992, N2
! N2O/5.0/ H2O/5.0/ N2/1.0/ CO2/1.5/ ! CO2/N2 per Tsang, others guessed
! NCO+NO=prods total is from MDHB92, 24th ISC, p702; branching based on
! 298 K work of Cooper and Hershberger, per Tsang,92. Prod ratio subject to
! revision pending higher T work.
!NCO+NO=N2O+CO    4.62E17  -1.73  763.    !
!NCO+NO=CO2+N2    6.16E17  -1.73  763.    !
!NCO+NO=CO+N2+O   3.22E17  -1.73  763.    !

```

```

!
! New revision for above rxns follows.
! Revised per newer results of Cooper, Park & Hershberger for the branching
! ratio (298 J) and fit to data from 7 sources for total. Mertens et al
! recommendation was shortened to their T range studied for this fit as
! they did not give a fit to their data over that range only. RRKM result
! of Lin, He and Melius is pretty close. They do predict a modest branching
! ratio variation vs T, if reaction(s) is sensitive, this ratio should
! possibly be reconsidered.
!
! NCO+NO=products 2.01E18 -1.78 790. ! fit described above
! NCO+NO=N2O+CO 8.80E17 -1.78 790. ! 0.44 @ 298
! NCO+NO=CO2+N2 1.13E18 -1.78 790. ! 0.56 @ 298
! NCO+NO=N2O+CO 3.98E19 -2.19 1743. ! ZL00, JPC A104, 10807, 2000
! NCO+NO=CO2+N2 1.46E21 -2.74 1824. ! ZL00, JPC A104, 10807, 2000
! NCO+H2=HNCO+H 2.07E06 2.0 6020. ! Tsang,1992
! NCO+NO2=CO+2NO 1.40E13 0.0 0. ! Tsang,1992,est
! NCO+NO2=CO2+N2O 0.40E13 0.0 0. ! Tsang,1992,est
! NCO+NO2=CO2+N2O 1.80E13 0.0 0. ! WRA, 1995, est
! 4/20/95 (WRA) CO+NO+NO doesn't seem to make sense as main channel of
! NCO+NO2.
! NCO+NO2=CO2+N2O 3.25E12 0.0 -707. ! WMHB, 25th ISC, 94
! NCO+NO2=CO2+N2O 2.98E12 0.0 -707. ! WMHB w/PH93 298 ratios
! NCO+NO2=CO+NO+NO 2.70E11 0.0 -707. ! WMHB w/PH93 298 ratios
! NCO+NO2=products 2.13E13 -0.258 -620. ! fit described below
! NCO+NO2=CO2+N2O 1.95E13 -0.258 -620. ! see below
! NCO+NO2=CO+NO+NO 1.77E12 -0.258 -620. ! see below

! NCO+NO2=products is taken from a fit to data from following 3 sources:
! WMHB94; 25th ISC, p983, 1994
! PH93; JPC 97, p13647, 1993
! JLW95; IJCK 27, p1111, 1995
! The branching ratio is taken from the room temperature measurement of PH93.
! Note WHMB95 recommendation above did not have the more recent data of
! PH93
!
! Effects of above branching need to be tested. Latter rxn could
! reverse (CO+NO+NO -> NCO+NO2) for DZ mixtures at high P. Have previously
! seen my predictions show this could matter. But that was using Tsang's
! (very large) estimate of the branching ratio to CO+NO+NO, which probably
! gives too high a k. No good measurements of the branching ratio for high T
! currently exist. - WRA, 2/2/96 -
!
! NH+O2=HNO+O 4.61E05 2.0 6500. ! M&M, 24th ISC, 92
! NH+O2=NO+OH 1.28E06 1.5 100. ! M&M, 24th ISC, 92
! the following reaction changed (slightly) ****
! NH+NO=N2O+H 3.50E14 -0.46 16.1 ! B.Williams fit of MM calc
! NH+NO=N2+OH 2.16E13 -0.23 0. ! M&M, 24th ISC, 92

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
! N2O+OH=N2+HO2 2.00E12 0.0 10000. ! MB89 ; removed per
! a number of studies, culminating with Glarborg's, C&F 95;
! note these were around 1250 K studies.
! N2O+OH=N2+HO2 1.29E-02 4.72 36561 ! Mebel et al 96, per DB00
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
! N2O+H=N2+OH 2.53E10 0.0 4550. ! MKF89
! DUP
! N2O+H=N2+OH 2.23E14 0.0 16750. ! MKF89
! DUP
!
! Following is WRA fit to selected experimental data for H+N2O=N2+OH.
!
! Best for the range 714 - 2850 K. The expression is:

```

```

!N2O+H=N2+OH      1.30E11    0.938  15210.  ! WRA01 (Fit#8, WRA, 3/16/01)

! Recommended error limits are a factor of 1.3 from 714 to 1200 K,
! increasing to a factor of 1.5 at 2850 K.
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

!N2O+H=NNH+O      5.00E-06    5.52  27420.    ! B&D93, July 1993 version
!NNH+O=N2O+H      1.40E14    -0.40   477.    ! B&D95,QRRK,preprint on O+NNH
!NNH+O=NO+NH      3.30E14    -0.23 -1013.    ! ditto
!N2O+O=N2+O2      1.00E14    0.0   28000.    ! HS85 (&TH91)
!N2O+O=N2+O2      1.40E12    0.0  10800.    ! DDCH92 (Shock Waves,813,1992)
!N2O+O=NO+NO      6.92E13    0.0  26600.    ! HS85 (&TH91)
!N2O+O=N2+O2      3.654E12    0.0  15900.    ! M&A97
!N2O+O=NO+NO      9.985E13    0.0  28040.    ! M&A97
!N2O+O=N2+O2      3.691E12    0.0  15930.    ! M&A99
!N2O+O=NO+NO      9.172E13    0.0  27690.    ! M&A99
!N2O+O=N2+O2      3.692E12    0.0  15940.    ! M&A00
!N2O+O=NO+NO      9.155E13    0.0  27680.    ! M&A00
!H+HNO=NH+OH      3.00E14    0.0  18000.    ! WRA, 1993 jannaf est
!NH+OH=N+H2O      5.00E11    0.5   2000.    ! MB89
!NH+N=N2+H        3.00E13    0.0    0.    ! MB89

! ***** N+H2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****
!N+H2=NH+H        1.60E14    0.0  25140.    ! DH90
!N+H2=NH+H        2.33E14    0.0  30830.    ! ZT00 (JCP 113, 6152, 2000)
! ***** End N+H2 revised per m-yet-wra.rdx.1.8.wNHx.wHC.5. *****

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH2+O=HNO+H      6.63E14    -0.5    0.    ! MB89
!HNO+H=NH2+O      3.50E15    -0.3  28200.    ! B&D July 93 preprint
!NH2+O=NH+OH      6.75E12    0.0    0.    ! MB89
!NH2+O=HNO+H      4.60E+13    0.00   0    ! DB00
!NH2+O=NH+OH      7.00E+12    0.00   0    ! DB00
!DUPLICATE
!NH2+O=NH+OH      3.33E+08    1.50  5077    ! DB00
!DUPLICATE
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

!NH2+OH=NH+H2O    4.00E06    2.0   1000.    ! MB89
!NH2+H=NH+H2      4.00E13    0.0   3650.    ! DKCH90
!NH2+NH=N2H2+H    1.50E15    -0.50   0.    ! DKCH90
!NH2+N=N2+H+H     7.20E13    0.0    0.    ! MB89
!NH2+O2=HNO+OH    4.50E12    0.0  25000.    ! MB89

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH2+NH2=N2H2+H2  5.00E11    0.0    0.    ! MB89
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

!NH2+NH2=NH+NH3   5.00E13    0.0  10000.    ! DKCH90
!NH2+NH2=N2H3+H   1.79E13    -0.35 11320.    ! B&D93, AMD, priv. comm.
!NH2+NH2+M=N2H4+M 2.98E47    -9.44 9680.    ! B&D93, AMD, priv. comm.

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH2+NO2=N2O+H2O  2.84E18    -2.2   0.    ! Baulch et al 84, per MB91
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH+NO2=N2O+OH    1.00E13    0.0    0.    ! from Harrison et al
!NH+NO2=N2O+OH    4.00E12    0.0    0.    ! branching per QH95
!NH+NO2=NO+HNO    5.70E12    0.0    0.    ! branching per QH95

```

! NH+NO2 total k=9.70E12 from HWP86, branching ratio from QH95  
! \*\*\*\*\* update taken from ketene2.072398.062701 to ketene2.060305 \*\*\*\*\*

! \*\*\*\*\*  
! Begin updates to DCS84 chem from ADN.051601. WRA, 5/22/03  
! \*\*\*\*\*

! You might think NxHy would matter a lot for MMH, but in fact the main  
! breakdown is likely scission of the N-N bond, rather than C-N.  
! I could have brought in lots of QRRK estimates I have for these  
! reactions, but it would seriously complicate things. I'm just  
! going to update the DCS84 reactions to DB00. WRA, 052203

!N2H4+H=N2H3+H2	1.00E12	0.50	2000.	! DCS84
!N2H4+OH=N2H3+H2O	3.00E10	0.68	1290.	! DCS84
!N2H4+O=N2H3+OH	2.00E13	0.00	1000.	! DCS84
!N2H3=N2H2+H	1.20E13	0.00	58000.	! DCS84
!N2H3+H=N2H2+H2	1.00E12	0.50	2000.	! DCS84
!N2H3+OH=N2H2+H2O	3.00E10	0.68	1290.	! DCS84
!N2H3+O=N2H2+OH	2.00E13	0.00	1000.	! DCS84

! NOTE, WRA has done QRRK on N2H3+M, but results are very complex to include, and  
! Ea is very large (> 50 kcal/mole) for all channels, so decided not to include  
! See ADN.051601 for QRRK results.

!N2H4+H=N2H3+H2	9.60E+08	1.50	4838	! HTRAN EST.	12/22/95	(DB00)
!N2H4+H=N2H3+H2	4.90E12	0.00	2130.	! fit to data from 6 sources in NIST (WRA)		
!N2H4+O=N2H3+OH	6.70E+08	1.50	2851	! HTRAN EST.	12/22/95	(DB00)
!N2H4+OH=N2H3+H2O	4.80E+06	2.00	-646	! HTRAN EST.	12/22/95	(DB00)
!N2H3+H=N2H2+H2	2.40E+08	1.50	-10	!ABSTRACTION	1/15/96	(DB00)
!N2H3+O=NH2+HNO	3.00E+13	0.00	0	!		(DB00)
!N2H3+O=NH2NO+H	3.00E+13	0.00	0			
!N2H3+O=N2H2+OH	1.70E+08	1.50	-646	!ABSTRACTION	1/15/96	(DB00)
!N2H3+OH=N2H2+H2O	1.20E+06	2.00	-1192	!ABSTRACTION	1/15/96	(DB00)
!N2H3+OH=H2NN+H2O (DB00)	3.00E+13	0.00	0	! 2/15/96 SAME AS ADDUCT FORMATION		
!N2H3+NH2=N2H2+NH3	9.20E+05	1.94	-1152	!ABSTRACTION	1/15/96	(DB00)
!N2H3+NH2=H2NN+NH3	3.00E+13	0.00	0	!SAME AS ADDUCT FORM.	(2/20/96)	(DB00)
!N2H3+HO2=H2NNHO+OH	3.00E+13	0.00	0	!RECOMBINATION (-5KCAL)		(DB00)
!N2H3+HO2=N2H2+H2O2	2.90E+04	2.69	-1600	! UPDATE	10/18/97	(DB00)
!N2H3+HO2=N2H4+O2	9.20E+05	1.94	2126	!NH2 WITH ADJUSTED THERMO		(DB00)

! \*\*\*\*\*  
! Begin updates to DCS84 chem from ADN.051601. WRA, 5/22/03  
! \*\*\*\*\*

!N2H2+M=NNH+H+M	5.00E16	0.0	50000.	! MB89
! H2O/15./ O2/2.0/ N2/2.0/ H2/2.0/				
!N2H2+H=NNH+H2	5.00E13	0.0	1000.	! MB89
!N2H2+O=NH2+NO	1.00E13	0.0	0.	! MB89
!N2H2+O=NNH+OH	2.00E13	0.0	1000.	! MB89
!N2H2+OH=NNH+H2O	1.00E13	0.0	1000.	! MB89
!N2H2+NH=NNH+NH2	1.00E13	0.0	1000.	! MB89
!N2H2+NH2=NH3+NNH	1.00E13	0.0	1000.	! MB89

! \*\*\*\*\*  
! Begin choices for NH2+NO taken from ADN.051601. WRA, 5/22/03  
!  
! NOTE!!! ADN.051601 contains QRRK results for many other  
! reactions and pressures on this PES. I'm just using the two  
! channels for Nusca's MMH mech with low P expressions because

```

! that's all that will matter at low P. Ratio of the two
! channels can be very sensitive in a number of systems.
!
! *****
! *****
! Begin reactions on NH2NO surface (Note NH2+NO=N2O+H2 is commented out
! earlier for reasons discussed there.
! *****
! *****

! history of WRA choices and comments

!NH2+NO=NNH+OH      6.40E15   -1.25    0.      ! MB89
!NH2+NO=N2+H2O      6.20E15   -1.25    0.      ! MB89
!NH2+NO=N2+H+OH     9.30E11    0.0     0.      ! BVV mdl, C&Fv98,402(1994)
!NH2+NO=N2+H2O      2.00E20   -2.6     924.    ! BVV mdl, C&Fv98,402(1994)
! Note, BVV had prods for radical channel as shown, but they are
! actually NNH+OH (which equally well model their NH3/NO flame
! experiment because all NNH->N2+H under their conditions).
! BVV expressions good for high T.
!NH2+NO=NNH+OH      4.90E11   -0.03   -362.   ! DYWL94 (lin), JPC1994
!NH2+NO=N2+H2O      4.70E15   -1.09   186.    ! DYWL94 (lin), JPC1994
! Above two expressions ignore DYWL's recomb channels
!NH2+NO=NNH+OH      3.50E10    0.335  -765.   ! DB00
!NH2+NO=N2+H2O      4.70E12   -0.247 -1200.  ! DB00
!NH2+NO=NNH+OH      1.43E07    1.40  -1777.  ! PL99 corrected typo per ADN.051601.2
!NH2+NO=N2+H2O      1.20E17   -1.61   298.   ! PL99 corrected typo per ADN.051601.2
!NH2+NO=NNH+OH      2.29E10    0.425  -815.   ! MG99
!NH2+NO=N2+H2O      2.77E20   -2.65  1258.   ! MG99
!
!
! Regarding NH2+NO:
! I used the BVV expressions for several years as these have
! a good representation of the high T branching ratio.
! T > 1000 is very important for combustion applications,
! The BVV expressions at T < 500 K have NNH+OH too low vs expts
! for T < 500 K, but good at higher T; total is mildly high.
! DB00 has good total from 298 - 2500, but NNH+OH branching too
! low for T > 1000 K. The branching may be extremely important.
! Note the PL99 branching ratio is similar to MG99. However,
! the total of the two channels is larger than the other
! expressions at high T. There is a minimum in the total
! at about 2000 K for PL99 expressions and then increases
! sharply towards higher T, which seems nonphysical.
! PL99 say the PL97 expression for the total was retained
! and just the branching ratio was changed. However, the
! total of PL99 expressions deviates to significantly
! higher values than the ktot expression given in PL97 for
! T > 2000 K. (PL97 ktot expression does not have minimum and
! then increase sharply towards higher T like PL99 does.)
! MG99 has good branching representation over 298 - 3000.
! MG99 maybe slightly low total (20%?) at high T (2500), but
! not terrible; certainly within error limits of experiments.
! Therefore these expressions were chosen. The branching ratio
! is typically very sensitive when these reactions come into
! play. WRA, 8/29 and 9/12/00
!
!
! *****
! End choices for NH2+NO taken from ADN.051601. WRA, 5/22/03
! *****

!NH3+OH=NH2+H2O     2.04E06    2.04   566.    ! MB89

```



```

!NH3+H=NH2+H2      6.36E05    2.39 10171.    ! MB89
!NH3+H=NH2+H2      5.42E05    2.40  9917.    ! KMF90 (Ko, Marshall...)
!NH3+O=NH2+OH      9.40E06    1.94  6460.    ! SUT/PAT/KLEMM90

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
!NH3+M=NH2+H+M     2.20E16    0.0  93470.    ! DKCH90; keyed for Ar=1.0
!NH3(+M)=NH2+H(+M) 5.50E15    0.00 107792.
! LOW/2.20E16 0.00 93470./
! Low pressure limit is from reevaluation by DKCH90.
! High pressure limit is from HW81 (assuming NH2+H products).
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

!NNH+NO=N2+HNO     5.00E13    0.0   0.    ! MB89
!NNH+NO=N2+HNO     2.00E13    0.0   0.    ! WRA, est, 040596
!NNH+H=N2+H2       1.00E14    0.0   0.    ! MB89
!NNH+OH=N2+H2O     5.00E13    0.0   0.    ! MB89
!NNH+NH2=N2+NH3    5.00E13    0.0   0.    ! MB89
!NNH+NH=N2+NH2     5.00E13    0.0   0.    ! MB89
! the next reaction rate changed *****
HNO+OH=NO+H2O      1.295E07   1.884 -958.    ! SPM91
H+HNO=H2+NO        4.46E11    0.72  655.    ! SP92
!HNO+NH2=NH3+NO    2.00E13    0.0  1000.    ! MB89
!N+NO=N2+O         3.27E12    0.3   0.    ! MB89
!O+NO=N+O2         3.80E09    1.0  41375.   ! TH91
!NO+H=N+OH         1.70E14    0.0  48800.   ! HS85
!HNO+HNO=N2O+H2O   3.63E-03   3.98  1190.    ! LHM92
!HNC+O=NH+CO       5.44E12    0.0   0.    ! TDLLM (Lin), 1994, preprint
!HNC+O=H+NCO       1.6E01     3.08 -224.   ! TDLLM, 1994
! note: 1st of two preceeding k's from experiment, 2nd from TST by TDLLM
! k's taken from the table (more digits than the abstract)
!HNC+OH=HNCO+H     2.80E13    0.0  3696.    ! HLM, IJCK 24, 1103, (1992).
!N2O+NO=N2+NO2     1.0E14     0.0  49675.   !added Yetter,
! traced source back to Smith and Thorne and then lost trail
!N2O+NO=N2+NO2     2.75E14    0.0  50000.   ! Borisov et al, 73, per NIST
!N2O+NO=N2+NO2     2.71E14    0.0  50700.   ! WRA, fit to selected (and
! some of it corrected) data from four sources
!N2O+NO=N2+NO2     4.29E13    0.00 47130.   ! WRA, 11/95; fit to reanalyzed
! lit results. This is not as different as old recommendation as it at first
! appears. Main difference is ~3 times smaller at high T. This has a strong
! effect on the A-factor, a more modest (but imp.) effect on Ea.
!NO+NO+NO=N2O+NO2 1.07E10    0.0  26800.   ! GVO 79
!HOCO+M=OH+CO+M    2.19E23   -1.89 35270.   ! LSG88, LP LIMIT
!HNC+OH=CN+H2O     1.5E12     0.00 7680.    ! TST result from TDLLM, 1994
!HNC+NO2=HNCO+NO   1.0E12     0.00 32000.   ! TST result from TDLLM, 1994
!
! New reactions, added 3/8/95, hlwm92 ISC
!
!HNCO+M=NH+CO+M     3.26E35   -5.11 109900. ! MCHB89,IJCK measured;best
! except Tsang 92 (used Tsang's expression earlier; has falloff)
!HNCO+M=H+NCO+M     5.00E15    0.0 120000. ! MCHB89,IJCK est
! per Tsang, better watch last reaction at low T, high P conditions,
! might get into falloff - could matter if reversed.
!HNCO+O=CO2+NH     9.80E07    1.41  8524. ! HLWM, 92 ISC, TST (Lin, p711)
!HNCO+O=NCO+OH     2.20E06    2.11 11430. ! HLWM, 92 ISC, TST
! NOTE: modeled exp results in T range of exp are very similar
! for previous two rxns. Next rxn could not be measured.
! Just noted Tsang 92 recommends these. Another product channel of the reverse
! of 2nd rxn is discussed earlier in this file and eliminated, per Tsang.
!HNCO+O=HNO+CO     1.49E08    1.57 44010. ! HLWM, 92 ISC, TST
!HNCO+OH=H2O+NCO   2.63E12    0.0  5544. ! Tully et al, 22nd ISC, 1989
!HNCO+OH=H2O+NCO   6.38E05    2.0  2560. ! Tsang,1992
!HNCO+OH=H2O+NCO   4.79E05    2.0  2560. ! Tsang,1992/MB91
!HNCO+OH=NH2+CO2   1.60E05    2.0  2560. ! Tsang,1992/MB91
! What's happening with HNCO+OH is Tsang's recommended total disappearance

```

```

! k for the rxn was used, but it was split into 2 channels 75:25 as
! recommended in MB91. This ratio is only established by the complex
! modeling work of MB91 (subject to error, especially the T dependence of
! the ratio), but seems reasonable. The total recommended by Tsang is
! close to that used by MB91, he just mentions having added a T**2
! dependence.      -WRA-

! ***** Update to HNCO+HO2 from m-yet-wra.rdx.1.8.wNHx.wHC.5*****
! Miller & Bowman
!HNCO+HO2=NCO+H2O2      3.00E+11  0.00  2.900E+04
!HNCO+HO2=NCO+H2O2  3.00E11  0.0  23700.      !
! WRA revised MB91's estimate due to updates
! in thermo.
! *****End update from m-yet-wra.rdx.1.8.wNHx.wHC.5*****

!HNCO+NH=NH2+NCO      2.00E13   0.0  23840. ! per Lin et al, 1991 jannaf,v2,337
!HNCO+NH=NH2+NCO      2.00E13   0.0  19300. ! WRA est, change due to new thermo
!HNCO+H=NH2+CO        2.10E14   0.0  16890. ! MK-HHB91 (Hanson)
!HNCO+H=NH2+CO        2.25E07   1.7  3800.  ! Miller&Melius IJCK92,TST,
!                                     ! agrees well w/Hanson
!HNCO+H=H2+NCO        1.05E05   2.50  13300. ! M&M,IJCK92, rev appears earlier
!                                     ! re prior reaction: am using Tsang's expression for the reverse
!HNCO+NO2=HNNO+CO2    2.50E12   0.0  26000. ! HLLM93
!CH+NO=HCN+O          1.10E14   0.0   0.    ! MB89
!
! added 3/10/95
!
!CN+NO=NCO+N           9.60E13   0.0  42100. ! Tsang 92
! see test estimates other channel at end
! Tsang's best est as of 1992 rev: remove cn+no -> n2+co
!
!CN+NO=NCO+N           5.5E12   0.0  30620. ! HWLM95 (Lin); Shock Waves Symp.
!CN+NO=N2+CO           3.9E11   0.0  27820. ! HWLM95, tst calc
!CN+NO=NCN+O           1.8E13   0.0  38190. ! HWLM95, tst calc
CO+NO2=NO+CO2         9.04E13   0.0  33780. ! TH91
!CO+NO2=CO2+NO        1.26E14   0.0  27600. ! Zabarnick, C&F91
!
! Just noted: Zabarnick misquoted Thorne & Melius who had 1.26E12;27600.
! Thorne and Melius' choice appears to be an estimate.
!
! *****
! Watch Princeton group for new info on prior rxn, they are working
! on it (see 1994 jannaf).
! *****
!
!CO+N2O=CO2+N2        left out per Princeton group and Lin recommendations.
!HO2+NO2=HONO+O2      4.64E11   0.0  -479. ! Zab, C&F91 cites Leeds, not there
!CH+NO2=HCO+NO        1.01E14   0.0   0. ! WCFS82
!HCO+NO2=CO+HONO      1.50E13   0.0  -430. ! T&M89, from TRG88 w/assumed prods
!HCO+NO2=CO2+H+NO     1.50E11   0.0  -430. ! T&M89, est?

! ***** H2+NO2 and HONO+ H revised per m-yet-wra.rdx.1.8.wNHx.wHC.5 *****
!H2+NO2=HONO+H        3.21E12   0.0  28810. ! Yetter et al, 29th Jannaf;
! ~k(S&G)/7.5; Ea somewhat tentative, Yetter et al didn't cover wide range;
! extrapolation out of range ~694-944 should be done with caution pending
! further work. On the other hand, considering the reverse rxn thermo and
! with the expectation the reverse rxn might have a small barrier, 28-31
! kcal is probably about right.
!HONO+H=H2+NO2        1.205E13   0.0  7326. ! TH91,est
!H2+NO2=HONO+H        2.40E13   0.0  29000. ! S&G78, as cited in nist
! Yetter et al criticised preceding expression as S&G
! depended on using high conc mixtures of H2/air (no inert) which
! calculations show would not have (T,P) constant during experiment.
! Conditions used by Skinner and coworkers (data cited and reduced by
! S&G as well as their own) were similar. Therefore, Princeton group
! presently best expression. (NOTE: T ranges used by S&G, Skinner et al

```

```

! and Princeton group were very similar, a fact I'd forgotten until
! recently. WRA, 3/31/95)
H2+NO2=HONO+H 1.30E04 2.76 29770. ! PGML98; see also MGYD00
HONO+H=HNO+OH 5.63E+10 0.86 4969. ! HLMM97
HONO+H=H2O+NO 8.13E+06 1.89 3847. ! HLMM97

! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****
2HONO=NO+NO2+H2O 0.349 3.64 12140. ! MLM98
! ***** update taken from ketene2.072398.062701 to ketene2.060305 *****

! **** End H2+NO2 and HONO+ H revised per m-yet-wra.rdx.1.8.wNHx.wHC.5 ****

!*****
! Begin NNH+M
!*****
!
! HEADS UP !!!!
!
! P dept rxns where I've used 3 param expressions; need attention in
! case of changing P.
!
! 12/22/00 NOTE: Don't worry about the above message anymore for NNH+M.
! I replaced old B&D95 limiting expressions with a Lindemann falloff form
! some time ago and forgot to clean the warning out. And JWB has gone
! over my Lindemann expression and tentatively approves. Above was an old
! note I forgot to clean out. I'm leaving it in to remind me what I did.
! Other P dept rxns in this section have been moved elsewhere and cleaned
! up to either falloff forms or specific P functions for which the user
! is instructed elsewhere what to do, i.e. chose from a list of
! functions. (see beginning of file in particular for a list of reactions
! thus affected). - WRA
!
!
!NNH=N2+H 1.00E04 0.0 0. ! MB89
!NNH(+M)=N2+H(+M) 4.10E09 1.13 5186. ! B&D95; high P limit
! LOW/ 1.00E13 0.5 3060./ ! B&D95; low P limit
! N2O/5.0/ H2O/9.0/ N2/1.0/ O2/0.82/ ! like N2O+M
! HNO3/5.0/ NH3/5.0/ NO3/5.0/ !
! CO2/3.2/
!DUP
!NNH=N2+H 3.00E08 0.0 0. ! tunneling term, B&D95
!DUP
! NOTE: Low and high P limits taken from estimates of B&D in IJCK95
! paper. Simple Lindemann form assumed, uncertainty doesn't seem
! to warrant better. Also, the reaction is not particularly
! sensitive for most propellant conditions as virtually all NNH is
! converted to N2+H. Finally, note B&D's low P expression
! includes a constant nonradiative decay (tunneling) term.

!*****
! End NNH+M
!*****

!*****
!
! HEADS UP !!!!
!
! P dept HCN=HNC rxn where I've used 3 param expressions; need attention in
! case of changing P.
!
!
!HCN=HNC 1.95E24 -4.23 49572. ! k(jwb, 1 atm;
! rcd 2/8/95)

```

```

!HCN=HNC          1.06E26   -4.34 50194.      ! 2 x k(jwb, 10 atm; i.e.for
!                  !                ! 20 atm; rcd 2/8/95)
!HCN=HNC          1.59E26   -4.34 50194.      ! 3 x k(jwb, 10 atm; i.e.for
!                  !                ! 30 atm; rcd 2/8/95)
!HCN+M=HNC+M      4.36E26   -3.34 50194.      ! 2nd order form, easiest to use
! above is low P limit, appropriate if T > ~600K; rxn is not sensitive for DZ.
! Reason is it is strongly into partial equilibrium.
! The expression is not bad (factor of 2ish error) even for T < 600 K, 10 atm.
! Of more concern would be hof(HNC).
!
!*****
!HNO+NO+NO=HNNO+NO2 1.70E11   0.00 2100.      ! Diau et al, IJCK 27,867(1995)
!HNNO+NO=NNH+NO2   3.2E12   0.00 270.       ! Diau et al, IJCK 27,867(1995)
!HNNO+NO=N2+HONO   2.6E11   0.0 810.       ! Diau et al, IJCK 27,867(1995)
!HNNO+M=H+N2O+M    2.2E15   0.0 21600.     ! Diau et al, IJCK 27,867(1995)
!HNNO+M=N2+OH+M    1.0E15   0.0 25600.     ! Diau et al, IJCK 27,867(1995)
!HNNO+OH=H2O+N2O   2.0E13   0.0 0.        ! wra est
!HNNO+H=H2+N2O     2.0E13   0.0 0.        ! wra est
!NNH+M=N2+H+M      1.0E14   0.0 3000.     ! Diau et al, IJCK 27,867(1995)
HCO+NO=HNO+CO     7.23E12   0.0 0.        ! TH91; test

```

```

!
! ***** REACTIONS GLEANED FROM GRI 3.0 *****
!
!O+CH2<=>H+HCO          8.000E+13   .000   .00
!O+CH2(S)<=>H2+CO       1.500E+13   .000   .00
!O+CH2(S)<=>H+HCO       1.500E+13   .000   .00
O+CH3<=>H+CH2O         5.060E+13   .000   .00
!O+CH4<=>OH+CH3        1.020E+09   1.500  8600.00
O+CH2O<=>OH+HCO        3.900E+13   .000  3540.00
!O+CH2OH<=>OH+CH2O     1.000E+13   .000   .00
O+CH3O<=>OH+CH2O       1.000E+13   .000   .00
!O+CH3OH<=>OH+CH2OH    3.880E+05   2.500  3100.00
!O+CH3OH<=>OH+CH3O     1.300E+05   2.500  5000.00
!O+C2H<=>CH+CO          5.000E+13   .000   .00
!O+C2H2<=>H+HCCO       1.350E+07   2.000  1900.00
!O+C2H2<=>OH+C2H        4.600E+19  -1.410 28950.00
!O+C2H2<=>CO+CH2        6.940E+06   2.000  1900.00
!O+C2H3<=>H+CH2CO       3.000E+13   .000   .00
!O+C2H4<=>CH3+HCO       1.250E+07   1.830  220.00
!O+C2H5<=>CH3+CH2O      2.240E+13   .000   .00
!O+C2H6<=>OH+C2H5       8.980E+07   1.920  5690.00
!O+CH2CO<=>OH+HCCO     1.000E+13   .000  8000.00
!O+CH2CO<=>CH2+CO2      1.750E+12   .000  1350.00
O2+CH2O<=>HO2+HCO      1.000E+14   .000 40000.00
!H+CH2(+M)<=>CH3(+M)    6.000E+14   .000   .00
!   LOW / 1.040E+26 -2.760 1600.00/
!   TROE/ .5620 91.00 5836.00 8552.00/
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ !C2H6/3.00/ ! AR/ .70/
!H+CH2(S)<=>CH+H2        3.000E+13   .000   .00
!H+CH3(+M)<=>CH4(+M)    13.90E+15  -0.534 536.00
!   LOW / 2.620E+33 -4.760 2440.00/
!   TROE/ .7830 74.00 2941.00 6964.00 /
!H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ !C2H6/3.00/ ! AR/ .70/
!H+CH4<=>CH3+H2         6.600E+08   1.620 10840.00
H+HCO(+M)<=>CH2O(+M)    1.090E+12   .480 -260.00
!   LOW / 2.470E+24 -2.570 425.00/
!   TROE/ .7824 271.00 2755.00 6570.00 /
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ !CH4/2.00/ C2H6/3.00/ ! AR/ .70/
!H+CH2O(+M)<=>CH2OH(+M) 5.400E+11   .454 3600.00
!   LOW / 1.270E+32 -4.820 6530.00/
!   TROE/ .7187 103.00 1291.00 4160.00 /
!H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ !CH4/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2        5.740E+07   1.900 2742.00
!H+CH2OH(+M)<=>CH3OH(+M) 1.055E+12   .500 86.00

```

```

!      LOW / 4.360E+31 -4.650 5080.00/
!      TROE/ .600 100.00 90000.0 10000.0 /
!H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ ! CH4/2.00/ C2H6/3.00/
!H+CH2OH<=>H2+CH2O 2.000E+13 .000 .00
!H+CH2OH<=>OH+CH3 1.650E+11 .650 -284.00
!H+CH2OH<=>CH2(S)+H2O 3.280E+13 -.090 610.00
H+CH3O(+M)<=>CH3OH(+M) 2.430E+12 .515 50.00
      LOW / 4.660E+41 -7.440 14080.0/
      TROE/ .700 100.00 90000.0 10000.0 /
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ !CH4/2.00/ C2H6/3.00/
!H+CH3O<=>H+CH2OH 4.150E+07 1.630 1924.00
H+CH3O<=>H2+CH2O 2.000E+13 .000 .00
H+CH3O<=>OH+CH3 1.500E+12 .500 -110.00
!H+CH3O<=>CH2(S)+H2O 2.620E+14 -.230 1070.00
!H+CH3OH<=>CH2OH+H2 1.700E+07 2.100 4870.00
H+CH3OH<=>CH3O+H2 4.200E+06 2.100 4870.00
!H+C2H(+M)<=>C2H2(+M) 1.000E+17 -1.000 .00
!      LOW / 3.750E+33 -4.800 1900.00/
!      TROE/ .6464 132.00 1315.00 5566.00 /
! H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
!H+C2H2(+M)<=>C2H3(+M) 5.600E+12 .000 2400.00
!      LOW / 3.800E+40 -7.270 7220.00/
!      TROE/ .7507 98.50 1302.00 4167.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
!H+C2H3(+M)<=>C2H4(+M) 6.080E+12 .270 280.00
!      LOW / 1.400E+30 -3.860 3320.00/
!      TROE/ .7820 207.50 2663.00 6095.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
!H+C2H3<=>H2+C2H2 3.000E+13 .000 .00
!H+C2H4(+M)<=>C2H5(+M) 0.540E+12 .454 1820.00
!      LOW / 0.600E+42 -7.620 6970.00/
!      TROE/ .9753 210.00 984.00 4374.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ !C2H6/3.00/ ! AR/ .70/
!H+C2H4<=>C2H3+H2 1.325E+06 2.530 12240.00
!H+C2H5(+M)<=>C2H6(+M) 5.210E+17 -.990 1580.00
!      LOW / 1.990E+41 -7.080 6685.00/
!      TROE/ .8422 125.00 2219.00 6882.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/
!H+C2H5<=>H2+C2H4 2.000E+12 .000 .00
!H+C2H6<=>C2H5+H2 1.150E+08 1.900 7530.00
!H+HCCO<=>CH2(S)+CO 1.000E+14 .000 .00
!H+HCCOH<=>H+CH2CO 1.000E+13 .000 .00
H2+CO(+M)<=>CH2O(+M) 4.300E+07 1.500 79600.00
      LOW / 5.070E+27 -3.420 84350.00/
      TROE/ .9320 197.00 1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ ! CH4/2.00/ C2H6/3.00/ ! AR/ .70/
!2OH(+M)<=>H2O2(+M) 7.400E+13 -.370 .00
!      LOW / 2.300E+18 -.900 -1700.00/
!      TROE/ .7346 94.00 1756.00 5182.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ ! C2H6/3.00/ ! AR/ .70/
!OH+CH2<=>H+CH2O 2.000E+13 .000 .00
!OH+CH2<=>CH+H2O 1.130E+07 2.000 3000.00
!OH+CH2(S)<=>H+CH2O 3.000E+13 .000 .00
OH+CH3(+M)<=>CH3OH(+M) 2.790E+18 -1.430 1330.00
      LOW / 4.000E+36 -5.920 3140.00/
      TROE/ .4120 195.0 5900.00 6394.00/
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ !CH4/2.00/ C2H6/3.00/
!OH+CH3<=>CH2+H2O 5.600E+07 1.600 5420.00
!OH+CH3<=>CH2(S)+H2O 6.440E+17 -1.340 1417.00
!OH+CH4<=>CH3+H2O 1.000E+08 1.600 3120.00
OH+CH2O<=>HCO+H2O 3.430E+09 1.180 -447.00
!OH+CH2OH<=>H2O+CH2O 5.000E+12 .000 .00
OH+CH3O<=>H2O+CH2O 5.000E+12 .000 .00
!OH+CH3OH<=>CH2OH+H2O 1.440E+06 2.000 -840.00
OH+CH3OH<=>CH3O+H2O 6.300E+06 2.000 1500.00
!OH+C2H<=>H+HCCO 2.000E+13 .000 .00

```

!OH+C2H2<=>H+CH2CO	2.180E-04	4.500	-1000.00
!OH+C2H2<=>H+HCCOH	5.040E+05	2.300	13500.00
!OH+C2H2<=>C2H+H2O	3.370E+07	2.000	14000.00
!OH+C2H2<=>CH3+CO	4.830E-04	4.000	-2000.00
!OH+C2H3<=>H2O+C2H2	5.000E+12	.000	.00
!OH+C2H4<=>C2H3+H2O	3.600E+06	2.000	2500.00
!OH+C2H6<=>C2H5+H2O	3.540E+06	2.120	870.00
!OH+CH2CO<=>HCCO+H2O	7.500E+12	.000	2000.00
!HO2+CH2<=>OH+CH2O	2.000E+13	.000	.00
!HO2+CH3<=>O2+CH4	1.000E+12	.000	.00
HO2+CH3<=>OH+CH3O	2.000E+13	.000	.00
!HO2+CH2O<=>HCO+H2O2	5.600E+06	2.000	12000.00
!C+CH2<=>H+C2H	5.000E+13	.000	.00
!C+CH3<=>H+C2H2	5.000E+13	.000	.00
!CH+H2<=>H+CH2	1.080E+14	.000	3110.00
!CH+H2O<=>H+CH2O	5.710E+12	.000	-755.00
!CH+CH2<=>H+C2H2	4.000E+13	.000	.00
!CH+CH3<=>H+C2H3	3.000E+13	.000	.00
!CH+CH4<=>H+C2H4	6.000E+13	.000	.00
!CH+CO (+M) <=>HCCO (+M)	5.000E+13	.000	.00
! LOW / 2.690E+28 -3.740 1936.00/			
! TROE/ .5757 237.00 1652.00 5069.00 /			
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ ! C2H6/3.00/ ! AR/ .70/			
!CH+CH2O<=>H+CH2CO	9.460E+13	.000	-515.00
!CH+HCCO<=>CO+C2H2	5.000E+13	.000	.00
!CH2+O2=>OH+H+CO	5.000E+12	.000	1500.00
!CH2+H2<=>H+CH3	5.000E+05	2.000	7230.00
!2CH2<=>H2+C2H2	1.600E+15	.000	11944.00
!CH2+CH3<=>H+C2H4	4.000E+13	.000	.00
!CH2+CH4<=>2CH3	2.460E+06	2.000	8270.00
!CH2+HCCO<=>C2H3+CO	3.000E+13	.000	.00
!CH2 (S) +N2<=>CH2+N2	1.500E+13	.000	600.00
!CH2 (S) +AR<=>CH2+AR	9.000E+12	.000	600.00
!CH2 (S) +O2<=>H+OH+CO	2.800E+13	.000	.00
!CH2 (S) +O2<=>CO+H2O	1.200E+13	.000	.00
!CH2 (S) +H2<=>CH3+H	7.000E+13	.000	.00
!CH2 (S) +H2O (+M) <=>CH3OH (+M)	4.820E+17	-1.160	1145.00
! LOW / 1.880E+38 -6.360 5040.00/			
! TROE/ .6027 208.00 3922.00 10180.0 /			
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
!CH2 (S) +H2O<=>CH2+H2O	3.000E+13	.000	.00
!CH2 (S) +CH3<=>H+C2H4	1.200E+13	.000	-570.00
!CH2 (S) +CH4<=>2CH3	1.600E+13	.000	-570.00
!CH2 (S) +CO<=>CH2+CO	9.000E+12	.000	.00
!CH2 (S) +CO2<=>CH2+CO2	7.000E+12	.000	.00
!CH2 (S) +CO2<=>CO+CH2O	1.400E+13	.000	.00
!CH2 (S) +C2H6<=>CH3+C2H5	4.000E+13	.000	-550.00
CH3+O2<=>O+CH3O	3.560E+13	.000	30480.00
CH3+O2<=>OH+CH2O	2.310E+12	.000	20315.00
!CH3+H2O2<=>HO2+CH4	2.450E+04	2.470	5180.00
!2CH3 (+M) <=>C2H6 (+M)	6.770E+16	-1.180	654.00
! LOW / 3.400E+41 -7.030 2762.00/			
! TROE/ .6190 73.20 1180.00 9999.00 /			
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ ! AR/ .70/			
!2CH3<=>H+C2H5	6.840E+12	.100	10600.00
!CH3+HCO<=>CH4+CO	2.648E+13	.000	.00
!CH3+CH2O<=>HCO+CH4	3.320E+03	2.810	5860.00
!CH3+CH3OH<=>CH2OH+CH4	3.000E+07	1.500	9940.00
!CH3+CH3OH<=>CH3O+CH4	1.000E+07	1.500	9940.00
!CH3+C2H4<=>C2H3+CH4	2.270E+05	2.000	9200.00
!CH3+C2H6<=>C2H5+CH4	6.140E+06	1.740	10450.00
!CH2OH+O2<=>HO2+CH2O	1.800E+13	.000	900.00
CH3O+O2<=>HO2+CH2O	4.280E-13	7.600	-3530.00
!C2H+O2<=>HCO+CO	1.000E+13	.000	-755.00
!C2H+H2<=>H+C2H2	5.680E+10	0.900	1993.00
!C2H3+O2<=>HCO+CH2O	4.580E+16	-1.390	1015.00

```

!C2H4 (+M) <=>H2+C2H2 (+M)          8.000E+12    .440    86770.00
!   LOW / 1.580E+51   -9.300  97800.00/
!   TROE/ .7345  180.00  1035.00  5417.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ ! C2H6/3.00/ ! AR/ .70/
!C2H5+O2<=>HO2+C2H4          8.400E+11    .000    3875.00
!2HCCO<=>2CO+C2H2          1.000E+13    .000     .00
!NNH+CH3<=>CH4+N2          2.500E+13    .000     .00
!NNH+O2<=>HO2+N2          5.000E+12    .000     .00
!NNH+O<=>OH+N2            2.500E+13    .000     .00
!NCO+O2<=>NO+CO2          2.000E+12    .000    20000.00
! NCO+O2 from MB89 w/same k appears above.
!H2CN+N<=>N2+CH2          6.000E+13    .000     400.00
!CH2+N2<=>HCN+NH          1.000E+13    .000    74000.00
!CH2 (S) +N2<=>NH+HCN      1.000E+11    .000    65000.00
!C+NO<=>CO+N              2.900E+13    .000     .00
!CH+NO<=>H+NCO            1.620E+13    .000     .00
!CH+NO<=>N+HCO            2.460E+13    .000     .00
!CH2+NO<=>H+HNCO          3.100E+17   -1.380    1270.00
!CH2+NO<=>OH+HCN          2.900E+14   -.690     760.00
!CH2+NO<=>H+HCNO          3.800E+13   -.360     580.00
!CH2 (S) +NO<=>H+HNCO      3.100E+17   -1.380    1270.00
!CH2 (S) +NO<=>OH+HCN      2.900E+14   -.690     760.00
!CH2 (S) +NO<=>H+HCNO      3.800E+13   -.360     580.00
!CH3+NO<=>HCN+H2O         9.600E+13    .000    28800.00
!CH3+NO<=>H2CN+OH         1.000E+12    .000    21750.00
!HCNO+H<=>H+HNCO          2.100E+15   -.690    2850.00
!HCNO+H<=>OH+HCN          2.700E+11    .180    2120.00
!HCNO+H<=>NH2+CO          1.700E+14   -.750    2890.00
!CH3+N<=>H2CN+H           6.100E+14   -.310     290.00
!CH3+N<=>HCN+H2           3.700E+12    .150    -90.00

```

```

! ***** END REACTIONS GLEANED FROM GRI 3.0 *****
!
!
```

```

! *****
! Following section from ketene2.020101.   WRA, 5/21/03
! *****

```

```

! *****
! Following reactions of HNO3 and NO3 taken from ADN.011701
! as of 1/25/01.   WRA
! *****

```

```

!*****
! Reactions added by WRA for HNO3/NO3 chem; see notes of 8/23/00
!*****

```

```

! HNO3+M
OH+NO2 (+M)=HNO3 (+M)  2.41E13    0.0    0.    ! TH91 keyed to N2
  LOW/ 6.42E32    -5.49  2350./
  !TSA/ 0.725  -2.5E-04 /
  H2O/9./ N2/1.0/ ! CO2/2.0/ ! N2O/5.0/    ! CO2/N2 from TH91;
  HNO3/5.0/ ! NH3/5.0/ NO3/5.0/

!HNO3+H=NO3+H2    2.40E08    1.5  11600.    ! WRA est following DB00 EP
!HNO3+H=NO2+H2O    6.00E13    0.0  9800.    ! WRA est following Laidler EP
!HNO3+H=HNO2+OH    6.00E13    0.0  7000.    ! WRA est following Laidler EP
!HNO3+H=HONO+OH    2.00E13    0.0  8000.    ! JWB est
! Above estimates agree with lower limit of Chapman & Wayne for H+HNO3
! of < 1.2e9 at 298 K. Seems reasonable the reactions should occur.

```

```

!HNO3+O=NO3+OH      2.00E13   0.0  12000.    ! WRA est following Laidler EP
!HNO3+O=NO2+HO2     2.00E13   0.0   6000.    ! possible channel, JWB thinks
!                                     ! unlikely
!HNO3+O=HNO2+O2     ! large exo would give
! fairly high k by EP method. But lit says no rxn at 298. Strange.
! DEM/SAN 97 has k(HNO3+O; 298) < 1.8E7. Above NO3+OH est works with this,
! but the other two estimates would not.

!*****
! HNO3+OH
!*****
!HNO3+OH=H2O+NO3     4.34E09   0.0  -1560.    ! DEM/SAN 97
!DUP
!HNO3+OH(+M)=H2O+NO3(+M) 2.47E08 0.0  -2860.    ! DEM/SAN 97
!   LOW/ 6.89E14   0.00 -1440./          !
!   N2O/5.0/ H2O/9./ N2/1.0/ ! CO2/2.0/   ! est.
!   HNO3/5.0/ NH3/5.0/ NO3/5.0/
!DUP
!
! Note Connell & Howard, 1985, conclude H2O2+NO2 is unimportant channel.
! DEM/SAN 97 cite works that state [OH] removed = [NO3] formed.
! This rxn deserves further attention. Didn't look into P dependence,
! which DEM/SAN 97 briefly discusses, carefully at this time (9/28/00; WRA).
! Must involve some stabilized species which perhaps should be put into the
! mech. NOTE: Duplicate rxns for HNO3+OH, as shown, are intended. These
! apparently represent an abstraction and an association channel. The
! version of the CHEMKIN interpreter used will allow these without DUP
! keywords; if DUP keywords are used where falloff and 'normal' reactions
! are specified, the version used flagged an error, though it shouldn't have.
! Some versions may have this 'bug' fixed and require the DUP keywords be
! uncommented.
!*****
! END HNO3+OH
!*****

!NO3+H2O2=HNO3+HO2  1.00E12   0.0   8500.    ! WRA est following Laidler EP
! HNO3+NH=HNO+HNO2, WRA est will not go, spin forbidden.
!HNO3+NH=HNOH+NO2   1.50E13   0.0   6000.    ! WRA est, EP Laidler
!HNO3+NH2=NO3+NH3   9.00E05   2.0   7300.    ! WRA est following DB00 EP
!HNO3+NH2=NH2O+HNO2 3.00E12   0.0   9000.    ! WRA est, EP Laidler
!HNO3+NH3=NH2O+H2O+NO 23.2   3.5  44930.    ! ML98 + Liau et al 1999 JANNAF
! for HNO3+NH3, see notes at beginning of file. Apparently
! Liau et al (note Lin was a coauthor) assume NH2ONO rapidly breaks down
! to NH2O+NO, so putting the reaction in with these products circumvents
! having to put in NH2ONO.
!HNO3+NO=HONO+NO2   8.00E06   2.0  11000.    ! est Ea from Laidler EP, set
!                                     ! A to pass through 298K data
!HONO+NO3=HNO3+NO2  1.00E12   0.0   6000.    ! WRA est, EP Laidler
!HNO2+NO3=HNO3+NO2  1.00E12   0.0   5000.    ! WRA est, EP Laidler

! NO3+M
!O+NO2(+M)=NO3(+M)  1.33E13   0.0   0.        ! TH91 keyed to N2
!   LOW/ 1.49E28    -4.08  2470./
!   !TSA/ 0.79    -1.8E-04/
!   N2O/5.0/ H2O/9./ N2/1.0/ ! CO2/2.7/   ! CO2/N2 from TH91;
!   HNO3/5.0/ NH3/5.0/ NO3/5.0/

!NO3+H=NO2+OH       6.00E13   0.0   0.        ! from refs in NIST database
!NO3+O=NO2+O2       1.00E13   0.0   0.        ! ATK/BAU 92/99
!NO3+OH=HO2+NO2     1.20E13   0.0   0.        ! ATK/BAU 99
!NO3+HO2=HNO3+O2    2.00E12   0.0   0.        ! from NIST, big error limits
!NO3+HO2=NO2+O2+OH  2.50E12   0.0   0.        ! controversial reaction
! For NO3+HO2 used recommendations from NIST for total, with C.J. Howard
! (most recent word on the rxn) that NO2+O2+OH is only channel.
! Some have the two channels of similar magnitudes at 298 K.
! Also note above is 298 K value for total, T dependence is unknown.

```



```

!
!NO3+NH=HNO+NO2 1.50E13 0.0 0. ! WRA est, EP Laidler
!NO3+NH=HNO3+N 1.00E12 0.0 5000. ! WRA est, EP Laidler
!NO3+NH2=HNO3+NH 1.00E12 0.0 10000. ! WRA est, EP Laidler
!NO3+NH2=NH2O+NO2 9.00E05 0.0 100. ! WRA est, EP DB00
!NO3+NO3=2NO2+O2 5.12E11 0.0 4870. ! DEM/SAN 97

!NO2+HO2=OH+NO3 1.00E12 0.0 16000. ! est, JWB/WRA
! Oops, this reaction already in as reverse above, with k established
! by experiment.
NO2+HO2=HONO+O2 1.00E12 0.0 5000. ! WRA est, EP Laidler
! From CJ Howard, JCP 77, per NIST, k(298) < 2E9. This reaction
! could be an important termination step in ADN model (if HO2 formed
! in abundance by OH+NO3). Per NIST database, the k of NO2+HO2 is
! very controversial. CJ Howard did excellent research on HO2+NO.
! This is an open issue. For now, I'm using an EP based
! estimate, which agrees with Howard's upper limit. The rxn is so
! poorly known, we could easily revise the estimate downwards.
! Presence of a much larger k for this rxn in Penn St mech may be
! reason for (unpublished) low predicted burn rates of ADN by both
! Penn St and ARL groups using that mech. WRA 9/1/00.
!
! Obtained Howard paper. Arguments that HONO+O2 does not contribute look
! pretty convincing, but it would be useful to obtain the other papers.
! Note they state SH74 assumed HONO+O2 was the main channel (which
! provides some confusion regarding limiting values in NIST), but no
! clear evidence for this was presented, looks like an assumption. A
! similar assumption clouds the interpretation of CD75. SH later (SH76)
! restudied the reaction. Later: also checked Demore et al, Eval 12, 1997.
! They cite k(300) < 3e8 from Tyndall et al 1995, must obtain that.
! Sounds like they are convinced by Tyndall. Not much discussion, but
! indication that the measurements included using FTIR to look for
! products. Note above estimate (just) agrees with this upper limit.
! WRA, 9/25/00
! Obtained Tyndall et al, and it is properly quoted as k(298)<3e8, and
! it does look pretty convincing. WRA, 10/17/00
!
! NOTE: The reactions (HNO3+NO=HONO+NO2 followed by
! HONO+M=OH+NO+M), NO2+HO2=HONO+O2, and NO3+NH3=HNO3+NH2 (put in as reverse
! above) likely do have reasonably fast rate constants and are potentially
! very important for ADN. Also, NO3+OH=HO2+NO2 followed by NO2+HO2=HONO+O2
! (termination).

! Ancillary HNOH, NH2O, and HNO2 rxns necessitated by addition
! of the HNO3 and NO3 rxns. Also obtained from ADN.011701.

!HNOH+NO2=HONO+HNO 6.00E11 0.0 2000. ! MG99, est.
!HNOH+H=NH2+OH 4.00E+13 0.00 0 !RECOMBINATION
!HNOH+H=HNO+H2 4.80E+08 1.50 378 !ABSTRACTION
!HNOH+O=HNO+OH 7.00E+13 0.00 0 !RECOMBINATION
!DUPLICATE
!HNOH+O=HNO+OH 3.30E+08 1.50 -358 !ABSTRACTION
!DUPLICATE
!HNOH+OH=HNO+H2O 2.40E+06 2.00 -1192 !ABSTRACTION
!NH2O+H=NH2+OH 4.00E+13 0.00 0 !RECOMBINATION
!NH2O+H=HNO+H2 4.80E+08 1.50 1560 !ABSTRACTION
!NH2O+O=HNO+OH 3.30E+08 1.50 487 !ABSTRACTION
!NH2O+OH=HNO+H2O 2.40E+06 2.00 -1192 !ABSTRACTION
!NH2O+NH2=HNO+NH3 1.80E+06 1.94 -1152 !ABSTRACTION
!HNO2+H=H2+NO2 2.40E+08 1.50 4163 ! HTRAN EST. 12/22/95
!HNO2+O=OH+NO2 1.70E+08 1.50 2365 ! HTRAN EST. 12/22/95
!HNO2+OH=H2O+NO2 1.20E+06 2.00 -795 ! HTRAN EST. 12/22/95
!HNO2+NH2=NO2+NH3 9.20E+05 1.94 874 ! HTRAN EST. 12/22/95

```

```

! *****
! End reactions of HNO3 and NO3 taken from ADN.011701
! as of 1/25/01.      WRA
! *****

! *****
! Reactions NO3 with carbon species brings in
! *****

!NO3+CH2O=HNO3+HCO  1.70E12  0.0  5000.      ! WRA est.
! NO3+CH2O: estimated A = 2x(8.4e11) from NO3+CH3CHO abstr,
! then with 298 value of k = 3.5E8 from 92ATK/BAU we have
! Ea~5 kcal/mole. The E-P estimate would normally be about
! 9 kcal/mole for Ea from 12 - 0.25(delta H = -12.7), but
! JWB points out the E/P factor for abstr by NO3 and ROO type
! rads is about 1/3 or even 1/2, not 1/4, so an Ea est around
! 5 or 6 kcal/mole is reasonable.

!NO3+HCO=H+CO2+NO2  2.00E13  0.0  0.      ! WRA est.
! This is just a first estimate. Other prod channels (see
! the following comments) could dominate at low T. Reaction
! needs further work if sensitive. Likely goes mainly by
! the activated complex H(C=O)-O-NO2. Complex could
! stabilize at high P, low T. Main high T products are
! likely HCO2+NO2, and HCO2 then mainly falls apart to
! H+CO2 under combustion conditions. Other channels (see
! following) could dominate at low T.
! NOTE: NO3+HCO=HONO+CO2 or HNO3+CO are also possible via
! the adduct with probably small or no barriers, but require
! H transfer through 5 center TS, so would have low A-factors.
! HCO2+NO2 is expected to have higher barrier (but below
! reactants), so dominates at high T. HNO3+CO can also
! result from H abstraction, but that's actually a
! disproportionation, so likely has a barrier. At first
! glance, this rxn looks like NO2+HCO, but it's not really
! very similar. NO2+HCO would make N-C bond in adduct,
! NO3+HCO would make O-C bond (ie, a nitro vs nitrate type
! adduct).
!NO3+C2H4=C2H4O+NO2  2.00E12  0.0  5720.
! Above k from 99ATK/BAU with WRA est of high T prods.
! NO3+C2H4 deserves more work, is more complex; a good one
! for QRRK or other study. Complex could stabilize.
! QM on PES surface, CNSTM, J.Org.Chem. 63, 6978, 1998, says
! C2H4O+NO2 is main channel.
!C2H4O=CH4+CO      1.21E13  0.0  57200.      ! LB83
!C2H4O=CH3CHO      7.26E13  0.0  57200.      ! LB83
!C2H4O=CH3+HCO     3.63E13  0.0  57200.      ! LB83

! In some of following rxns, WRA has replaced oxiranyl
! (cyclo c2h3o) with ch2cho because reaction to that species
! should happen rapidly at high T, and it greatly simplifies.

!C2H4O+CH3=CH4+CH2CHO  1.10E12  0.0  11800.      ! BK84

!C2H4O+O=OH+CH2CHO  results on this reaction are very
! scattered. Am leaving it out because either H or OH or
! both are always present in higher conc, and reactions
! with each are rapid. Therefore, O+C2H4O will not
! be imp.

!C2H4O+OH=H2O+CH2CHO  1.40E13  0.0  3360.
! C2H4O+OH from fit to 88WAL/LIU, 84BAL/KEE, and 84LOR/ZEL

!C2H4O+H=H2+CH2CHO    3.80E13  0.0  9197.
! C2H4O+H from fit to 84BAL/KEE and 83LIF/BEN. C2H4+OH and
! H2O+C2H3 channels are much less significant and therefore

```

```

! ignored.

!C2H4O+NO=HNO+CH2CHO   delta H = +22 kcal/mole, ignore.

!C2H4O+NO2=HONO+CH2CHO 1.30E12  0.0   3700.
! C2H4O+NO2 k from Jaffe 71, WRA assigned products.

!C2H4O+NO3=HNO3+CH2CHO 1.00E12  0.0   6000.      ! WRA est. E/P

! ignore CH2CHO+M for now

!CH2CHO+H=CH3+HCO      1.00E14  0.0     0.      ! WRA est.

!CH2CHO+H=H2+CH2CO     1.00E13  0.0     0.      ! WRA est.
! CH2CHO+H=CH3+HCO est. is so large because this is add/diss,
! and the A-factor is large due to low H entropy compared to
! typical complex entropy (compare to H+C2H4 and H+N2O).

!CH2CHO+OH=CH2OH+HCO   2.00E13  0.0     0.      ! WRA est.

!CH2CHO+OH=CH2CO+H2O   1.20E06  2.0     0.
! last rxn est. by WRA using Ea = 0 and E/P method of DB00

! CH2CHO+OH=H2O+HCOOH is exothermic and possibly even fast
! (addition of OH at C of C=O), but left out at present
! because of lack of thermo and chem for HCOOH and need to
! finish mech rapidly.

!CH2CHO+NO=HNO+CH2CO   1.00E12  0.0   8600.      ! WRA est. E/P
! per Gutman, ON-CH2CHO can stabilize at low T. This seems
! unlikely at high T, and I don't have time to work up
! chemistry on that species. Possible future topic.
! WRA 1/30/01

!CH2CHO+NO2=HONO+CH2CO 8.90E12  0.0   -160.
! C2H4O+NO2 k is from Barnhard et al, WRA estimated prods.
! O2N-CH2CHO could stabilize at low T.
!

!CH2CHO+NO3=HNO3+CH2CO 1.00E12  0.0     0.      ! WRA est., E/P
! adduct formation is also possible, not considered

!CH3+NO2=CH3O+NO      1.40E13  0.0     0.      ! ave GT74, YSG81,
!! and BC93. Williams & Fleming, C&F 97 is close.
!Identical reaction appears in HC/NO2 block below.

!CH3+NO3=CH3O+NO2     2.00E13  0.0     0.      ! WRA est.

!
! *****
! pertinent CH3CHO and CH2CHO chem from GRImech3.0:
! *****
!
!O+C2H5<=>H+CH3CHO      1.096E+14   .000   .00
!O+CH3CHO<=>OH+CH2CHO   2.920E+12   .000  1808.00
!O+CH3CHO=>OH+CH3+CO    2.920E+12   .000  1808.00
!O2+CH3CHO=>HO2+CH3+CO  3.010E+13   .000 39150.00
!H+CH3CHO<=>CH2CHO+H2   2.050E+09   1.160  2405.00
!H+CH3CHO=>CH3+H2+CO    2.050E+09   1.160  2405.00
!OH+CH3CHO=>CH3+H2O+CO  2.343E+10   0.730 -1113.00
!HO2+CH3CHO=>CH3+H2O2+CO 3.010E+12   .000 11923.00
!CH3+CH3CHO=>CH3+CH4+CO 2.720E+06   1.770  5920.00
!O+C2H4<=>H+CH2CHO     6.700E+06   1.830   220.00
!C2H3+O2<=>O+CH2CHO    3.030E+11   .290    11.00
!C2H3+O2<=>HO2+C2H2    1.337E+06   1.610 -384.00
!H+CH2CO (+M) <=>CH2CHO (+M) 4.865E+11   0.422 -1755.00

```

```

!   LOW/ 1.012E+42  -7.63  3854.0/
!   TROE/ 0.465  201.0  1773.0  5333.0 /
!H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/
!CH4/2.00/ C2H6/3.00/ AR/ .70/
!O+CH2CHO=>H+CH2+CO2          1.500E+14   .000   .00

!O2+CH2CHO=>OH+CO+CH2O          1.810E+10   .000   .00
!O2+CH2CHO=>OH+2HCO             2.350E+10   .000   .00
!   WRA on O2+CH2CHO: GRI uses above two channels, but the first has a
!   5c TS with likely only a small barrier and low A factor; second has
!   a 4c TS and it seems this would have a much more significant
!   barrier. JWB and student(s) have considered this rxn by QRRK. They
!   do not consider the second channel to be significant, and it does
!   not appear in NIST database. QRRK results indicate OCH2CHO will
!   significantly stabilize at temperatures even as high as 1000 K at
!   modest P (1 atm); not important at very low P. At very low P, the
!   first channel is T independent, and the k value obtained is close
!   to that given above (traced to BAU/COB92). At modest P and low to
!   intermediate T, the first channel falls off. It seems unlikely
!   this reaction (to any products) can matter much to propellant
!   combustion because conditions are rich, and there is little O2.
!   I was originally going to leave the reaction out, but decided to
!   keep it in for test purposes. It will be necessary to examine
!   modeling results to watch for unexpected influence of this reaction.
!   If it matters, further thought and a more elaborate treatment, and
!   possibly also addition of reactions with OCH2CHO, will be
!   necessary.          WRA, 2/1/01

! *****
! end pertinent CH3CHO and CH2CHO chem from GRImech3.0:
! *****
! *****
! End reactions for NO3 with carbon species brings in
! *****

! *****
! End section from ketene2.020101.          WRA, 5/21/03
! *****

! *****
! Begin section of updates from ketene2.020101 to
! ketene2.051601 and other key rxns from 051601.  WRA, 5/22/03
! NOTE: some of these overlap reactions in ketene2.020101.
! (Went carefully over all reactions towards the end of
! those files, prior sections are from DZ mech core of
! small molecule reactions I started with above. Chose
! not to include CHOCHO or CH2CO.)
! *****

!CH3+NH=H2CN+H2          3.50E13   0.0   290. ! WF97
! Above was an estimate by W&F, C&F 110, 1, 1997, used in modeling
! CH4/O2 flames doped with NH3, CH3NH2 or CH3CN. Reasonable estimate
! explained some of their results.

!
! ***** These reactions could be very imppt for CH2O/NO2 mixtures.
! k's taken from th91. CH2O+NO is obtained by reversing Tsang's estimate
! for HCO+HNO = CH2O+NO. Should be better than his forward k, as that is
! obtained from Keq, and he didn't have best thermo at time of his review.
!
!HCO+HNO=CH2O+NO          6.00E11   0.0   2000. ! TH91 - estimated
!
! Following 3 reactions are potentially very important in DB modeling.
! They are recommended by Tsang (TH91). There are a few studies, but the
! most complete work includes RPKM modeling of HCO+NO2 by the Emory group.
! Note the reaction involves activated intermediate complexes which could

```

```

! stabilize at high P, low T, a factor which may need future study. Note
! NIST database contains a couple bad typos re these rxns. Note the 2nd
! of these was included in earlier reactions previously, is commented out
! now.
!
CH2O+NO2=HCO+HONO  8.02E02   2.77  13730. ! Lin et al; TH91
HCO+NO2=CO+HONO   1.24E23   -3.29  2355. ! Lin et al; TH91
HCO+NO2=H+CO2+NO  8.39E15   -0.75  1930. ! Lin et al; TH91

! HCO+HCO only measured at 298
HCO+HCO=CH2O+CO   3.00E13   0.0    0. ! Bau 92
HCO+HCO=H2+CO+CO  5.20E12   0.0    0. ! ratioed to CH2O per TH86

! *****
! Begin hydrocarbon - NO2 reactions.
! *****

!CH4+NO2=CH3+HONO  1.20E13  0.0  30000. ! SG81
! Note, other workers, e.g. Yetter/Dryer group, have pointed out
! possible systematic errors in temperatures in the similar
! experiments of S&G on the H2+NO2=H+HONO reaction.

CH3+NO2=CH3O+NO   1.40E13  0.0    0. ! ave GT74, YSG81,
! and BC93. Williams & Fleming, C&F 100, 571, 1995 uses
! a very close value (1.5E13) in modeling of CH4/O2/NO2/N2 flames,
! and states the results are sensitive.

!CH2+NO2=CH2O+NO  5.00E13  0.0    0. ! ave STWW89 & DM95
! Study of CH2+NO2 at 298 K indicates that it is fast, as shown,
! but products have not been measured. (No measurements at other
! than 298 K.) CH2O+NO is highly exothermic and would appear to
! be the most likely, but HCO+H+NO is mildly exothermic and could
! easily and justifiably be tried in modeling. The stabilized
! radical adducts H2C-ONO or H2C-NO2 would also be formed
! exothermally. However, the experiments were performed at
! pressures of only a few torr, so it seems unlikely that those
! products were formed in the experiments.

! CH+NO2 is included in an earlier section.

! The reaction CH3+N2O=CH3O+N2 may eventually deserve some
! thought. However, it is beyond the scope of the present work.
! There is only one measurement and one upper limit in NIST
! database.
! *****
! End hydrocarbon - NO2 reactions.
! *****

! *****
! End section of updates from ketene2.020101 to
! ketene2.051601 and other key rxns from 051601. WRA, 5/22/03
! *****

!*****
! Following H2CN rxns taken from m-yet-wra.rdx.1.8.wNHx.wHC.5.
!
! WRA added three reactions of H2CN.
! First two k's taken from Marston & Stief, 1989 NASA tech note.
! Need to get their open lit paper. k for H2CN+H is lower limit.
! Measurements were at low T, long extrapolation necessary for
! combustion.
! Last k estimated.
!*****
!H2CN+N=HCN+NH      7.20E+13  0.00  4.000E+02
!H2CN+H=HCN+H2      4.00E+13  0.00  0.0    ! lower limit
! see H2CN+OH=HCN+H2O from Catoire et al 98 below.

```

```

!H2CN+OH=HCN+H2O          2.00E+13   0.00   0.0      ! WRA est
!*****
! end addition of H2CN reactions from m-yet-wra.rdx.1.8.wNHx.WHC.5.
!*****

!*****
! Following HOCN+H rxns taken from m-yet-wra.rdx.1.8.wNHx.WHC.5.
!
! Begin WRA mods to HOCN+H; also note one rev rxn commented out
! earlier.
!*****
! 17.5, 4
! Glarborg and Miller, Combust. Flame, 1994.
!HOCN+H=HNCO+H            2.00E+07   2.00   2.000E+03
! following lines from B&D 97 preprint and private communication
!H+HOCN=HCN+OH 2.00E+13   -0.04  2136   ! REV. OF 41B2
! WRA comment: B&D switched to and recommend reverse expression:
!OH+HCN=HOCN+H 1.10E+06   2.03   13373   !MILLER/MELIUS
!HOCN+H=HNCO+H 3.10E+08   0.84   1917
!HOCN+H=NH2+CO 1.20E+08   0.61   2076
!HOCN+H=H2+NCO 2.40E+08   1.50   6617   ! HTRAN EST. 12/22/95
! end B&D 97 preprint and private communication lines
!*****
! End WRA mods to HOCN+H
!*****

!*****
! Begin section on MMH and large fragment reactions.
!*****

! Rxns 1 - 16 of Catoire et al, 96 (Shock Waves, v6, 139, 1996):

!CH3NHNH2+M=CH3NH+NH2+M   2.5E14   0.0   40940. ! Catoire et al, 96
CH3NHNH2+H=CH3NNH2+H2     1.3E13   0.0   2500. ! Catoire et al, 96
!CH3NHNH2+H=CH3NH+NH3     4.46E09  0.0   3100. ! Catoire et al, 96
!CH3NHNH2+CH3=CH4+CH3NNH2  1.0E13   0.0   6990. ! Catoire et al, 96
!CH3NHNH2+NH2=NH3+CH3NNH2  1.0E11   0.5   1990. ! Catoire et al, 96
CH3NNH2+M=CH3NNH+H+M      1.0E17   0.0   35770. ! Catoire et al, 96
!CH3NH+M=CH3+NH+M         1.0E14   0.0   18000. ! Catoire et al, 96
!CH3NH+M=CH2NH+H+M        1.0E16   0.0   23800. ! Catoire et al, 96
!CH3NH+H=CH2NH+H2         1.0E08   2.0    0. ! Catoire et al, 96
!CH3NH+H=CH3+NH2          6.0E13   0.0    0. ! Catoire et al, 96
!CH3NNH+CH3=CH4+CH3NN     4.6E13   0.0   4850. ! Catoire et al, 96
!CH3NNH+NH2=NH3+CH3NN     4.6E13   0.0   4850. ! Catoire et al, 96
CH3NN=CH3+N2              3.0E06   0.0    0. ! Catoire et al, 96
!CH3NNCH3=CH3NN+CH3       6.9E15   0.0   50880. ! Catoire et al, 96
!CH3NNCH3=C2H6+N2         2.0E11   0.0   33000. ! Catoire et al, 96
!CH2NH+M=HCN+H2+M         1.0E14   0.0   10000. ! Catoire et al, 96

! Rxns 1 - 30 of Catoire et al, 98 (Proc. Instn. Mech. Engrs., v212,
! 393, 1998):

CH3NHNH2=CH3NNH+H2        3.16E13  0.0   57000. ! Golden et al, 72
!CH3NHNH2=CH2NH+NH3       1.58E13  0.0   54000. ! Golden et al, 72
CH3NNH2+HO2=CH3NHNH2+O2   1.0E06   2.0    0. ! Catoire et al, 98
CH3NN+HO2=CH3NNH+O2       1.0E06   2.0    0. ! Catoire et al, 98
CH3NHNH2+O=CH3NNH+H2O     9.6E12   0.0    0. ! Catoire et al, 98
CH3NHNH2+OH=CH3NNH+H2O    1.0E08   2.0    0. ! Catoire et al, 98
CH3NNH2+O=CH3NNH+OH       1.0E08   2.0    0. ! Catoire et al, 98
!CH3NNH2+HO2=CH3NNH+H2O2  1.0E08   2.0    0. ! Catoire et al, 98
CH3NNH2+O2=CH3NNH+HO2     4.0E12   0.0    0. ! Catoire et al, 98
!CH3NHNH2+HO2=CH3NNH2+H2O2 2.7E11   0.0   1987. ! Catoire et al, 98
!CH3NNH+HO2=CH3NN+H2O2    1.0E11   0.0   1987. ! Catoire et al, 98

```

CH3NHNH2+OH=CH3NNH2+H2O	3.92E13	0.0	0.	! Catoire et al, 98
CH3NNH+OH=CH3NN+H2O	3.92E13	0.0	0.	! Catoire et al, 98
CH3NHNH2+O=CH3NNH2+OH	9.6E12	0.0	0.	! Catoire et al, 98
CH3NNH+O=CH3NN+OH	9.6E12	0.0	0.	! Catoire et al, 98
!CH3NH+OH=CH2NH+H2O	1.0E08	2.0	0.	! Catoire et al, 98
!CH3NH+O=CH2NH+OH	1.0E08	2.0	0.	! Catoire et al, 98
!CH3NH+O2=CH2NH+HO2	1.0E07	2.0	6300.	! Catoire et al, 98
!CH3NH+O=CH3O+NH	6.0E13	0.0	0.	! Catoire et al, 98
!CH3NH+OH=CH4+HNO	6.0E12	0.0	0.	! Catoire et al, 98
!CH3NH+O2=CH3O+HNO	6.0E12	0.0	4000.	! Catoire et al, 98
!CH2NH+O=CH2O+NH	1.0E07	2.0	2800.	! Catoire et al, 98
!CH2NH+OH=CH2O+NH2	1.8E05	2.0	14800.	! Catoire et al, 98
!CH2NH+O=H2CN+OH	3.16E08	2.0	6100.	! Catoire et al, 98
!H2CN+HO2=CH2NH+O2	7.87E04	2.0	21700.	! Catoire et al, 98
!CH2NH+OH=H2CN+H2O	1.0E07	2.0	4000.	! Catoire et al, 98
!H2CN+O=HCN+OH	1.0E07	2.0	6100.	! Catoire et al, 98
!H2CN+OH=HCN+H2O	1.0E07	2.0	3700.	! Catoire et al, 98
!H2CN+O2=HCN+HO2	2.7E04	2.0	17300.	! Catoire et al, 98
!H2CN+NO=HCN+HNO	1.0E07	2.0	4400.	! Catoire et al, 98

! Reactions taken from Catoire et al, JPP 20, 87, 2004, these matter  
! mainly at low T, and they are mostly quite rough estimates:

!CH3NNH2+NO2 (+M)=CH3N(NH2)NO2 (+M)	1.0E13	0.0	0.	! Catoire et al, 04
! LOW/	1.0E17	0.0	0. /	!
!CH3NNH2+NO2 (+M)=CH3N(NH2)ONO (+M)	1.0E13	0.0	0.	! Catoire et al, 04
! LOW/	1.0E17	0.0	0. /	!
CH3NHNH2+NO2=CH3NNH2+HONO	2.2E11	0.0	5900.	! Catoire et al, 04
CH3NNH+NO2=CH3NN+HONO	2.2E11	0.0	5900.	! Catoire et al, 04
CH3NNH2+NO2=CH3NNH+HONO	1.0E08	2.0	0.	! Catoire et al, 04
!CH3NN=CH3+N2	3.0E06	0.0	0.	! Catoire et al, 04 THIS RXN ALREADY IN ABOVE

! \*\*\*\*\*  
! End section on MMH and large fragment reactions.  
! \*\*\*\*\*

! \*\*\*\*\*  
! Section on further small molecule reactions mentioned by  
! Catoire et al and of interest WRA, 060203  
! \*\*\*\*\*

! \*\*\*\*\*  
! NH2+HO2=NH3+O2  
! \*\*\*\*\*  
! following rxn, not used previously by WRA, cited as sensitive in  
! Catoire et al, 27th ISC, 1998 (ignition delay in MMH/O2/AR  
! mixtures):  
  
!NH2+HO2=NH3+O2           2.0E13    0.0        0. ! DEM/SAN 97, 298 K  
!NH2+HO2=NH3+O2           4.52E13  0.0        0. ! Catoire et al, 98  
! Looking at NIST database (and my expectations), the Catoire  
! cited value seems a bit large.

! \*\*\*\*\*  
! HO2+HO2=H2O2+O2  
! \*\*\*\*\*  
! See 2HO2=H2O2+O2 used previously by WRA above.  
! Catoire et al cite HO2+HO2=H2O2+O2 k = 4.2E14exp(-11980/RT), this  
! traces to 94 BAU/COB, 850- 1250 K per NIST. But the Ea is WIERD!!  
! Extrapolate to 298 = BAD agreement with expt. (per NIST). And that Ea  
! seems way too big to me. MB89 used 2E12, and TH86 recommended

```

! 1.8E12. I've kept TH86, which I've been using for a long time.
! I don't think anything I ever did was sensitive to this rxn.
! Catoire et al state this rxn is sensitive for MMH, better keep an
! eye on it.

! Further comments on some small moc rxns Catoire et al say are
! sensitive:
! For H2O2+M=OH+OH+M, I use reverse from GRI, with falloff.
! For CH3+CH3(+M)=C2H6(+M), I use GRI. Both GRI and Catoire had
! falloff. Expressions are slightly different.
! For CH4+HO2=CH3+H2O2, I have reverse from GRI.
! For CH3+NO2=CH4+O2, I use same expression as Catoire.
! My expression for O2+H=O+OH from MHB90, slightly different from
! Catoire, I'm sure is excellent.

!*****
! End section on further small molecule reactions mentioned by
! Catoire et al and of interest WRA, 060203
!*****

!*****
! Catoire et al 2004 recommend using NO2=N2O4 WRA, 062104
!*****

! *****
! NO2 = N2O4
! *****
! Atkinson et al, JPCRD 1997, as cited by Catoire et al,
! JPP 20, 87, 2004.

N2O4 (+M)=NO2+NO2 (+M) 4.05E18 -1.1 12840.
LOW/ 1.96E28 -3.8 12800. /

!*****
! End NO2=N2O4 WRA, 062104
!*****

! Initially inserted NAMMH complex formation at high P limit only,
! for testing.
!CH3NHNH2+HNO3=NAMMH 7.83E21 -3.46 -276. ! WRA EMAIL 1/18/2005

!CH3NHNH2+HNO3=NAMMH 2.00E13 0.0 0. ! WRA est, hi P lim.
!CH3NHNH2+HNO3=CH3NHNH2-HNO3 2.00E13 0.0 0. ! WRA est, hi P lim.

! *****
! Block of reactions for CH3NO2
! *****

! Reactions are taken from: Glarborg, Bendtsen, and Miller, IJCK 31,
! 591, 1999, Appendix A.

! NOTES:
!
! 1. These authors considered CH3+NO2(+M)=CH2ONO(+M) to be negligible.
! 2. Species CH3NO2 CH3NO H2CNO2 CH3ONO CH3ONO2 had to be added.
! Thermo from Sandia database used.
! 3. CH3+NO2=CH3O+NO is already in above. I kept the k(T) I have
! been using for years, it is only slightly different (about
! 20-60 % larger) than that of GBD99 commented out below.
! at combustion T.
! 4. CH4+NO2=CH3+HONO is already in above with k(T) identical to
! that of GBD99 commented out below.

```



!CH3NO2 (+M)=CH3+NO2 (+M)	1.80E16	0.00	58500.	!GBD99
!	LOW/	1.30E17	0.00	42000. /
!	!TSA/	0.183	0.0 /	!
!CH3NO2+H=CH3+HONO	3.30E12	0.00	3730.	!GBD99
!CH3NO2+H=CH3NO+OH	1.40E12	0.00	3730.	!GBD99
!CH3NO2+H=H2CNO2+H2	5.40E02	3.50	5200.	!GBD99
!CH3NO2+O=H2CNO2+OH	1.50E13	0.00	5350.	!GBD99
!CH3NO2+OH=H2CNO2+H2O	5.00E05	2.00	1000.	!GBD99
!CH3NO2+OH=CH3OH+NO2	2.00E10	0.00	-1000.	!GBD99
!CH3NO2+CH3=H2CNO2+CH4	5.50E-01	4.00	8300.	!GBD99
!CH3NO2+CH2 (S)=H2CNO2+CH3	1.20E14	0.00	0.	!GBD99
!CH3NO2+CH2=H2CNO2+CH3	6.50E12	0.00	7900.	!GBD99
!H2CNO2=CH2O+NO	1.00E13	0.00	36000.	!GBD99
!CH3+NO (+M)=CH3NO (+M)	9.00E12	0.00	119.	!GBD99
!	LOW/	3.20E23	-1.87	0. /
!CH3+NO2=CH3O+NO	4.00E13	-0.20	0.	!GBD99
!CH4+NO2=CH3+HONO	1.20E13	0.00	30000.	!GBD99
CH3O+NO=CH2O+HNO	1.30E14	-0.70	0.	!GBD99
!CH3O+NO (+M)=CH3ONO (+M)	6.60E14	-0.60	0.	!GBD99
!	LOW/	2.70E27	-3.50	0. /
CH3O+NO2=CH2O+HONO	6.00E12	0.00	2285.	!GBD99
!CH3O+NO2 (+M)=CH3ONO2 (+M)	1.20E13	0.00	0.	!GBD99
!	LOW/	1.40E30	-4.50	0. /

### A.3 HFO-1234yf

#### Thermochemical parameters in CHEMKIN format

```

THERMO
 298.000 1000.000 5000.000
N2          121286N  2          G  0300.00  5000.00  1000.00      1
 0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13      2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-0.03963222E-04      3
 0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02      4
AR          120186AR  1          G  0300.00  5000.00  1000.00      1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00      2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00      3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02      4
HE          L10/90HE  1  0  0  0G  200.000  6000.000  1000.      1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00      2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00      3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01 0.00000000E+00      4
NE          L10/92NE  1  0  0  0G  200.000  6000.000  1000.00      1
 0.25000000E+01 0.          0.          0.          0.          2
-0.74537500E+03 0.33553227E+01 0.25000000E+01 0.          0.          3
 0.          0.          -0.74537498E+03 0.33553227E+01 0.00000000E+00      4
C(S)       P 4/83C  1  0  0  0C  200.000  5000.000  12.01100      1
 0.14556924e+01 0.17170638e-02-0.69758410e-06 0.13528316e-09-0.96764905e-14      2
-0.69512804e+03-0.85256842e+01-0.31087207e+00 0.44035369e-02 0.19039412e-05      3
-0.63854697e-08 0.29896425e-11-0.10865079e+03 0.11138295e+01      4
O          L 1/90O  1  00  00  00G  200.000  3500.000  1000.000      1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15      2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06      3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00 6.72540300E+03      4
O2         TPIS89O  2  00  00  00G  200.000  3500.000  1000.000      1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14      2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06      3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00 8.68010400E+03      4

```

```

H      L 7/88H  1  00  00  00G  200.000  3500.000  1000.00  1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22 2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15 3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01 6.19742800E+03 4
H2     TPIS78H  2  00  00  00G  200.000  3500.000  1000.00  1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14 2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05 3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01 8.46810200E+03 4
OH     S 9/01O  1H  1  0  0  0G  200.000  6000.000  1000.00  1
 2.86472886E+00 1.05650448E-03-2.59082758E-07 3.05218674E-11-1.33195876E-15 2
 3.71885774E+03 5.70164073E+00 4.12530561E+00-3.22544939E-03 6.52764691E-06 3
-5.79853643E-09 2.06237379E-12 3.38153812E+03-6.90432960E-01 4.51532273E+03 4
OH"OLD" RUS 78O  1H  1  00  00G  200.000  3500.000  1000.00  1
 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11 1.17412376E-14 2
 3.85865700E+03 4.47669610E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06 3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01 8.81310600E+03 4
H2O    L 8/89H  2O  1  00  00G  200.000  3500.000  1000.00  1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14 2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06 3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01 9.90409200E+03 4
HO2    L 5/89H  1O  2  00  00G  200.000  3500.000  1000.00  1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14 2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05 3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00 1.00021620E+04 4
H2O2   L 7/88H  2O  2  00  00G  200.000  3500.000  1000.00  1
 4.16500285E+00 4.90831694E-03-1.90139225E-06 3.71185986E-10-2.87908305E-14 2
-1.78617877E+04 2.91615662E+00 4.27611269E+00-5.42822417E-04 1.67335701E-05 3
-2.15770813E-08 8.62454363E-12-1.77025821E+04 3.43505074E+00 1.11588350E+04 4
C      L11/88C  1  00  00  00G  200.000  3500.000  1000.00  1
 2.49266888E+00 4.79889284E-05-7.24335020E-08 3.74291029E-11-4.87277893E-15 2
 8.54512953E+04 4.80150373E+00 2.55423955E+00-3.21537724E-04 7.33792245E-07 3
-7.32234889E-10 2.66521446E-13 8.54438832E+04 4.53130848E+00 6.53589500E+03 4
CH     TPIS79C  1H  1  00  00G  200.000  3500.000  1000.00  1
 2.87846473E+00 9.70913681E-04 1.44445655E-07-1.30687849E-10 1.76079383E-14 2
 7.10124364E+04 5.48497999E+00 3.48981665E+00 3.23835541E-04-1.68899065E-06 3
 3.16217327E-09-1.40609067E-12 7.07972934E+04 2.08401108E+00 8.62500000E+03 4
CH2    L S/93C  1H  2  00  00G  200.000  3500.000  1000.00  1
 2.87410113E+00 3.65639292E-03-1.40894597E-06 2.60179549E-10-1.87727567E-14 2
 4.62636040E+04 6.17119324E+00 3.76267867E+00 9.68872143E-04 2.79489841E-06 3
-3.85091153E-09 1.68741719E-12 4.60040401E+04 1.56253185E+00 1.00274170E+04 4
CH2*   L S/93C  1H  2  00  00G  200.000  3500.000  1000.00  1
 2.29203842E+00 4.65588637E-03-2.01191947E-06 4.17906000E-10-3.39716365E-14 2
 5.09259997E+04 8.62650169E+00 4.19860411E+00-2.36661419E-03 8.23296220E-06 3
-6.68815981E-09 1.94314737E-12 5.04968163E+04-7.69118967E-01 9.93967200E+03 4
CH3    L11/89C  1H  3  00  00G  200.000  3500.000  1000.00  1
 2.28571772E+00 7.23990037E-03-2.98714348E-06 5.95684644E-10-4.67154394E-14 2
 1.67755843E+04 8.48007179E+00 3.67359040E+00 2.01095175E-03 5.73021856E-06 3
-6.87117425E-09 2.54385734E-12 1.64449988E+04 1.60456433E+00 1.03663400E+04 4
CH4    L 8/88C  1H  4  00  00G  200.000  3500.000  1000.00  1
 7.48514950E-02 1.33909467E-02-5.73285809E-06 1.22292535E-09-1.01815230E-13 2
-9.46834459E+03 1.84373180E+01 5.14987613E+00-1.36709788E-02 4.91800599E-05 3
-4.84743026E-08 1.66693956E-11-1.02466476E+04-4.64130376E+00 1.00161980E+04 4
CO     TPIS79C  1O  1  00  00G  200.000  3500.000  1000.00  1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14 2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06 3
 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00 8.67100000E+03 4
CO2    L 7/88C  1O  2  00  00G  200.000  3500.000  1000.00  1
 3.85746029E+00 4.41437026E-03-2.21481404E-06 5.23490188E-10-4.72084164E-14 2
-4.87591660E+04 2.27163806E+00 2.35677352E+00 8.98459677E-03-7.12356269E-06 3
 2.45919022E-09-1.43699548E-13-4.83719697E+04 9.90105222E+00 9.36546900E+03 4
HCO    L12/89H  1C  1O  1  00G  200.000  3500.000  1000.00  1
 2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-5.33508711E-14 2
 4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05 3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 9.98945000E+03 4
CH2O   L 8/88H  2C  1O  1  00G  200.000  3500.000  1000.00  1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14 2

```

-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05 3  
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01 1.00197170E+04 4  
CH2OH"OLD" GUNL93C 1H 30 1 00G 200.000 3500.000 1000.0 1  
3.69266569E+00 8.64576797E-03-3.75101120E-06 7.87234636E-10-6.48554201E-14 2  
-3.24250627E+03 5.81043215E+00 3.86388918E+00 5.59672304E-03 5.93271791E-06 3  
-1.04532012E-08 4.36967278E-12-3.19391367E+03 5.47302243E+00 1.18339080E+04 4  
CH2OH IU2/03C 1H 30 1 00G 200.000 6000.00 1  
5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-14 2  
-4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-05 3  
-3.64869060E-08 1.47907450E-11-3.50072890E+03 3.30913500E+00-2.04462770E+03 4  
CH3O"OLD" 121686C 1H 30 1 G 0300.00 3000.00 1000.00 1  
0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12 2  
0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04 3  
-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02 4  
CH3O IU1/03C 1H 30 1 G 200.000 6000.00 1  
4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-14 2  
3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-05 3  
-4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00 2.52571660E+03 4  
CH3OH L 8/88C 1H 40 1 00G 200.000 3500.000 1000.000 1  
1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-1.17060220E-13 2  
-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02 6.52441155E-05 3  
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00 1.14352770E+04 4  
C2H L 1/91C 2H 1 00 00G 200.000 3500.000 1000.000 1  
3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-1.77232770E-14 2  
6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-2.84769501E-05 3  
2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00 1.04544720E+04 4  
C2H2 L 1/91C 2H 2 00 00G 200.000 3500.000 1000.000 1  
4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-3.61235213E-14 2  
2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-3.55171815E-05 3  
2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01 1.00058390E+04 4  
H2CC L12/89H 2C 2 0 0G 200.000 6000.000 1000.000 1  
0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-13 2  
0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-05 3  
-0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01 0.49887266E+05 4  
C2H3 L 2/92C 2H 3 00 00G 200.000 3500.000 1000.000 1  
3.01672400E+00 1.03302292E-02-4.68082349E-06 1.01763288E-09-8.62607041E-14 2  
3.46128739E+04 7.78732378E+00 3.21246645E+00 1.51479162E-03 2.59209412E-05 3  
-3.57657847E-08 1.47150873E-11 3.48598468E+04 8.51054025E+00 1.05750490E+04 4  
C2H4 L 1/91C 2H 4 00 00G 200.000 3500.000 1000.000 1  
2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-1.25706061E-13 2  
4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03 5.70990292E-05 3  
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00 1.05186890E+04 4  
C2H5 L12/92C 2H 5 00 00G 200.000 3500.000 1000.000 1  
1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-1.49641576E-13 2  
1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03 4.97142807E-05 3  
-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00 1.21852440E+04 4  
C2H6 L 8/88C 2H 6 00 00G 200.000 3500.000 1000.000 1  
1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-1.90002890E-13 2  
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03 5.99438288E-05 3  
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00 1.18915940E+04 4  
CH2CO"OLD" L 5/90C 2H 20 1 00G 200.000 3500.000 1000.000 1  
4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-7.94838201E-14 2  
-7.55105311E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-1.73947474E-05 3  
9.34397568E-09-2.01457615E-12-7.04291804E+03 1.22156480E+01 1.17977430E+04 4  
CH2CO D05/90C 2H 20 1 00G 200.000 3500.000 1000.000 1  
4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-7.94838201E-14 2  
-7.77850000E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-1.73947474E-05 3  
9.34397568E-09-2.01457615E-12-7.27000000E+03 1.22156480E+01 1.17977430E+04 4  
CH2CHO"OLD" T04/83O 1H 3C 2 0G 300.000 5000.000 1  
0.59756699E+01 0.81305914E-02-0.27436245E-05 0.40703041E-09-0.21760171E-13 2  
0.49032178E+03-0.50320879E+01 0.34090624E+01 0.10738574E-01 0.18914925E-05 3  
-0.71585831E-08 0.28673851E-11 0.15214766E+04 0.95714535E+01 0.30474436E+04 4  
CH2CHO D05/83O 1H 3C 2 0G 300.000 5000.000 1  
0.59756699E+01 0.81305914E-02-0.27436245E-05 0.40703041E-09-0.21760171E-13 2  
-0.96950000E+03-0.50320879E+01 0.34090624E+01 0.10738574E-01 0.18914925E-05 3  
-0.71585831E-08 0.28673851E-11 0.62000000E+02 0.95714535E+01 0.30474436E+04 4

CH2OCH"OLD" T 9/92C 2H 3O 1 OG 298.150 3000.000 1000.0 1
0.48131470E+00 0.20711914E-01-0.12693155E-04 0.34579642E-08-0.35399703E-12 2
0.15648642E+05 0.34629876E+02 0.10854772E+01 0.12845259E-01 0.24138660E-05 3
-0.44642672E-08-0.29381916E-12 0.15910655E+05 0.33395312E+02 0.16817588E+05 4
CH2OCH A12/04C 2H 3O 1 OG 298.150 3000.000 500.0 1
0.44994054E+01 0.11552625E-01-0.48144129E-05 0.89234919E-09-0.56870585E-13 2
0.17473963E+05 0.33925515E+00-0.38396084E+00 0.23879038E-01-0.12467587E-04 3
-0.17686411E-08 0.28142438E-11 0.18836203E+05 0.25741745E+02 4
CH2OCH2 T 6/92C 2H 4O 1 OG 298.150 3000.0 1000.0 1
0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-13 2
-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-04 3
-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-0.63304657E+04 4
CH3CO T 9/92C 2H 3O 1 OG 200.000 6000.0 1000.0 1
0.59447731E+01 0.78667205E-02-0.28865882E-05 0.47270875E-09-0.28599861E-13 2
-0.37873075E+04-0.50136751E+01 0.41634257E+01-0.23261610E-03 0.34267820E-04 3
-0.44105227E-07 0.17275612E-10-0.26574529E+04 0.73468280E+01-0.12027167E+04 4
CH3CHO L 8/88C 2H 4O 1 OG 200.000 6000.0 1000.0 1
0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13 2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04 3
-0.14585611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05 4
HCCO SRIC91H 1C 2O 1 G 0300.00 4000.00 1000.00 1
0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13 2
0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04 3
0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02 4
HCCOH SRI91C 2O 1H 2O OG 300.000 5000.000 1000.G 1
0.59238291E+01 0.67923600E-02-0.25658564E-05 0.44987841E-09-0.29940101E-13 2
0.72646260E+04-0.76017742E+01 0.12423733E+01 0.31072201E-01-0.50866864E-04 3
0.43137131E-07-0.14014594E-10 0.80316143E+04 0.13874319E+02 4
C2O RUS 79C 2O 1 0 OG 200.000 6000.000 1
0.51512722E+01 0.23726722E-02-0.76135971E-06 0.11706415E-09-0.70257804E-14 2
0.33241888E+05-0.22183135E+01 0.28648610E+01 0.11990216E-01-0.18362448E-04 3
0.15769739E-07-0.53897452E-11 0.33749932E+05 0.88867772E+01 0.35003406E+05 4
C3H2 T12/00C 3H 2 0 OG 200.000 6000.000 1
0.73481207E+01 0.44476404E-02-0.12610332E-05 0.78131814E-10 0.13216298E-13 2
0.62551656E+05-0.91040211E+01 0.45094776E+01 0.17438605E-01-0.24516321E-04 3
0.18993967E-07-0.57996520E-11 0.63080191E+05 0.42892461E+01 4
C3H2-2 S 4/01C 3H 2 0 OG 200.000 3000.000 1
7.47247827E+00 4.57765160E-03-1.56482125E-06 2.43991965E-10-1.42462924E-14 2
8.83321441E+04-1.27113314E+01 3.74356467E+00 2.51955211E-02-4.62608277E-05 3
4.34360520E-08-1.53992558E-11 8.89297787E+04 4.22612394E+00 9.08356403E+04 4
cc3H2 121686C 3H 2 G 0300.00 5000.00 1000.00 1
0.06530853E+02 0.05870316E-01-0.01720777E-04 0.02127498E-08-0.08291910E-13 2
0.05115214E+06-0.01122728E+03 0.02691077E+02 0.01480366E+00-0.03250551E-04 3
-0.08644363E-07 0.05284878E-10 0.05219072E+06 0.08757391E+02 4
C3H3 T 5/97C 3H 3 0 OG 200.000 6000.000 1
7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-2.51475415E-14 2
3.89087427E+04-1.25848436E+01 1.35110927E+00 3.27411223E-02-4.73827135E-05 3
3.76309808E-08-1.18540923E-11 4.01057783E+04 1.52058924E+01 4.16139977E+04 4
ac3H4 L 8/89C 3H 4 0 OG 200.000 6000.000 1
0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13 2
0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04 3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05 4
pc3H4 T 2/90H 4C 3 0 OG 200.000 6000.000 1
0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13 2
0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05 3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05 4
cc3H4 T12/81C 3H 4 0 OG 300.000 5000.000 1
0.66999931E+01 0.10357372E-01-0.34551167E-05 0.50652949E-09-0.26682276E-13 2
0.30199051E+05-0.13378770E+02-0.24621047E-01 0.23197215E-01-0.18474357E-05 3
-0.15927593E-07 0.86846155E-11 0.32334137E+05 0.22729762E+02 0.3332728 E+05 4
C3H8 P11/94C 3H 8 0 OG 300.000 3000.000 1
0.75244152E+01 0.18898282E-01-0.62921041E-05 0.92161457E-09-0.48684478E-13 2
-0.16564394E+05-0.17838375E+02 0.92851093E+00 0.26460566E-01 0.60332446E-05 3
-0.21914953E-07 0.94961544E-11-0.14057907E+05 0.19225538E+02 4
nc3H7 P11/94C 3H 7 0 OG 300.000 3000.000 1
0.77097479E+01 0.16031485E-01-0.52720238E-05 0.75888352E-09-0.38862719E-13 2

0.79762236E+04-0.15515297E+02	0.10491173E+01	0.26008973E-01	0.23542516E-05	3					
-0.19595132E-07	0.93720207E-11	0.10312346E+05	0.21136034E+02	4					
ic3H7	P11/94C	3H	7	0	OG	300.000	3000.000	1	
0.65192741E+01	0.17220104E-01	-0.57364217E-05	0.84130732E-09	-0.44565913E-13	2				
0.73227193E+04-0.90830215E+01	0.14449199E+01	0.20999112E-01	0.77036222E-05	3					
-0.18476253E-07	0.71282962E-11	0.94223724E+04	0.20116317E+02	4					
C3H6	120186C	3H	6	G	0300.00	5000.00	1000.00	1	
0.06732257E+02	0.01490834E+00	-0.04949899E-04	0.07212022E-08	-0.03766204E-12	2				
-0.09235703E+04-0.01331335E+03	0.01493307E+02	0.02092518E+00	0.04486794E-04	3					
-0.01668912E-06	0.07158146E-10	0.01074826E+05	0.01614534E+03	4					
CH2CHCO	T05/99C	3H	30	1	OG	200.000	6000.0	1000.0	1
6.95842227E+00	1.07193211E-02	-3.85218494E-06	6.22009064E-10	-3.72401640E-14	2				
5.64826498E+03-1.14745786E+01	3.21169467E+00	1.18422105E-02	1.67462582E-05	3					
-3.06947176E-08	1.33048816E-11	7.12815750E+03	1.00881663E+01	8.70564832E+03	4				
CH2CHCO	USC/07C	3H	30	1	OG	300.000	5000.000	1	
0.72938666E+01	0.11401899E-01	-0.45696443E-05	0.79430967E-09	-0.44163078E-13	2				
0.83094941E+04-0.11019943E+02	0.23135836E+01	0.28253129E-01	-0.25737754E-04	3					
0.12222654E-07-0.21353429E-11	0.95213496E+04	0.14105129E+02		4					
CH3CHOCH2	T 6/92C	3H	60	1	OG	298.150	3000.0	1000.0	1
0.86900558E 01	0.16020987E-01	-0.53971753E-05	0.79941542E-09	-0.42656366E-13	2				
-0.15420691E 05-0.22485016E 02	0.48733836E 00	0.28519690E-01	0.30096162E-05	3					
-0.22652642E-07	0.10706728E-10	-0.12556434E 05	0.22605270E 02	-0.11156446E 05	4				
CH3CH2CHO	USC/07C	3H	60	1	OG	300.000	5000.000	1	
0.62637410E+01	0.19976260E-01	-0.76195147E-05	0.11687118E-08	-0.41959993E-13	2				
-0.25885953E+05-0.57786498E+01	0.27255676E+01	0.23236005E-01	0.29740656E-05	3					
-0.16613415E-07	0.74250103E-11	-0.24556711E+05	0.14166277E+02	4					
CH3COCH3	T 5/92C	3H	60	1	OG	200.000	6000.000	1000.0	1
0.72975991E+01	0.17566207E-01	-0.63170456E-05	0.10203086E-08	-0.61094016E-13	2				
-0.29817680E+05-0.12756981E+02	0.55557943E+01	-0.28365428E-02	0.70568945E-04	3					
-0.87810488E-07	0.34028266E-10	-0.28113337E+05	0.23226600E+01	-0.26116945E+05	4				
C2H3CHO	USC/07C	3H	40	1	OG	300.000	5000.000	1	
0.58111868E+01	0.17114256E-01	-0.74834161E-05	0.14252249E-08	-0.91746841E-13	2				
-0.10784054E+05-0.48588004E+01	0.12713498E+01	0.26231054E-01	-0.92912305E-05	3					
-0.47837272E-08	0.33480543E-11	-0.93357344E+04	0.19498077E+02	4					
ac3H5	PD5/98C	3H	5	0	OG	300.000	3000.000	1	
0.65007877E+01	0.14324731E-01	-0.56781632E-05	0.11080801E-08	-0.90363887E-13	2				
0.17482449E+05-0.11243050E+02	0.13631835E+01	0.19813821E-01	0.12497060E-04	3					
-0.33355555E-07	0.15846571E-10	0.19245629E+05	0.17173214E+02	4					
CH3CCH2	PD5/98C	3H	5	0	OG	300.000	3000.000	1	
0.54255528E+01	0.15511072E-01	-0.56678350E-05	0.79224388E-09	-0.16878034E-13	2				
0.27843027E+05-0.33527184E+01	0.17329209E+01	0.22394620E-01	-0.51490611E-05	3					
-0.67596466E-08	0.38253211E-11	0.29040498E+05	0.16568878E+02	4					
CH3CHCH	PD5/98C	3H	5	0	OG	300.000	3000.000	1	
0.53725281E+01	0.15780509E-01	-0.59922850E-05	0.93089664E-09	-0.36550966E-13	2				
0.29614760E+05-0.34186478E+01	0.91372931E+00	0.26432343E-01	-0.11758950E-04	3					
-0.23035678E-08	0.27715488E-11	0.30916867E+05	0.19989269E+02	4					
C4H	P 1/93C	4H	1	0	OG	300.000	3000.000	1	
0.77697593E+01	0.49829976E-02	-0.17628546E-05	0.28144284E-09	-0.16689869E-13	2				
0.94345900E+05-0.14165274E+02	0.13186295E+01	0.38582956E-01	-0.71385623E-04	3					
0.65356359E-07-0.22617666E-10	0.95456106E+05	0.15567583E+02		4					
C4H2	D11/99C	4H	2	0	OG	300.000	3000.000	1	
0.91576328E+01	0.55430518E-02	-0.13591604E-05	0.18780075E-10	0.23189536E-13	2				
0.52588039E+05-0.23711460E+02	0.10543978E+01	0.41626960E-01	-0.65871784E-04	3					
0.53257075E-07-0.16683162E-10	0.54185211E+05	0.14866591E+02		4					
nc4H3	USC/07C	4H	30	0	OG	300.000	5000.000	1	
0.78045716E+01	0.10712364E-01	-0.41939124E-05	0.70446277E-09	-0.36271326E-13	2				
0.62987805E+05-0.14129741E+02	0.81667686E+00	0.38716201E-01	-0.48045651E-04	3					
0.32066808E-07-0.85628215E-11	0.64455754E+05	0.19740503E+02		4					
ic4H3	USC/07C	4H	30	0	OG	300.000	5000.000	1	
0.76538548E+01	0.11204055E-01	-0.46401342E-05	0.86786639E-09	-0.57430562E-13	2				
0.57954363E+05-0.11756476E+02	0.37221482E+01	0.25957543E-01	-0.26356343E-04	3					
0.15508920E-07-0.38040565E-11	0.58837121E+05	0.75637245E+01		4					
H2C4O	USC/07C	4H	20	1	OG	300.000	5000.000	1	
0.84292183E+01	0.10502701E-01	-0.42066836E-05	0.71184902E-09	-0.35796602E-13	2				
0.22907807E+05-0.16511997E+02	0.31811900E+01	0.29840752E-01	-0.32832409E-04	3					
0.20631813E-07-0.54200598E-11	0.24125576E+05	0.94210100E+01		4					

C4H4 USC/07C 4H 4O 0 OG 300.000 5000.000 1  
0.72539601E+01 0.13914094E-01-0.52932214E-05 0.83480450E-09-0.35197882E-13 2  
0.31766016E+05-0.12629521E+02 0.58857048E+00 0.36546685E-01-0.34106968E-04 3  
0.16652619E-07-0.30064623E-11 0.33359492E+05 0.20657881E+02 4  
nC4H5 USC/07C 4H 5O 0 OG 300.000 5000.000 1  
0.74087291E+01 0.17752748E-01-0.75601506E-05 0.14203795E-08-0.91100182E-13 2  
0.40438762E+05-0.13150027E+02 0.22611290E+00 0.36742371E-01-0.22120474E-04 3  
0.14390138E-08 0.26435809E-11 0.42428410E+05 0.24066401E+02 4  
iC4H5 USC/07C 4H 5O 0 OG 300.000 5000.000 1  
0.69646029E+01 0.18274333E-01-0.78133735E-05 0.15292154E-08-0.10920493E-12 2  
0.34725098E+05-0.10649321E+02 0.11308105E+00 0.40950615E-01-0.35413581E-04 3  
0.15530969E-07-0.23355122E-11 0.36383371E+05 0.23692457E+02 4  
C4H5-2 H6W/94C 4H 5 0 OG 300.000 3000.000 1  
1.45381710E+01-8.56770560E-03 2.35595240E-05-1.36763790E-08 2.44369270E-12 2  
3.32590950E+04-4.53694970E+01 2.96962800E+00 2.44422450E-02-9.12514240E-06 3  
-4.24668710E-18 1.63047280E-21 3.55033160E+04 1.20360510E+01 3.73930550E+04 4  
c-C4H5 PUPM3 C 4H 5 0 OG 300.000 3000.000 1  
0.67467155E+01 0.17283000E-01-0.65168579E-05 0.98917574E-09-0.34604908E-13 2  
0.32808359E+05-0.12912880E+02-0.26397593E+01 0.41549157E-01-0.21920954E-04 3  
-0.46959014E-08 0.61348890E-11 0.35373828E+05 0.35701797E+02 4  
C4H7 USC/07C 4H 7O 0 OG 300.000 5000.000 1  
0.70134835E+01 0.22634558E-01-0.92545470E-05 0.16807927E-08-0.10408617E-12 2  
0.20955008E+05-0.88893080E+01 0.74449432E+00 0.39678857E-01-0.22898086E-04 3  
0.21352973E-08 0.23096375E-11 0.22653328E+05 0.23437878E+02 4  
C4H6 H6W/94C 4H 6 0 OG 300.000 3000.000 1  
0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-12 2  
0.91338516E+04-0.23328171E+02 0.11284465E+00 0.34369022E-01-0.11107392E-04 3  
-0.92106660E-08 0.62065179E-11 0.11802270E+05 0.23089996E+02 4  
C4H612 A 8/83C 4H 6 0 OG 300. 3000. 1000.0 1  
0.1781557E 02 -0.4257502E-02 0.1051185E-04 -0.4473844E-08 0.5848138E-12 2  
0.1267342E 05 -0.6982662E 02 0.1023467E 01 0.3495919E-01 -0.2200905E-04 3  
0.6942272E-08 -0.7879187E-12 0.1811799E 05 0.1975066E 02 0.1950807E+05 4  
C4H6-2 A 8/83C 4H 6 0 OG 300. 3000. 1000.0 1  
9.0338133E+00 8.2124510E-03 7.1753952E-06 -5.8834334E-09 1.0343915E-12 2  
1.4335068E+04 -2.0985762E+01 2.1373338E+00 2.6486229E-02 -9.0568711E-06 3  
-5.5386397E-19 2.1281884E-22 1.5710902E+04 1.3529426E+01 1.7488676E+04 4  
C4H10 P11/94C 4H 10 0 OG 300.000 3000.000 1  
0.10526774E+02 0.23590738E-01-0.78522480E-05 0.11448408E-08-0.59827703E-13 2  
-0.20479223E+05-0.32198579E+02 0.15685419E+01 0.34652278E-01 0.68168129E-05 3  
-0.27995097E-07 0.12307742E-10-0.17129977E+05 0.17908045E+02 4  
iC4H10 P11/94C 4H 10 0 OG 300.000 3000.000 1  
0.10846169E+02 0.23338389E-01-0.77833962E-05 0.11393807E-08-0.59918289E-13 2  
-0.21669854E+05-0.35870573E+02 0.54109489E+00 0.37860301E-01 0.55459804E-05 3  
-0.30500110E-07 0.14033357E-10-0.17977644E+05 0.21150935E+02 4  
pC4H9 USC/07C 4H 9O 0 OG 300.000 5000.000 1  
0.86822395E+01 0.23691071E-01-0.75948865E-05 0.66427136E-09 0.54845136E-13 2  
0.49644058E+04-0.17891747E+02 0.12087042E+01 0.38297497E-01-0.72660509E-05 3  
-0.15428547E-07 0.86859435E-11 0.73221040E+04 0.22169268E+02 4  
sc4H9 P11/94C 4H 9 0 OG 300.000 3000.000 1  
0.94263839E+01 0.21918998E-01-0.72868375E-05 0.10630334E-08-0.55649464E-13 2  
0.31965874E+04-0.22406051E+02 0.69428423E+00 0.33113346E-01 0.62942577E-05 3  
-0.27025274E-07 0.11989315E-10 0.64175654E+04 0.26279789E+02 4  
tC4H9 P11/94C 4H 9 0 OG 300.000 3000.000 1  
0.76607261E+01 0.23879414E-01-0.80890353E-05 0.12057521E-08-0.65009814E-13 2  
0.16207623E+04-0.14800281E+02 0.96167553E+00 0.25735856E-01 0.15609033E-04 3  
-0.26656519E-07 0.89418010E-11 0.46564412E+04 0.24805366E+02 4  
iC4H9 USC/07C 4H 9O 0 OG 300.000 5000.000 1  
0.84981728E+01 0.24689538E-01-0.86487589E-05 0.10779325E-08-0.64340570E-15 2  
0.44288174E+04-0.18441397E+02 0.97527862E+00 0.41613799E-01-0.14467331E-04 3  
-0.93852393E-08 0.68797377E-11 0.66688267E+04 0.21277582E+02 4  
C4H81 T 6/83C 4H 8 0 OG 300.000 5000.000 1  
0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12 2  
-0.21397231E+04 0.15543201E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05 3  
-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21062469E+02 4  
C4H82 T 6/83C 4H 8 0 OG 300.000 5000.00 1  
0.82797676E+00 0.35864539E-01-0.16634498E-04 0.34732759E-08-0.26657398E-12 2

-0.30521033E+04 0.21342545E+02 0.12594252E+01 0.27808424E-01 0.87013932E-05 3  
-0.24402205E-07 0.98977710E-11-0.29647742E+04 0.20501129E+02 4  
iC4H8 T 6/83H 8C 4 0 OG 300.000 5000.0 1  
0.44609470E+01 0.29611487E-01-0.13077129E-04 0.26571934E-08-0.20134713E-12 2  
-0.50066758E+04 0.10671549E+01 0.26471405E+01 0.25902957E-01 0.81985354E-05 3  
-0.22193259E-07 0.88958580E-11-0.40373069E+04 0.12676388E+02 4  
iC4H7 USC/07C 4H 7O 0 OG 300.000 5000.000 1  
0.71485939E+01 0.22189671E-01-0.84400172E-05 0.13133353E-08-0.51617927E-13 2  
0.12712294E+05-0.12131183E+02-0.10375890E+01 0.45566667E-01-0.30476231E-04 3  
0.71102568E-08 0.99685722E-12 0.14896458E+05 0.29863663E+02 4  
C2H3CHOCH2 A 8/83C 4H 6O 1 OG 300. 3000. 1000.0 1  
-4.72093360E+00 3.91413780E-02-6.52872650E-06-7.68209500E-09 2.51473310E-12 2  
1.75352252E+03 5.17190420E+01 7.97985440E-01 3.44034320E-02-1.24598510E-05 3  
-5.18062790E-18 1.99359540E-21-6.48927540E+02 2.18896980E+01 1.00654250E+03 4  
CH3CHCHCHO T 5/92C 4H 6O 1 OG 298.150 3000.0 1000.0 1  
0.78794540E+01-2.09130550E-02 4.45360508E-05-2.60374870E-08 4.86836120E-12 2  
-1.95278768E+04-6.87200320E+01-1.55577660E+00 4.09640630E-02-1.69868810E-05 3  
-6.00928140E-18 2.31368530E-21-1.41394920E+04 3.74707580E+01-1.29340710E+04 4  
CH2CHCOCH3 T 3/97C 4H 6O 1 OG 200.000 3000.0 1000.0 1  
1.98794540E+01-2.09130550E-02 4.45360508E-05-2.60374870E-08 4.86836120E-12 2  
-1.90786168E+04-6.97265750E+01-1.55577660E+00 4.09640630E-02-1.69868810E-05 3  
-6.00928140E-18 2.31368530E-21-1.49447258E+04 3.64642160E+01-1.66079520E+04 4  
C4H4O T03/97C 4H 4O 1 OG 200.000 6000.0 1000.0 1  
9.38935003E+00 1.40291241E-02-5.07755110E-06 8.24137332E-10-4.95319963E-14 2  
-8.68241814E+03-2.79162920E+01 8.47469463E-01 1.31773796E-02 5.99735901E-05 3  
-9.71562904E-08 4.22733796E-11-5.36785445E+03 2.14945172E+01-4.17166616E+03 4  
CH3CHCHCO USC/07C 4H 5O 1 OG 300.000 5000.000 1  
0.77608204E+01 0.20031804E-01-0.80631016E-05 0.13361392E-08-0.62308408E-13 2  
0.45708291E+04-0.11095638E+02 0.53053460E+01 0.15749373E-01 0.21623913E-04 3  
-0.36607769E-07 0.14932489E-10 0.57588633E+04 0.42043533E+01 4  
CH2CHCHCHO USC/07C 4H 5O 1 OG 300.000 5000.000 1  
0.83010607E+01 0.19945331E-01-0.82903771E-05 0.15100753E-08-0.91581155E-13 2  
0.15788387E+03-0.16910566E+02 0.12108673E+01 0.35205878E-01-0.10939090E-04 3  
-0.11720642E-07 0.76174908E-11 0.22665703E+04 0.20613544E+02 4  
CH2CHCH2CHO T 5/92C 4H 6O 1 OG 298.150 3000.0 1000.0 1  
1.98794540E+01-2.09130550E-02 4.45360508E-05-2.60374870E-08 4.86836120E-12 2  
-1.58539966E+04-6.71095639E+01-1.55577660E+00 4.09640630E-02-1.69868810E-05 3  
-6.00928140E-18 2.31368530E-21-1.04656118E+04 3.90812260E+01-1.29340710E+04 4  
C4H6O25 T 3/97C 4H 6O 1 OG 200.000 5000.000 1000.0 1  
8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-13 2  
-1.76177415E+04-2.32464750E+01 2.67053463E+00 4.92586420E-03 8.86967406E-05 3  
-1.26219194E-07 5.23991321E-11-1.46572472E+04 1.45722395E+01-1.30831522E+04 4  
C4H6O23 T 3/97C 4H 6O 1 OG 200.000 5000.000 1000.0 1  
8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-13 2  
-1.32392815E+04-2.32464750E+01 2.67053463E+00 4.92586420E-03 8.86967406E-05 3  
-1.26219194E-07 5.23991321E-11-1.02787872E+04 1.45722395E+01-1.30831522E+04 4  
sC4H9 T07/95C 4H 9 0 OG 200.000 6000.000 1000.0 1  
0.88057265E+01 0.23630381E-01-0.84564737E-05 0.13612584E-08-0.81313232E-13 2  
0.37941169E+04-0.19996770E+02 0.46457042E+01 0.79313214E-02 0.70027013E-04 3  
-0.95973349E-07 0.38628890E-10 0.62341181E+04 0.79642808E+01 0.84190169E+04 4  
C5H2 20587C 5H 2 G 0300.00 5000.00 1000.00 1  
0.01132917E+03 0.07424057E-01-0.02628189E-04 0.04082541E-08-0.02301333E-12 2  
0.07878706E+06-0.03617117E+03 0.03062322E+02 0.02709998E+00-0.01009170E-03 3  
-0.01272745E-06 0.09167219E-10 0.08114969E+06 0.07071078E+02 4  
C5H3 20387C 5H 3 G 0300.00 5000.00 1000.00 1  
0.01078762E+03 0.09539619E-01-0.03206745E-04 0.04733323E-08-0.02512135E-12 2  
0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-04 3  
-0.01215449E-06 0.07726478E-10 0.06588531E+06 0.04173259E+02 4  
C5H6 T 1/90C 5H 6 0 OG 200.000 6000.000 1  
0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-13 2  
0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-04 3  
-0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02 0.16152485E+05 4  
C5H5"OLD" D10/01C 5H 5 0 OG 300.000 3000.000 1  
-0.18328686E+01 0.41817095E-01-0.26248981E-04 0.80593523E-08-0.98131702E-12 2  
0.30725047E+05 0.32755760E+02-0.14847748E+02 0.14919417E+00-0.29516959E-03 3  
0.27862689E-06-0.96990506E-10 0.31251482E+05 0.83555710E+02 4

C5H5	T12/89C	5H	5	0	OG	300.00	2000.000	1000.00	1
									2
									3
									4
cC5H8	T03/97C	5H	80	0	OG	200.000	6000.000	1000.0	1
									2
									3
									4
lC5H9	T03/97C	5H	90	0	OG	200.000	6000.000	1000.0	1
									2
									3
									4
cC5H9	T03/97C	5H	90	0	OG	200.000	6000.000	1000.0	1
									2
									3
									4
C5H40	T 8/99C	5H	40	1	OG	200.000	6000.000		1
									2
									3
									4
C5H40H	T 8/99C	5H	50	1	OG	200.000	6000.000		1
									2
									3
									4
C5H50(2,4)	D 9/97C	5H	50	1	OG	300.000	3000.000		1
									2
									3
									4
C5H50(1,3)	DU0997C	5H	50	1	OG	300.000	3000.000	1000.00	1
									2
									3
									4
C5H50H	HWZD99C	5H	60	1	OG	300.000	3000.000		1
									2
									3
									4
bi-C5H40	DU0997C	5H	40	1	OG	300.000	3000.000	1000.00	1
									2
									3
									4
lC5H6	HWZD99C	5H	6	0	OG	300.	3000.	1000.	1
									2
									3
									4
lC5H7	HWZD99C	5H	7	0	OG	300.000	3000.000		1
									2
									3
									4
C6H2	D11/99C	6H	2	0	OG	300.000	3000.000		1
									2
									3
									4
C6H	P 1/93C	6H	1	0	OG	300.000	3000.000		1
									2
									3
									4
l-C6H4	H6W/94C	6H	4	0	OG	300.000	3000.000		1
									2
									3
									4
l-C6H6	H6W/94C	6H	6	0	OG	300.000	3000.000		1
									2
									3
									4
c-C6H7	H6W/94C	6H	7	0	OG	300.000	3000.000		1
									2



0.16730059E+05-0.83746933E+02-0.30328493E+01	0.50804518E-01-0.69150292E-05	3			
-0.29715974E-07	0.16296353E-10	4			
0.23895383E+05	0.38909180E+02	4			
n-C6H7	H6W/94C 6H 7 0 OG	300.000 3000.000	1		
0.22577469E+02-0.30737517E-02	0.14225234E-04-0.69880848E-08	0.10232874E-11	2		
0.41228980E+05-0.91568619E+02	0.13248032E+00	0.57103366E-01-0.43712644E-04	3		
0.15538603E-07-0.12976356E-11	0.47730512E+05	0.25339081E+02	4		
C6H8	H6W/94C 6H 8 0 OG	300.000 3000.000	1		
0.28481979E+02-0.15702948E-01	0.26771697E-04-0.11780109E-07	0.16573427E-11	2		
0.93346445E+04-0.12500226E+03	0.15850439E+01	0.40215142E-01	0.78439543E-05	3	
-0.38761325E-07	0.18545207E-10	0.17949613E+05	0.19112625E+02	4	
cc6H8	T03/97C 6H 80 0 OG	200.000 6000.000	1000.0	1	
0.11779870E+02	0.25519980E-01-0.92666947E-05	0.15068122E-08-0.90658701E-13	2		
0.65486686E+04-0.41618805E+02	0.17265319E+01	0.14887612E-01	0.94809230E-04	3	
-0.14083394E-06	0.58859873E-10	0.11021297E+05	0.19130886E+02	0.12784878E+05	4
lc6H9	T 2/92C 6H 90 0 OG	200.000 3000.000	1000.0	1	
0.23165919E+02	0.10813608E-01-0.17638168E-05	0.00000000E+00	0.00000000E+00	2	
0.11162402E+05-0.98600332E+02	0.31671271E+00	0.52069818E-01-0.21965057E-04	3		
0.00000000E+00	0.00000000E+00	0.19926824E+05	0.27879902E+02	0.22141533E+05	4
cc6H9	T 2/92C 6H 90 0 OG	200.000 3000.000	1000.0	1	
0.26295828E+02	0.86828857E-02-0.15770376E-05	0.00000000E+00	0.00000000E+00	2	
0.20863563E+04-0.12573825E+03-0.35714300E+01	0.61696043E-01-0.26928803E-04	3			
0.00000000E+00	0.00000000E+00	0.13657039E+05	0.39986250E+02	0.15096500E+05	4
cc6H10	T03/97C 6H 100 0 OG	200.000 6000.000	1000.0	1	
0.11773904E+02	0.30947360E-01-0.11234330E-04	0.18262494E-08-0.10985119E-12	2		
-0.72028376E+04-0.42658688E+02	0.23662378E+01	0.10681712E-01	0.11822112E-03	3	
-0.16567854E-06	0.67612802E-10-0.24824973E+04	0.16769357E+02-0.55324968E+03	4		
C6H3	H6W/94C 6H 3 0 OG	300.000 3000.000	1		
0.58188343E+01	0.27933408E-01-0.17825427E-04	0.53702536E-08-0.61707627E-12	2		
0.85188250E+05-0.92147827E+00	0.11790619E+01	0.55547360E-01-0.73076168E-04	3		
0.52076736E-07-0.15046964E-10	0.85647312E+05	0.19179199E+02	4		
i-C6H5	H6W/94C 6H 5 0 OG	300.000 3000.000	1		
0.22501663E+02-0.81009977E-02	0.15955695E-04-0.72310371E-08	0.10310424E-11	2		
0.58473410E+05-0.91224777E+02-0.78585434E+00	0.60221825E-01-0.62890264E-04	3			
0.36310730E-07-0.87000259E-11	0.64942270E+05	0.28658905E+02	4		
i-C6H7	H6W/94C 6H 7 0 OG	300.000 3000.000	1		
0.20481506E+02	0.79439697E-03	0.11450761E-04-0.60991177E-08	0.91756724E-12	2	
0.37728426E+05-0.81812073E+02-0.17099094E+01	0.62486034E-01-0.54290707E-04	3			
0.26959682E-07-0.58999090E-11	0.44086621E+05	0.33344772E+02	4		
o-C6H4	D11/99C 6H 4 0 OG	300.000 3000.000	1		
0.88432961E+01	0.20301474E-01-0.88674269E-05	0.17264292E-08-0.11786047E-12	2		
0.49317113E+05-0.24014301E+02-0.38454189E+01	0.58391564E-01-0.48644750E-04	3			
0.16770320E-07-0.78580680E-12	0.52592500E+05	0.40587132E+02	4		
m-C6H4	D11/99C 6H 4 0 OG	300.000 3000.000	1		
0.95307283E+01	0.19178549E-01-0.80941481E-05	0.14811132E-08-0.88632260E-13	2		
0.5686535E+05-0.27623203E+02-0.39450364E+01	0.59887171E-01-0.50811577E-04	3			
0.17603140E-07-0.72608743E-12	0.60323117E+05	0.40899506E+02	4		
p-C6H4	D11/99C 6H 4 0 OG	300.000 3000.000	1		
0.98300371E+01	0.18499156E-01-0.75165058E-05	0.12727610E-08-0.61767120E-13	2		
0.64446117E+05-0.29418266E+02-0.39744728E+01	0.58399867E-01-0.44950713E-04	3			
0.10307744E-07	0.22412619E-11	0.68058992E+05	0.41168865E+02	4	
l-C6H4Z	D11/99C 6H 4 0 OG	300.000 3000.000	1		
0.11186811E+02	0.17122138E-01-0.73898623E-05	0.14678845E-08-0.10733922E-12	2		
0.60743207E+05-0.29537384E+02	0.20895090E+01	0.53276263E-01-0.63299172E-04	3		
0.40811642E-07-0.10598600E-10	0.62662203E+05	0.14613283E+02	4		
nC6H5	D11/99C 6H 5 0 OG	300.000 3000.000	1		
0.11263281E+02	0.19379666E-01-0.76874276E-05	0.12866819E-08-0.63244650E-13	2		
0.68052773E+05-0.30487534E+02-0.27013230E+00	0.59389681E-01-0.60963321E-04	3			
0.33169378E-07-0.71466453E-11	0.70785828E+05	0.26953651E+02	4		
C6H5	D11/99C 6H 5 0 OG	300.000 3000.000	1		
0.85973110E+01	0.22241630E-01-0.87199978E-05	0.13788785E-08-0.53146056E-13	2		
0.36261047E+05-0.22954643E+02-0.36931453E+01	0.52178968E-01-0.25558427E-04	3			
-0.70661121E-08	0.75833975E-11	0.39779590E+05	0.41332535E+02	4	
C6H6	D11/99C 6H 6 0 OG	300.000 3000.000	1		
0.91381245E+01	0.23854433E-01-0.88127726E-05	0.12099021E-08-0.18221503E-13	2		
0.52043462E+04-0.29115665E+02-0.48437734E+01	0.58427613E-01-0.29485855E-04	3			
-0.69390440E-08	0.82125253E-11	0.91817773E+04	0.43889832E+02	4	

C5H5CH3 P 1/93C 6H 8 0 OG 300.000 2500.000 1  
0.14628364E+02 0.19849248E-01-0.50529134E-05 0.10556275E-10 0.11381723E-12 2  
0.55674092E+04-0.56114021E+02-0.45763016E-01 0.29978730E-01 0.61898092E-04 3  
-0.11171783E-06 0.49435803E-10 0.10927480E+05 0.26558569E+02 4  
C5H4CH2 P 1/93C 6H 6 0 OG 300.000 2500.000 1  
0.75731055E+04-0.18843678E+02 0.17058320E-01-0.65980571E-05 0.93053393E-09 2  
-0.22894220E+07-0.40003195E+05 0.78428810E+02-0.43919629E+00 0.13370259E-02 3  
-0.14196110E-05 0.56357985E-09 0.22226365E+05-0.41005380E+03 4  
C6H5C6H5 HW /94C 12H 10 0 OG 300.000 3000.000 1  
0.50761871E+02-0.34501564E-01 0.50293413E-04-0.21559579E-07 0.30097192E-11 2  
0.21538867E+04-0.24670712E+03-0.10283234E+02 0.12428707E+00-0.95990268E-04 3  
0.32294793E-07-0.23045229E-11 0.20165258E+05 0.72707947E+02 4  
C6H5C2H H6W/94C 8H 6 0 OG 300.000 3000.000 1  
0.24090759E+02 0.78232400E-03 0.11453964E-04-0.61620504E-08 0.93346685E-12 2  
0.27429445E+05-0.10499631E+03-0.52645016E+01 0.84511042E-01-0.76597848E-04 3  
0.33216978E-07-0.47673063E-11 0.35566242E+05 0.46378815E+02 4  
C6H5CH3 L 6/87C 7H 8 0 OG 200.000 6000.000 1  
0.12940034E+02 0.26691287E-01-0.96838505E-05 0.15738629E-08-0.94663601E-13 2  
-0.69764908E+03-0.46728785E+02 0.16152663E+01 0.21099438E-01 0.85366018E-04 3  
-0.13261066E-06 0.55956604E-10 0.40756300E+04 0.20282210E+02 0.60135835E+04 4  
C6H5CH2 T08/90C 7H 7 0 OG 200.000 6000.000 1  
0.14043980E+02 0.23493873E-01-0.85375367E-05 0.13890841E-08-0.83614420E-13 2  
0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01 0.32861492E-04 3  
-0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02 0.25317186E+05 4  
C6H5C2H3 T12/94C 8H 8 0 OG 298.150 5000.000 1  
0.16139277E+02 0.24210847E-01-0.72678359E-05 0.11392276E-08-0.72984881E-13 2  
0.10249251E+05-0.61169437E+02-0.10717708E+02 0.12666725E+00-0.17762493E-03 3  
0.14344049E-06-0.47616577E-10 0.16597133E+05 0.71526331E+02 0.17723291E+05 4  
C6H5CH2OH L 7/87C 7H 80 1 OG 200.000 6000.000 1000.00 1  
0.15281154E+02 0.27208501E-01-0.98584660E-05 0.16012183E-08-0.96278057E-13 2  
-0.19700471E+05-0.59418673E+02 0.20642021E+01 0.22775140E-01 0.95972053E-04 3  
-0.15085110E-06 0.64175832E-10-0.14285021E+05 0.18148312E+02-0.12077200E+05 4  
C6H5CHO L 3/86C 7H 60 1 OG 298.150 5000.000 1000.00 1  
0.13650737E+02 0.25680419E-01-0.10466729E-04 0.19413430E-08-0.13483792E-12 2  
-0.11019744E+05-0.47965796E+02-0.31627334E+01 0.66369245E-01-0.34816353E-04 3  
-0.62999377E-08 0.85807101E-11-0.61169349E+04 0.40231735E+02-0.44259974E+04 4  
C6H5CO EST/BUR P 1/93C 7H 50 1 OG 300.000 2500.000 1  
0.13374409E+02 0.23999289E-01-0.10465724E-04 0.21669131E-08-0.18007045E-12 2  
0.69147837E+04-0.44659218E+02-0.20251155E+01 0.61512541E-01-0.31603653E-04 3  
-0.69724599E-08 0.79835149E-11 0.11255803E+05 0.35778175E+02 4  
C6H4O2 PURL96C 6H 40 2 OG 300.000 5000.000 1000.000 1  
0.11730840E+02 0.23614995E-01-0.10234576E-04 0.19532174E-08-0.12746022E-12 2  
-0.21085770E+05-0.36300453E+02-0.95193005E+00 0.57842445E-01-0.38214439E-04 3  
0.46312656E-08 0.36296651E-11-0.17611047E+05 0.29239513E+02 4  
C6H5O T05/02C 6H 50 1 OG 200.000 6000.000 1000.000 1  
1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-14 2  
2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-05 3  
-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01 6.49467016E+03 4  
C6H5OH L 4/84C 6H 60 1 OG 300.000 5000.000 1  
0.14912073E 02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-13 2  
-0.18375199E 05-0.55924103E 02-0.16956539E 01 0.52271299E-01-0.72024050E-05 3  
-0.35859603E-07 0.20449073E-10-0.13284121E 05 0.32542160E 02-0.11594207E 05 4  
C6H5C2H5 A 6/83C 8H 10 0 OG 300. 3000. 1000.00 1  
0.3878978E 01 0.5810059E-01 -0.3196380E-04 0.8448993E-08 -0.8694825E-12 2  
-0.5024922E 03 0.3837099E 01 -0.7266845E 01 0.1003089E 00 -0.9651715E-04 3  
0.5565908E-07 -0.1453370E-10 0.1987290E 04 0.5857746E 02 0.3529492E+04 4  
HOC6H4CH3 AVG CRESOL6/87C 7H 80 1 OG 200.000 6000.000 1000.00 1  
0.15932987E+02 0.27011160E-01-0.99448722E-05 0.16296689E-08-0.98513298E-13 2  
-0.23592065E+05-0.59732841E+02 0.42258267E+00 0.45551636E-01 0.32012513E-04 3  
-0.81121959E-07 0.37665658E-10-0.18202621E+05 0.26032903E+02-0.15911701E+05 4  
OC6H4CH3 EST/BUR P 1/93C 7H 70 1 OG 300.000 2500.000 1  
0.22609371E+02 0.75646150E-02 0.65960894E-05-0.47150865E-08 0.80409063E-12 2  
-0.82025244E+04-0.97292511E+02-0.28855777E+00 0.48003536E-01 0.18032993E-04 3  
-0.61741488E-07 0.28852587E-10-0.68945581E+03 0.26720068E+02 4  
bi-C6H5CH2 A 6/83C 14H 14 0 OG 300. 3000. 1000.00 1  
0.7292035E 01 0.9250200E-01 -0.5168641E-04 0.1362709E-07 -0.1381148E-11 2

```

0.1031673E 05 -0.1132738E 02 -0.1388958E 02 0.1720984E 00 -0.1700660E-03 3
0.9601888E-07 -0.2373253E-10 0.1503234E 05 0.9270736E 02 0.1721641E+05 4
C10H8 H6W/94C 10H 8 0 0G 300.000 3000.000 1
0.36468643E+02-0.15419513E-01 0.30160038E-04-0.13700120E-07 0.19582730E-11 2
0.35091445E+04-0.17329489E+03-0.94505043E+01 0.11137849E+00-0.10345667E-03 3
0.52800392E-07-0.11804439E-10 0.16695594E+05 0.65187668E+02 4
C6H4CH3 P 1/93C 7H 7 0 0G 300.000 2500.000 1
0.11615498E+02 0.27431838E-01-0.10899345E-04 0.18641830E-08-0.10191607E-12 2
0.31209334E+05-0.38994637E+02-0.31415942E+01 0.56723077E-01-0.86885111E-05 3
-0.34249616E-07 0.19266902E-10 0.35738547E+05 0.39742840E+02 4
C2H5OH L 8/88C 2H 60 1 0G 200.000 6000.000 1000. 1
0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4
CH3CHOH T 4/83C 2O 1H 5 0G 300.000 5000. 1000. 1
0.7665424E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-13 2
-0.56092969E+04-0.93980442E+01 0.24813328E+01 0.16790036E-01 0.37755499E-05 3
-0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02-0.25172860E+04 4
C2H4OH T 4/83H 5C 2O 1 0G 300.000 5000. 1000. 1
0.759444014E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-13 2
-0.57727852E+04-0.13955572E+02 0.14019508E+01 0.21543175E-01-0.22326512E-05 3
-0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19148981E+02-0.25154820E+04 4
CH3CH2O T11/82O 1C 2H 5 0G 300.000 5000.0 1000. 1
0.60114346E+01 0.12165219E-01-0.40449604E-05 0.59076588E-09-0.30969595E-13 2
-0.49366992E+04-0.67901798E+01 0.17302504E+01 0.16908489E-01 0.39996221E-05 3
-0.13711180E-07 0.57643603E-11-0.32922483E+04 0.17336115E+02-0.20138288E+04 4
HOC2H4O2 C 2H 5O 3 0G 300.000 5000.000 1391.000 01
1.00941573E+01 1.23879015E-02-3.73811683E-06 5.46874551E-10-3.09943951E-14 2
-2.37710522E+04-2.00956526E+01 4.44209543E+00 2.52880383E-02-1.51605275E-05 3
5.24921198E-09-7.91470852E-13-2.17507126E+04 1.04122371E+01 4
!*****
!*** Hydrogen/Oxygen/Fluorine ***
!*****
F 71STUPRO F 1 0 0 0G 300.00 3000.00 1400.00 1
0.26511661E+01-0.14012971E-03 0.51923643E-07-0.88495445E-11 0.59028014E-15 2
0.87582901E+04 0.40785743E+01 0.29037076E+01-0.63529632E-03 0.26473487E-06 3
0.76906306E-10-0.54525355E-13 0.86722692E+04 0.27082800E+01 4
HF 71STUPRO H 1F 1 0 0G 300.00 3000.00 1250.00 1
0.27812981E+01 0.10395908E-02-0.24173550E-06 0.26841590E-10-0.10976637E-14 2
-0.33504174E+05 0.50197012E+01 0.34365739E+01 0.48602072E-03-0.12523971E-05 3
0.13647500E-08-0.40957404E-12-0.33800089E+05 0.12068184E+01 4
F2 71STUPRO F 2 0 0 0G 300.00 3000.00 1150.00 1
0.40577420E+01 0.60003376E-03-0.21921787E-06 0.43150757E-10-0.31258842E-14 2
-0.13243860E+04 0.86321366E+00 0.26695504E+01 0.52941846E-02-0.64709095E-05 3
0.39183347E-08-0.93845135E-12-0.98080128E+03 0.78265913E+01 4
HOF 71STU/H 1O 1F 1 0G 300.00 3000.00 1360.00 1
0.26247602E+01 0.49878675E-02-0.26043122E-05 0.66588051E-09-0.66785970E-13 2
-0.16464887E+05 0.11045392E+02 0.32404377E+01 0.33052621E-02-0.97045369E-07 3
-0.12711684E-08 0.49087999E-12-0.16710688E+05 0.77199944E+01 4
F2O 71STU/F 2O 1 0 0G 300.00 3000.00 1245.00 1
0.60502237E+01 0.11801203E-02-0.62998049E-06 0.16265308E-09-0.16630594E-13 2
0.86796609E+03-0.55559173E+01 0.23117985E+01 0.14403418E-01-0.18975198E-04 3
0.11788725E-07-0.28156285E-11 0.17661785E+04 0.13044809E+02 4
FO 71STU/F 1O 1 0 0G 300.00 3000.00 1440.00 1
0.35749648E+01 0.14752427E-02-0.87370400E-06 0.25045480E-09-0.27149179E-13 2
0.11918373E+05 0.51764106E+01 0.27886566E+01 0.39705102E-02-0.37470082E-05 3
0.16844357E-08-0.29009936E-12 0.12107603E+05 0.91359916E+01 4
FO2 71STU/F 1O 2 0 0G 300.00 3000.00 1360.00 1
0.56242097E+01 0.17066411E-02-0.89995239E-06 0.22561211E-09-0.22048285E-13 2
-0.40013089E+03-0.17257001E+01 0.36727894E+01 0.76317941E-02-0.79426701E-05 3
0.40752038E-08-0.83001063E-12 0.13887520E+03 0.82723509E+01 4
!*****
!*** Cl Fluorocarbons ***
!*****
CH3F 78KOL74CHEROD C 1H 3F 1 0G 300.00 3000.00 1100.00 1
0.26440009E+01 0.99725077E-02-0.39849725E-05 0.72514762E-09-0.48843996E-13 2

```

```

-0.29427146E+05 0.84230576E+01 0.25962366E+01 0.36531694E-02 0.13103231E-04 3
-0.14532989E-07 0.44801427E-11-0.29006808E+05 0.10482267E+02 4
CH2F2 78KOL74CHEROD C 1H 2F 2 OG 300.00 3000.00 1100.00 1
0.45584984E+01 0.83197879E-02-0.33715698E-05 0.61879687E-09-0.41951543E-13 2
-0.56506221E+05 0.43663670E+00 0.17390054E+01 0.11937925E-01-0.26932091E-06 3
-0.55189353E-08 0.21813549E-11-0.55439684E+05 0.16234241E+02 4
CHF3 78KOL74CHEROD C 1H 1F 3 OG 300.00 3000.00 1300.00 1
0.75241689E+01 0.52300472E-02-0.20360032E-05 0.35729556E-09-0.23099727E-13 2
-0.87022508E+05-0.14611191E+02 0.68075829E+00 0.23985910E-01-0.21833598E-04 3
0.99802568E-08-0.18517901E-11-0.84989416E+05 0.21061742E+02 4
CF4 78KOL74CHEROD C 1F 4 0 OG 300.00 3000.00 1250.00 1
0.98083153E+01 0.32826930E-02-0.13404484E-05 0.24373829E-09-0.16286158E-13 2
-0.11602499E+06-0.27000237E+02 0.32957353E+00 0.33269603E-01-0.38826706E-04 3
0.22059347E-07-0.49483733E-11-0.11350361E+06 0.21201651E+02 4
CH2F 82MCMGOL96ZAC C 1H 2F 1 OG 300.00 3000.00 1300.00 1
0.40601301E+01 0.54664229E-02-0.21094939E-05 0.37445811E-09-0.24740006E-13 2
-0.55927678E+04 0.30137878E+01 0.21179745E+01 0.10239270E-01-0.66208892E-05 3
0.23785703E-08-0.38933587E-12-0.49574186E+04 0.13339356E+02 4
CHF2 82MCMGOL96ZAC C 1H 1F 2 OG 300.00 3000.00 1150.00 1
0.54482814E+01 0.44116540E-02-0.17418858E-05 0.30919959E-09-0.20176188E-13 2
-0.31960950E+05-0.22945525E+01 0.18327633E+01 0.13416380E-01-0.95432838E-05 3
0.29592968E-08-0.27919992E-12-0.30857056E+05 0.16758883E+02 4
CF3 82MCMGOL71STU C 1F 3 0 OG 300.00 3000.00 1250.00 1
0.77316707E+01 0.22711464E-02-0.89049640E-06 0.15293834E-09-0.95083758E-14 2
-0.59145675E+05-0.14020193E+02 0.13572871E+01 0.21575805E-01-0.23901982E-04 3
0.12961109E-07-0.28017315E-11-0.57391273E+05 0.18647376E+02 4
CHF 84PRINIL71STU C 1H 1F 1 OG 300.00 3000.00 1300.00 1
0.44836570E+01 0.17496353E-02-0.50479025E-06 0.10895265E-09-0.98789823E-14 2
0.17958123E+05 0.28922230E+00 0.33448388E+01 0.23546052E-02 0.19398293E-05 3
-0.26525057E-08 0.79116937E-12 0.18514014E+05 0.70528597E+01 4
CF2 78ROD71STUPRO C 1F 2 0 OG 300.00 3000.00 1300.00 1
0.53312066E+01 0.19774838E-02-0.96024791E-06 0.21070369E-09-0.15953977E-13 2
-0.24371370E+05-0.25636718E+01 0.22859133E+01 0.10760786E-01-0.10538201E-04 3
0.48988138E-08-0.88638428E-12-0.23521183E+05 0.13134773E+02 4
CF 91GURVEY71STU C 1F 1 0 OG 300.00 3000.00 1100.00 1
0.36649678E+01 0.97368064E-03-0.41098236E-06 0.80062875E-10-0.56498068E-14 2
0.27724177E+05 0.42816350E+01 0.33538391E+01 0.20909703E-03 0.32077431E-05 3
-0.36687537E-08 0.11986311E-11 0.27907743E+05 0.63346309E+01 4
!*****
!*** Oxidized C1 Fluorocarbons ***
!*****
CHF:O 71STUPRO C 1H 1O 1F 1G 300.00 3000.00 1150.00 1
0.48192546E+01 0.50541823E-02-0.20142117E-05 0.36359085E-09-0.24472407E-13 2
-0.47263078E+05 0.97225119E-01 0.21184975E+01 0.10773988E-01-0.55158163E-05 3
0.58151932E-09 0.21704209E-12-0.46356705E+05 0.14652434E+02 4
CF2:O 71STUPRO C 1O 1F 2 OG 300.00 3000.00 1150.00 1
0.67913103E+01 0.33830542E-02-0.14301173E-05 0.27122572E-09-0.19052381E-13 2
-0.79453977E+05-0.94831193E+01 0.11761386E+01 0.21086988E-01-0.23921571E-04 3
0.13994913E-07-0.33760536E-11-0.77951303E+05 0.19113367E+02 4
CF:O 71STUPRO C 1O 1F 1 OG 300.00 3000.00 1250.00 1
0.51499637E+01 0.18493847E-02-0.74023187E-06 0.13278499E-09-0.88305997E-14 2
-0.22488372E+05-0.49683000E+00 0.29406080E+01 0.74709168E-02-0.62183316E-05 3
0.26291635E-08-0.47322188E-12-0.21792255E+05 0.11168908E+02 4
CF3O 82BATWAL96ZAC C 1O 1F 3 OG 300.00 3000.00 1250.00 1
0.98204084E+01 0.33891583E-02-0.14465389E-05 0.27696170E-09-0.19558034E-13 2
-0.82586582E+05-0.23197115E+02 0.13872398E+01 0.29895540E-01-0.34274496E-04 3
0.19180570E-07-0.42495935E-11-0.80336902E+05 0.19727594E+02 4
!*****
!*** Fluoroethanes ***
!*****
CH3-CH2F 75CHEROD C 2H 5F 1 OG 300.00 3000.00 1150.00 1
0.49574949E+01 0.16347645E-01-0.68027900E-05 0.12680240E-08-0.85810885E-13 2
-0.34339539E+05-0.21487264E+01 0.15235718E+00 0.28409823E-01-0.18754566E-04 3
0.73293263E-08-0.15029738E-11-0.32810924E+05 0.23294000E+02 4
CH2F-CH2F 95BURZAC96ZAC C 2H 4F 2 OG 300.00 3000.00 1150.00 1
0.84689627E+01 0.11513919E-01-0.36912381E-05 0.48219219E-09-0.20057166E-13 2

```

```

-0.56187065E+05-0.19218729E+02 0.95024582E+00 0.26764954E-01-0.13062727E-04 3
0.19592248E-08 0.52805697E-13-0.53549479E+05 0.21647110E+02 4
CH3-CHF2 75CHEROD C 2H 4F 2 OG 300.00 3000.00 1150.00 1
0.67084006E+01 0.15029444E-01-0.64189642E-05 0.12317783E-08-0.86169635E-13 2
-0.63428609E+05-0.97388704E+01 0.22571398E+00 0.34009513E-01-0.28684769E-04 3
0.13949828E-07-0.30824021E-11-0.61591943E+05 0.23706746E+02 4
CH2F-CHF2 68LACSKI96ZAC C 2H 3F 3 OG 300.00 3000.00 1100.00 1
0.92726485E+01 0.12040181E-01-0.48605999E-05 0.88656689E-09-0.59650602E-13 2
-0.83983519E+05-0.21387996E+02 0.64737590E+00 0.36292494E-01-0.31143200E-04 3
0.14464592E-07-0.30120967E-11-0.81526562E+05 0.23295333E+02 4
CH3-CF3 75CHEROD C 2H 3F 3 OG 300.00 3000.00 1150.00 1
0.95647119E+01 0.12054064E-01-0.51100096E-05 0.97284274E-09-0.67507209E-13 2
-0.93737598E+05-0.24901030E+02-0.21413884E+00 0.44477304E-01-0.48570862E-04 3
0.28726062E-07-0.70658104E-11-0.91218867E+05 0.24457644E+02 4
CHF2-CHF2 95BURZAC96ZAC C 2H 2F 4 OG 300.00 3000.00 1150.00 1
0.11513612E+02 0.98876231E-02-0.39914064E-05 0.72604359E-09-0.48678100E-13 2
-0.11030753E+06-0.31717002E+02 0.95286488E+00 0.41252814E-01-0.40681792E-04 3
0.21161088E-07-0.46600599E-11-0.10738264E+06 0.22558208E+02 4
CH2F-CF3 75CHEROD C 2H 2F 4 OG 300.00 3000.00 1150.00 1
0.11788997E+02 0.10127942E-01-0.43242826E-05 0.82543702E-09-0.57605133E-13 2
-0.11251398E+06-0.33875106E+02-0.21952401E+00 0.48986991E-01-0.53501350E-04 3
0.29784889E-07-0.67393540E-11-0.10944369E+06 0.26825948E+02 4
CHF2-CF3 75CHEROD C 2H 1F 5 OG 300.00 3000.00 1150.00 1
0.14058914E+02 0.79984131E-02-0.34820007E-05 0.67492657E-09-0.47789563E-13 2
-0.13834703E+06-0.44385372E+02 0.41067599E+00 0.52272371E-01-0.60122547E-04 3
0.34643557E-07-0.80647608E-11-0.13484115E+06 0.24624084E+02 4
CF3-CF3 75CHEROD C 2F 6 0 OG 300.00 3000.00 1150.00 1
0.17150062E+02 0.46114319E-02-0.19268956E-05 0.35553332E-09-0.23964360E-13 2
-0.16795100E+06-0.61723795E+02 0.14806601E+00 0.61793558E-01-0.78409584E-04 3
0.48371551E-07-0.11822352E-10-0.16368577E+06 0.23729541E+02 4
!*****
!*** Fluoroethyls ***
!*****
CH2F-CH2 90CHERAU C 2H 4F 1 OG 300.00 3000.00 1100.00 1
0.45367287E+01 0.14322536E-01-0.61958858E-05 0.12056208E-08-0.85530181E-13 2
-0.76283536E+04 0.31255507E+01 0.14016944E+01 0.22391057E-01-0.13868676E-04 3
0.45731402E-08-0.72649168E-12-0.66832515E+04 0.19587617E+02 4
CH3-CHF 95BURZAC90CHE C 2H 4F 1 OG 300.00 3000.00 1100.00 1
0.44008317E+01 0.14474236E-01-0.62438522E-05 0.12096797E-08-0.85419919E-13 2
-0.11355555E+05 0.31912492E+01 0.24004317E+01 0.17057379E-01-0.43206917E-05 3
0.26797414E-08 0.12865753E-11-0.10589455E+05 0.14418634E+02 4
CH2F-CHF 95BURZAC91CHE C 2H 3F 2 OG 300.00 3000.00 1250.00 1
0.87214510E+01 0.86815505E-02-0.35422910E-05 0.66313495E-09-0.44742292E-13 2
-0.32272851E+05-0.18251835E+02 0.22898344E+01 0.25577305E-01-0.19912795E-04 3
0.75880439E-08-0.11237829E-11-0.30343295E+05 0.15431326E+02 4
CHF2-CH2 90CHERAU C 2H 3F 2 OG 300.00 3000.00 1100.00 1
0.67982556E+01 0.12130852E-01-0.52871420E-05 0.10362364E-08-0.74087387E-13 2
-0.36291249E+05-0.72160920E+01 0.12123746E+01 0.29952820E-01-0.27809679E-04 3
0.14586627E-07-0.33536338E-11-0.34840005E+05 0.21112708E+02 4
CH3-CF2 78ROD90CHERAU C 2H 3F 2 OG 300.00 3000.00 1150.00 1
0.64772061E+01 0.12487615E-01-0.53578191E-05 0.10304861E-08-0.72450865E-13 2
-0.39201981E+05-0.63195346E+01 0.23142186E+01 0.23701830E-01-0.16389184E-04 3
0.57257237E-08-0.80729590E-12-0.37994895E+05 0.15358357E+02 4
CH2F-CF2 91CHERAU C 2H 2F 3 OG 300.00 3000.00 1150.00 1
0.88702445E+01 0.10089497E-01-0.43915564E-05 0.85758186E-09-0.61164127E-13 2
-0.57295496E+05-0.17248955E+02 0.20900802E+01 0.29390131E-01-0.25553336E-04 3
0.11710794E-07-0.23112930E-11-0.55373132E+05 0.17813614E+02 4
CHF2-CHF 91CHERAU C 2H 2F 3 OG 300.00 3000.00 1250.00 1
0.94245630E+01 0.93845534E-02-0.40694952E-05 0.79548881E-09-0.56874376E-13 2
-0.58166030E+05-0.20313155E+02 0.18136794E+01 0.32776675E-01-0.32420504E-04 3
0.16831319E-07-0.36002411E-11-0.56094627E+05 0.18591066E+02 4
CF3-CH2 78ROD90CHERAU C 2H 2F 3 OG 300.00 3000.00 1150.00 1
0.95879571E+01 0.92998799E-02-0.40774688E-05 0.80571741E-09-0.58185489E-13 2
-0.65995251E+05-0.22107686E+02 0.71700835E+00 0.40531459E-01-0.47864066E-04 3
0.29440811E-07-0.73125849E-11-0.63850063E+05 0.22103248E+02 4
CHF2-CF2 95BURZAC91CHE C 2H 1F 4 OG 300.00 3000.00 1250.00 1

```

```

0.11627462E+02 0.71020241E-02-0.30321751E-05 0.58031013E-09-0.40595926E-13 2
-0.84517281E+05-0.30486515E+02 0.30303759E+01 0.31363562E-01-0.29518978E-04 3
0.13983874E-07-0.27124342E-11-0.82031363E+05 0.14088813E+02 4
CF3-CHF 95BURZAC91CHE C 2H 1F 4 OG 300.00 3000.00 1250.00 1
0.11753063E+02 0.71311773E-02-0.31225055E-05 0.61530080E-09-0.44414594E-13 2
-0.86403865E+05-0.31333337E+02 0.21777569E+01 0.37699208E-01-0.41607296E-04 3
0.23110573E-07-0.51391529E-11-0.83881248E+05 0.17267626E+02 4
CF3-CF2 78ROD91CHERAU C 2F 5 0 OG 300.00 3000.00 1150.00 1
0.13959451E+02 0.49126632E-02-0.21053836E-05 0.39913356E-09-0.27648992E-13 2
-0.11242354E+06-0.41910578E+02 0.15747871E+01 0.46149396E-01-0.56963498E-04 3
0.34834336E-07-0.85235376E-11-0.10927738E+06 0.20480869E+02 4
!*****
!*** Fluoroethylenes ***
!*****
CH2:CHF 91GURVEY92DAU C 2H 3F 1 OG 300.00 3000.00 1100.00 1
0.48490759E+01 0.11146324E-01-0.46698155E-05 0.87478288E-09-0.59497855E-13 2
-0.19152550E+05-0.81788291E-01 0.62671121E-01 0.25703433E-01-0.22550142E-04 3
0.11676847E-07-0.27702203E-11-0.17842347E+05 0.24442171E+02 4
CHF:CHF[E] 82STAVOY95ZA C 2H 2F 2 OG 300.00 3000.00 1100.00 1
0.74872205E+01 0.80010682E-02-0.30483755E-05 0.51756316E-09-0.31970208E-13 2
-0.38340681E+05-0.13945178E+02 0.10952163E+01 0.26752037E-01-0.25108206E-04 3
0.13345970E-07-0.31849488E-11-0.36546538E+05 0.19001110E+02 4
CHF:CHF[Z] 82STAVOY95ZA C 2H 2F 2 OG 300.00 3000.00 1100.00 1
0.73420093E+01 0.821193890E-02-0.31754900E-05 0.54928213E-09-0.34743441E-13 2
-0.38823315E+05-0.13112868E+02 0.38315180E+00 0.29489609E-01-0.29414493E-04 3
0.16433649E-07-0.40175881E-11-0.36926877E+05 0.22508279E+02 4
CH2:CF2 91GURVEY69STU C 2H 2F 2 OG 300.00 3000.00 1100.00 1
0.75269154E+01 0.81672748E-02-0.32464823E-05 0.58546604E-09-0.39018495E-13 2
-0.43575506E+05-0.14492913E+02-0.54464109E+00 0.36101293E-01-0.42452205E-04 3
0.26867821E-07-0.70049045E-11-0.41578875E+05 0.25913851E+02 4
CHF:CF2 91GURVEY69STU C 2H 1F 3 OG 300.00 3000.00 1100.00 1
0.92978219E+01 0.66906598E-02-0.27184096E-05 0.49759041E-09-0.33586660E-13 2
-0.62705082E+05-0.20939116E+02 0.13552072E+01 0.32311285E-01-0.35790356E-04 3
0.20975806E-07-0.51422015E-11-0.60645808E+05 0.19293753E+02 4
CF2:CF2 71STUPRO C 2F 4 0 OG 300.00 3000.00 1100.00 1
0.11324277E+02 0.49963111E-02-0.21178179E-05 0.39861912E-09-0.27503925E-13 2
-0.83426613E+05-0.31270209E+02 0.25973529E+01 0.33905883E-01-0.41223935E-04 3
0.26050696E-07-0.67880509E-11-0.81178922E+05 0.12797244E+02 4
!*****
!*** Fluorovinyls ***
!*****
CHF:CH[E] 96ZACWES C 2H 2F 1 OG 300.00 3000.00 1050.00 1
0.58993136E+01 0.70760772E-02-0.28887543E-05 0.53085830E-09-0.35873561E-13 2
0.12541439E+05-0.53585386E+01 0.26848631E+00 0.27945434E-01-0.35411860E-04 3
0.25148746E-07-0.73773052E-11 0.13892575E+05 0.22559566E+02 4
CHF:CH[Z] 96ZACWES C 2H 2F 1 OG 300.00 3000.00 1050.00 1
0.52720505E+01 0.81754708E-02-0.34673780E-05 0.64788558E-09-0.43922904E-13 2
0.12647789E+05-0.19972542E+01 0.44420192E+00 0.26606878E-01-0.31480981E-04 3
0.20535551E-07-0.55252516E-11 0.13722215E+05 0.21668910E+02 4
CH2:CF 96ZACWES C 2H 2F 1 OG 300.00 3000.00 1050.00 1
0.59366687E+01 0.65440923E-02-0.23741343E-05 0.38223533E-09-0.22535997E-13 2
0.10745181E+05-0.55730445E+01 0.93664567E+00 0.23455005E-01-0.26099122E-04 3
0.16833431E-07-0.46658292E-11 0.12014041E+05 0.19594667E+02 4
CHF:CF[E] 96ZACWES C 2H 1F 2 OG 300.00 3000.00 1050.00 1
0.77099314E+01 0.51456246E-02-0.20013569E-05 0.34607509E-09-0.21864903E-13 2
-0.80621915E+04-0.12513673E+02 0.22126254E+01 0.22498052E-01-0.24414477E-04 3
0.14815361E-07-0.39398084E-11-0.66036801E+04 0.15471005E+02 4
CHF:CF[Z] 96ZACWES C 2H 1F 2 OG 300.00 3000.00 1050.00 1
0.77264612E+01 0.50029540E-02-0.18613080E-05 0.31199442E-09-0.19536071E-13 2
-0.79003013E+04-0.12864265E+02 0.14830603E+01 0.25289629E-01-0.28989928E-04 3
0.18356855E-07-0.49865919E-11-0.62750421E+04 0.18768190E+02 4
CF2:CH 96ZACWES C 2H 1F 2 OG 300.00 3000.00 1050.00 1
0.74110309E+01 0.64817026E-02-0.30631409E-05 0.62562526E-09-0.45512604E-13 2
-0.11017369E+05-0.11617089E+02 0.64712617E+00 0.31659599E-01-0.41452904E-04 3
0.28609364E-07-0.80609769E-11-0.94385390E+04 0.21799374E+02 4
CF2:CF 96ZACWES C 2F 3 0 OG 300.00 3000.00 1050.00 1

```

```

0.93845078E+01 0.38715458E-02-0.15369592E-05 0.26964434E-09-0.17640575E-13 2
-0.29433542E+05-0.19475848E+02 0.28683294E+01 0.25255065E-01-0.30028721E-04 3
0.18868899E-07-0.49993607E-11-0.27765224E+05 0.13444472E+02 4
!*****
!*** Fluoroacetylenes ***
!*****
C2HF 71STUPRO C 2H 1F 1 OG 300.00 3000.00 1050.00 1
0.59505136E+01 0.42683355E-02-0.16949802E-05 0.31112356E-09-0.21296349E-13 2
0.13021557E+05-0.75725301E+01 0.21892326E+01 0.21270501E-01-0.31679826E-04 3
0.24157264E-07-0.71274619E-11 0.13736471E+05 0.10227633E+02 4
C2F2 71STUPRO C 2F 2 0 OG 300.00 3000.00 1150.00 1
0.78096893E+01 0.27447408E-02-0.11104124E-05 0.19909478E-09-0.13059569E-13 2
-0.30353682E+03-0.16774334E+02 0.30593062E+01 0.17876216E-01-0.20807590E-04 3
0.12624164E-07-0.31567150E-11 0.97108585E+03 0.74032107E+01 4
!*****
!*** Fluoroketenes ***
!*****
CHFCO 96ZACWES C 2H 1F 1O 1G 300.00 3000.00 1050.00 1
0.67776435E+01 0.62335944E-02-0.25595800E-05 0.47531383E-09-0.32595082E-13 2
-0.20336925E+05-0.85911299E+01 0.19623675E+01 0.22507519E-01-0.25638947E-04 3
0.16791690E-07-0.47348234E-11-0.19104027E+05 0.15674252E+02 4
CF2CO 96ZACWES C 2F 2O 1 OG 300.00 3000.00 1050.00 1
0.88684122E+01 0.42627717E-02-0.17381349E-05 0.31228667E-09-0.20426586E-13 2
-0.38145628E+04-0.17907486E+02 0.34054339E+01 0.22694311E-01-0.28035260E-04 3
0.19124705E-07-0.55121984E-11-0.36737327E+05 0.96487236E+01 4
CFCO 96ZACWES C 2F 1O 1 OG 300.00 3000.00 1050.00 1
0.73033099E+01 0.29793943E-02-0.13058250E-05 0.25407405E-09-0.18103465E-13 2
0.57355650E+04-0.98434103E+01 0.37594179E+01 0.14231997E-01-0.16010254E-04 3
0.98885732E-08-0.26613184E-11 0.66747250E+04 0.81859183E+01 4
CF3OF 71STU/C 1O 1F 4 OG 300.00 3000.00 1440.00 1
0.12399629E+02 0.32529590E-02-0.14291450E-05 0.29960628E-09-0.25133306E-13 2
-0.96721165E+05-0.34715971E+02 0.24959868E+01 0.32773790E-01-0.35901194E-04 3
0.18734756E-07-0.37862643E-11-0.93915478E+05 0.16231910E+02 4
!BR J 6/74BR 1 0 0 OG 300.00 5000.00 1000.00 1
! 0.20843207E+01 0.71949483E-03-0.27419924E-06 0.42422650E-10-0.23791570E-14 2
! 0.12858837E+05 0.90838003E+01 0.24611551E+01 0.33319275E-03-0.10080655E-05 3
! 0.12262126E-08-0.44283510E-12 0.12711920E 05 0.69494733E+01 4
BR J 6/74BR 1 0 0 OG 200.00 6000.00 1000.00 1 Burcat
2.08902355E+00 7.11612338E-04-2.69886632E-07 4.15012215E-11-2.31379689E-15 2
1.28556222E+04 9.07042853E+00 2.48422309E+00 1.61406290E-04-5.63460901E-07 3
7.46724224E-10-2.58956029E-13 1.27084065E+04 6.86656618E+00 1.34526268E+04 4
!BR2 J12/61BR 20 00 00 OG 300.00 5000.00 1000.00 1
! 0.44479495E+01 0.10051208E-03-0.16393816E-07 0.22685621E-11-0.10236774E-15 2
! 0.23659941E+04 0.40888431E+01 0.38469580E+01 0.26111841E-02-0.40034147E-05 3
! 0.28120689E-08-0.73256202E-12 0.24846984E+04 0.69696985E+01 4
BR2 J12/61BR 20 00 00 OG 200.00 6000.00 1000.00 1 Burcat
5.18755860E+00-1.38705071E-03 9.35013276E-07-2.07120920E-10 1.41849439E-14 2
2.10348349E+03 7.61702748E-02 3.34375055E+00 6.34803695E-03-1.36288984E-05 3
1.31573020E-08-4.67760593E-12 2.53163737E+03 9.07775332E+00 3.71410943E+03 4
!HBR J 9/65H 1BR 1 0 OG 300.00 5000.00 1000.00 1
! 0.27935804E+01 0.15655925E-02-0.56171064E-06 0.95783142E-10-0.61813990E-14 2
! -0.52338384E+04 0.76423703E+01 0.36056690E+01-0.59529431E-03 0.65029568E-06 3
! 0.93781219E-09-0.71141852E-12-0.54389455E+04 0.34831774E+01 4
HBR J 9/65H 1BR 1 0 OG 200.00 6000.00 1000.00 1 Burcat
2.83372014E+00 1.48517671E-03-5.13137154E-07 8.73711119E-11-5.72363001E-15 2
-5.17620691E+03 7.43754245E+00 3.48117971E+00 3.42734055E-04-1.80532777E-06 3
3.61180553E-09-1.74298435E-12-5.35537141E+03 4.01309183E+00-4.31185963E+03 4
!CF3BR OC 1F 3BR 1 OG 300.000 4000.000 1000.00 1
! 0.10835589E+02+0.15757806E-02-0.20505728E-06-0.81578432E-10 0.17003094E-13 2
! -0.81927266E+05-0.27720734E+02 0.44576893E+01 0.14666174E-01-0.20081193E-05 3
! -0.10235016E-07+0.52610143E-11-0.80003992E+05 0.62208567E+01 4
CF3BR OC 1F 3BR 1 OG 200.000 6000.000 1000.00 1 Burcat
1.02441971E+01 2.82088779E-03-1.10430609E-06 1.88474696E-10-1.17193712E-14 2
-8.19308539E+04-2.45567155E+01 1.92067214E+00 3.10919159E-02-3.85950853E-05 3
2.31847352E-08-5.46470390E-12-7.99043849E+04 1.71123451E+01-7.82475456E+04 4
!CH3BR DIPPR C 1H 3BR 1 OG 300.00 3000.00 1100.00 1

```

! 0.26622491E+01 0.10938679E-01-0.49091741E-05 0.97218827E-09-0.69039725E-13 2  
!-0.58748252E+04 0.11128287E+02 0.13844668E+01 0.15781927E-01-0.13119413E-04 3  
! 0.77319100E-08-0.21949811E-11-0.55462775E+04 0.17495386E+02 4  
CH3BR C 1H 3BR 1 OG 200.00 6000.00 1000.00 1 Burcat  
4.14293955E+00 7.61096796E-03-2.67015354E-06 4.24035809E-10-2.50883825E-14 2  
-6.20545949E+03 3.21432559E+00 3.61367184E+00-8.86540422E-04 2.94669395E-05 3  
-3.76504049E-08 1.49390354E-11-5.61401651E+03 8.24978857E+00-4.38301716E+03 4  
CH2BR MCMGOlest C 1H 2BR 1 OG 300.00 1500.00 1040.00 1  
-0.28798719E+00 0.10936174E-01-0.47249918E-05 0.90419016E-09-0.62866972E-13 2  
0.20433462E+05 0.28715322E+02-0.14987932E+01 0.14414354E-01-0.83676316E-05 3  
0.25675561E-08-0.35151943E-12 0.20761287E+05 0.34940128E+02 4  
!CH2:CHBR DIPPR C 2H 3BR 1 OG 300.00 3000.00 1100.00 1  
! 0.48816714E+01 0.11872023E-01-0.54511750E-05 0.10926716E-08-0.77674167E-13 2  
! 0.72374120E+04 0.14265356E+01 0.63704010E+00 0.26976451E-01-0.26856586E-04 3  
! 0.15318821E-07-0.37691556E-11 0.82471016E+04 0.22526875E+02 4  
!CH3-CH2BR DIPPR C 2H 5BR 1 OG 300.00 3000.00 1140.00 1  
! 0.10484190E+01 0.25329179E-01-0.13151664E-04 0.28967557E-08-0.22319548E-12 2  
!-0.88946358E+04 0.21877824E+02 0.52438083E+00 0.30080803E-01-0.22248551E-04 3  
! 0.93023889E-08-0.17393510E-11-0.90132273E+04 0.23537494E+02 4  
!C2H3BR DIPPR C 2H 3BR 1 OG 300.00 3000.00 1100.00 1  
! 0.48816714E+01 0.11872023E-01-0.54511750E-05 0.10926716E-08-0.77674167E-13 2  
! 0.72374120E+04 0.14265356E+01 0.63704010E+00 0.26976451E-01-0.26856586E-04 3  
! 0.15318821E-07-0.37691556E-11 0.82471016E+04 0.22526875E+02 4  
C2H3BR C 2H 3BR 1 OG 200.00 6000.00 1000.00 1 Burcat  
6.26544676E+00 8.40448044E-03-2.96022704E-06 4.71565331E-10-2.79679290E-14 2  
6.27917135E+03-5.89080021E+00 2.44081829E+00 1.33416754E-02 7.36029379E-06 3  
-2.10890514E-08 1.00995615E-11 7.55967704E+03 1.50863318E+01 8.90852257E+03 4  
!C2H5BR DIPPR C 2H 5BR 1 OG 300.00 3000.00 1140.00 1  
! 0.10484190E+01 0.25329179E-01-0.13151664E-04 0.28967557E-08-0.22319548E-12 2  
!-0.88946358E+04 0.21877824E+02 0.52438083E+00 0.30080803E-01-0.22248551E-04 3  
! 0.93023889E-08-0.17393510E-11-0.90132273E+04 0.23537494E+02 4  
C2H5BR C 2H 5BR 1 OG 200.00 6000.00 1000.00 1 Burcat  
6.95002116E+00 1.28709161E-02-4.60446763E-06 7.41067324E-10-4.42632344E-14 2  
-1.06394105E+04-1.00517817E+01 3.62900361E+00 6.37387681E-03 3.97846545E-05 3  
-5.78493445E-08 2.39750833E-11-9.02251371E+03 1.07167737E+01-7.40873485E+03 4  
FBR JANAF BR 1F 1 OG 300.00 2000.00 1120.00 1  
0.42965810E+01 0.21597634E-03-0.94250398E-08-0.10763197E-10 0.32730061E-15 2  
-0.83889498E+04 0.28342494E+01 0.27913390E+01 0.60536896E-02-0.87848912E-05 3  
0.59839505E-08-0.15549082E-11-0.80648880E+04 0.10172832E+02 4  
!BRO 82WAG/EVA BR 1O 1 OG 300.00 2000.00 593.00 1  
! 0.38423535E+01 0.29818127E-03-0.10111621E-08-0.45536224E-11-0.12545159E-14 2  
! 0.13986282E+05 0.65954140E+01 0.34409032E+01 0.19365875E-02-0.11562326E-05 3  
!-0.23853307E-08 0.26881704E-11 0.14050726E+05 0.84726383E+01 4  
BRO BR 1O 1 OG 200.00 6000.00 1000.00 1 Burcat  
5.13722924E+00-5.16463629E-04 2.06071880E-07-3.26108430E-11 1.97330917E-15 2  
1.32089286E+04-1.47001990E+00 2.48296400E+00 6.85676900E-03-3.78833758E-06 3  
-4.21357998E-09 3.45838452E-12 1.38620073E+04 1.20185205E+01 1.48669014E+04 4  
!BROH 76BEN H 1BR 1O 1 OG 300.00 2000.00 895.00 1  
! 0.44804555E+01 0.72687612E-03 0.42097174E-07-0.49948238E-11-0.24686600E-14 2  
!-0.10963203E+05 0.39700594E+01 0.40847205E+01 0.15786399E-02-0.21558384E-06 3  
!-0.41121729E-09 0.20176279E-12-0.10846878E+05 0.60649913E+01 4  
BROH Burc H 1BR 1O 1 OG 200.00 6000.00 1000.00 1 Burcat  
4.52559122E+00 1.88368072E-03-6.04303745E-07 8.98998654E-11-5.06961671E-15 2  
-8.92977368E+03 3.31036380E+00 3.31731799E+00 5.05328752E-03-1.73682519E-06 3  
-2.67712334E-09 1.93314146E-12-8.62468312E+03 9.49126178E+00-7.43074457E+03 4  
!  
CH300 86TSA/HAM C 1H 3O 2 OG 300.00 1500.00 1000.00 1  
0.52292572E+01 0.86924298E-02 0.39167105E-06-0.27944819E-08 0.82817431E-12 2  
0.12289245E+04-0.13037471E+01 0.10026689E+01 0.23475309E-01-0.18768121E-04 3  
0.80828167E-08-0.14456237E-11 0.21861054E+04 0.19632191E+02 4  
CH300H estBEN C 1H 4O 2 OG 300.00 1500.00 1000.00 1  
0.52292572E+01 0.86924298E-02 0.39167105E-06-0.27944819E-08 0.82817431E-12 2  
0.14807183E+05 0.73953418E+00 0.10026689E+01 0.23475309E-01-0.18768121E-04 3  
0.80828167E-08-0.14456237E-11 0.15764364E+05 0.21675472E+02 4  
C3F7H Burcat C 3H 1F 7 OG 300.000 5000.000 1  
0.1944626E+02 0.1296430E-01 -0.6579523E-05 0.1579046E-08 -0.1494170E-12 2



-0.1912779E+06	-0.6759355E+02	0.3892091E+00	0.7478753E-01	-0.8484074E-04	3						
0.4842886E-07	-0.1150851E-10	-0.1864860E+06	0.2857845E+02		4						
C3F7	Burcat	C	3F	7	0	OG	300.000	5000.000		1	
0.1611692E+02	0.1602694E-01	-0.8663088E-05	0.2211648E-08	-0.2208344E-12	2						
-0.1668943E+06	-0.4996330E+02	0.1874186E+01	0.6455843E-01	-0.7452887E-04	3						
0.4482470E-07	-0.1126337E-10	-0.1634068E+06	0.2137972E+02		4						
C3F6	Hynes	C	3F	6	0	OG	300.000	5000.000		1	
0.1459909E+02	0.1404826E-01	-0.8270140E-05	0.2255100E-08	-0.2342412E-12	2						
-0.1408496E+06	-0.4123436E+02	0.2559720E+01	0.6406888E-01	-0.9602950E-04	3						
0.7705808E-07	-0.2527435E-10	-0.1382602E+06	0.1711541E+02		4						
CF3O2	NIST	C	1F	3O	2	OG	300.000	5000.000		1	
0.1005499E+02	0.8205633E-02	-0.5062363E-05	0.1433123E-08	-0.1534602E-12	2						
-0.1015453E+06	-0.2260937E+02	0.4379631E+00	0.4555659E-01	-0.6176471E-04	3						
0.4131473E-07	-0.1106784E-10	-0.8164120E+05	0.2413379E+02		4						
C3F7O	Hynes	C	3F	7O	1	OG	300.000	5000.000		1	
0.2287185E+02	0.7640052E-02	-0.1657346E-05	-0.2941549E-09	0.1035168E-12	2						
-0.1880432E+06	-0.8666051E+02	0.1136218E+01	0.7336590E-01	-0.7413762E-04	3						
0.3256982E-07	-0.4255755E-11	-0.1823545E+06	0.2413339E+02		4						
C3F7O2	Hynes	C	3F	7O	2	OG	300.000	5000.000		1	
0.1787408E+02	0.2373510E-01	-0.1367114E-04	0.3718392E-08	-0.3930683E-12	2						
-0.1860711E+06	-0.5607585E+02	0.1641474E+01	0.8751624E-01	-0.1100224E-03	3						
0.7251820E-07	-0.2041578E-10	-0.1828074E+06	0.2252190E+02		4						
CF3COF	hynes	C	2F	4O	1	OG	300.000	5000.000		1	
0.1006273E+02	0.1214340E-01	-0.7263414E-05	0.2011440E-08	-0.2118963E-12	2						
-0.1282302E+06	-0.2073074E+02	0.1769974E+01	0.4245083E-01	-0.5069665E-04	3						
0.3111379E-07	-0.7895977E-11	-0.1263522E+06	0.2018299E+02		4						
C3F6O	hynes	C	3F	6O	1	OG	300.000	5000.000		1	
0.1704561E+02	0.1455861E-01	-0.8812300E-05	0.2462951E-08	-0.2613377E-12	2						
-0.1744044E+06	-0.5524056E+02	0.2606280E+01	0.7231953E-01	-0.1005112E-03	3						
0.7052793E-07	-0.1995183E-10	-0.1713574E+06	0.1482562E+02		4						
CF3CHO	NIST	C	2F	3H	1O	1G	300.000	5000.000		1	
0.8047711E+01	0.1377502E-01	-0.7751215E-05	0.2053101E-08	-0.2090976E-12	2						
-0.9645195E+05	-0.1217682E+02	0.2986401E+01	0.2819500E-01	-0.2091598E-04	3						
0.5048025E-08	0.6025630E-12	-0.9512344E+05	0.1374664E+02		4						
CF3CO	NIST	C	2F	3O	1	OG	300.000	5000.000		1	
0.8273660E+01	0.9456556E-02	-0.5544948E-05	0.1509502E-08	-0.1566714E-12	2						
-0.7681196E+05	-0.1889926E+02	-0.7058443E+01	0.1041643E+00	-0.2377523E-03	3						
0.2500676E-06	-0.9594719E-10	-0.7441268E+05	0.4950205E+02		4						
C3F7OH	hynes	C	3F	7O	1H	1G	300.000	5000.000		1	
0.1696278E+02	0.2565773E-01	-0.1513042E-04	0.4192663E-08	-0.4490027E-12	2						
-0.2188921E+06	-0.5534448E+02	0.1429132E+01	0.8909125E-01	-0.1141049E-03	3						
0.7694099E-07	-0.2212097E-10	-0.2159364E+06	0.1918044E+02		4						
C2F5COC3F7	OC	6F	12O	1	G	300.000	3000.000	1000.00		1	Hf -
650.8;Cp,S-Smith KD data^M											
0.30630959E+02	0.38184828E-01	-0.24308864E-04	0.70308675E-08	-0.76600556E-12	2	^M					
-0.33931382E+06	-0.11703101E+03	0.47864609E+01	0.12945436E+00	-0.14305048E-03	3	^M					
0.74083490E-07	-0.14502047E-10	-0.33353949E+06	0.10680870E+02		4	^M					
C2F5CO	OC	3F	5O	1H	OG	300.000	2500.000	1000.00		1	^M
0.10993560E+02	0.22635009E-01	-0.16215860E-04	0.53906966E-08	-0.68205687E-12	2	^M					
-0.12892516E+06	-0.29543968E+02	0.58825005E+01	0.31427282E-01	-0.11926324E-04	3	^M					
-0.91209576E-08	0.58588476E-11	-0.12732035E+06	-0.19730690E+01		4	^M					
C2F5CHO	OC	3F	5O	1H	1G	300.000	2500.000	1000.00		1	^M
0.70011481E+01	0.36515406E-01	-0.27132992E-04	0.93304054E-08	-0.12151653E-11	2	^M					
-0.14764381E+06	-0.28355041E+01	0.23841549E+01	0.57546395E-01	-0.62523998E-04	3	^M					
0.35487425E-07	-0.83951742E-11	-0.14684857E+06	0.18798064E+02		4	^M					
C3F7CO	OC	4F	7O	1	G	300.000	2500.000	1000.00		1	^M
0.49092940E+01	0.56218006E-01	-0.44870281E-04	0.16215609E-07	-0.21904541E-11	2	^M					
-0.18448922E+06	0.12881551E+02	0.45819062E+01	0.62040688E-01	-0.60374001E-04	3	^M					
0.31064553E-07	-0.70309731E-11	-0.18464940E+06	0.13332725E+02		4	^M					
C3F7CHO	OC	4F	7O	1H	1G	300.000	2500.000	1000.00		1	^M
0.10618414E+02	0.46140362E-01	-0.34401925E-04	0.11943552E-07	-0.15745340E-11	2	^M					
-0.20345971E+06	-0.11769315E+02	0.45903305E+01	0.62406189E-01	-0.47030908E-04	3	^M					
0.12516368E-07	0.24388842E-12	-0.20186177E+06	0.19274330E+02		4	^M					
CH3CL	P10/94C	1H	3CL	1	OG	300.000	5000.000			1	
0.32689390E+01	0.92516765E-02	-0.36359988E-05	0.65624309E-09	-0.44634275E-13	2						
-0.11414660E+05	0.65114729E+01	0.14974829E+01	0.13280178E-01	-0.67253280E-05	3						

	0.15378357E-08-0.93943118E-13-0.10838215E+05	0.15982884E+02	4
HCL	P10/94C 0H 1CL 1 OG	300.000 5000.000	1
	0.26698947E+01 0.16795019E-02-0.65570902E-06	0.11805238E-09-0.80157173E-14	2
	-0.11895735E+05 0.69596723E+01 0.37513903E+01	-0.15701609E-02 0.29359076E-05	3
	-0.16186063E-08 0.30519358E-12-0.12178082E+05	0.14434038E+01	4
C2H3CL	P10/94C 2H 3CL 1 G	300.000 5000.000	1
	0.77008685E+01 0.60307727E-02-0.17425522E-05	0.23259663E-09-0.11821483E-13	2
	-0.69747985E+03-0.15386004E+02-0.51604284E+00	0.29082193E-01-0.25283043E-04	3
	0.10575896E-07-0.16491385E-11 0.15821904E+04	0.27054797E+02	4
CH2CL2	P10/94C 1H 2CL 2 G	300.000 5000.000	1
	0.61242234E+01 0.63982922E-02-0.24562633E-05	0.43617380E-09-0.29351029E-13	2
	-0.13932398E+05-0.50325787E+01 0.19851337E+01	0.17541990E-01-0.13471231E-04	3
	0.52453911E-08-0.82820866E-12-0.12736034E+05	0.16519668E+02	4
CL2	P10/94CL 2 G	300.000 5000.000	1
	0.44090056E+01 0.84541656E-04 0.50853202E-07	-0.22772696E-10 0.22776700E-14	2
	-0.13854860E+04 0.15162125E+01 0.33381039E+01	0.34455271E-02-0.38269443E-05	3
	0.19303847E-08-0.36316601E-12-0.11176785E+04	0.69319611E+01	4
CCLO	P10/94C 1H 0O 1CL 1G	300.000 5000.000	1
	0.54527492E+01 0.14905796E-02-0.55361447E-06	0.99210376E-10-0.67908086E-14	2
	-0.37913489E+04 0.26021378E+00 0.44134244E+01	0.43130716E-02-0.33850152E-05	3
	0.13681372E-08-0.22748414E-12-0.34925629E+04	0.56650213E+01	4
COCL2	P10/94C 1H 0O 1CL 2G	300.000 5000.000	1
	0.81774233E+01 0.13049061E-02-0.18321398E-06	-0.17078037E-10 0.38207222E-14	2
	-0.29258002E+05-0.13549749E+02 0.33382932E+01	0.16730762E-01-0.18232525E-04	3
	0.91587907E-08-0.17094629E-11-0.28066674E+05	0.10846275E+02	4
CLO	P10/94C 0H 0O 1CL 1G	300.000 5000.000	1
	0.41921985E+01 0.24638425E-03 0.13541307E-07	-0.20121881E-10 0.23209407E-14	2
	0.10829101E+05 0.30529724E+01 0.27140057E+01	0.49285501E-02-0.54084281E-05	3
	0.26949409E-08-0.49474554E-12 0.11194181E+05	0.10512031E+02	4
HOCL	P10/94C 0H 1O 1CL 1G	300.000 5000.000	1
	0.43822240E+01 0.19622493E-02-0.59643407E-06	0.83821951E-10-0.44831988E-14	2
	-0.10421134E+05 0.27262922E+01 0.30026838E+01	0.65029353E-02-0.60264081E-05	3
	0.28518366E-08-0.50366961E-12-0.10094111E+05	0.96322441E+01	4
CL	P10/94CL 1 G	300.000 5000.000	1
	0.13872418E+01 0.28203241E-02-0.19779163E-05	0.47591700E-09-0.38228847E-13	2
	0.14185898E+05 0.11573212E+02 0.19662441E+01	0.37102780E-02-0.63901296E-05	3
	0.45205485E-08-0.11396033E-11 0.13841773E+05	0.78168915E+01	4
C2H5CL	P10/94C 2H 5CL 1 OG	300.000 5000.000	1
	0.63900159E+01 0.13589931E-01-0.49262673E-05	0.83954462E-09-0.54774319E-13	2
	-0.16519378E+05-0.82724200E+01 0.32824488E+00	0.29650049E-01-0.20331928E-04	3
	0.71824487E-08-0.99036476E-12-0.14751053E+05	0.23363119E+02	4
CHCLO	P10/94C 1H 1O 1CL 1G	300.000 5000.000	1
	0.54425752E+01 0.40740978E-02-0.13713436E-05	0.21131457E-09-0.12406439E-13	2
	-0.21737678E+05-0.14684490E+01 0.24871004E+01	0.13707166E-01-0.12902424E-04	3
	0.62192414E-08-0.11668459E-11-0.21026138E+05	0.13365688E+02	4
CH2CCL2	P10/94C 2H 2CL 2 G	300.000 5000.000	1
	0.94631375E+01 0.51515079E-02-0.16778675E-05	0.25891876E-09-0.15525513E-13	2
	-0.33484740E+04-0.21968365E+02 0.20329971E+01	0.25629377E-01-0.22238923E-04	3
	0.91865536E-08-0.14298341E-11-0.12526302E+04	0.16537584E+02	4
CH2CLCHCL	P12/94C 2H 3CL 2 OG	300.000 5000.000	1
	0.81636744E+01 0.97785815E-02-0.35228452E-05	0.59069797E-09-0.37788540E-13	2
	0.25106412E+04-0.12163959E+02 0.11649524E+01	0.32017583E-01-0.29638153E-04	3
	0.14003846E-07-0.25759087E-11 0.42493019E+04	0.23163632E+02	4
CH2CHCL2	P01/95C 2H 3CL 2 OG	300.000 5000.000	1
	0.92271004E+01 0.88715451E-02-0.34804373E-05	0.63719324E-09-0.44031043E-13	2
	0.44947378E+04-0.19140724E+02 0.24135213E+01	0.26192989E-01-0.18614366E-04	3
	0.54654912E-08-0.24626088E-12 0.65256143E+04	0.16612469E+02	4
CH3CCL3	P01/95C 2H 3CL 3 OG	300.000 5000.000	1
	0.12974936E+02 0.63293413E-02-0.14376318E-05	0.11646843E-09-0.72959289E-15	2
	-0.22258066E+05-0.37838493E+02 0.44153862E+01	0.28668961E-01-0.19700710E-04	3
	0.32678982E-08 0.13308499E-11-0.19834807E+05	0.66973190E+01	4
CH2CLCHCL2	P01/95C 2H 3CL 3 OG	300.000 5000.000	1
	0.12001616E+02 0.75028380E-02-0.18939955E-05	0.19200949E-09-0.52870818E-14	2
	-0.22729797E+05-0.31100998E+02 0.25047257E+01	0.34007359E-01-0.25102949E-04	3
	0.46573314E-08 0.17307150E-11-0.20212381E+05	0.17678709E+02	4
CH2CCL3	P01/95C 2H 2CL 3 OG	300.000 5000.000	1

0.11523775E+02	0.57698204E-02	-0.14441449E-05	0.14252104E-09	-0.35470915E-14	2		
0.17564395E+04	-0.26912674E+02	0.32407036E+01	0.29974939E-01	-0.25205449E-04	3		
0.79379490E-08	0.40280980E-13	0.38997676E+04	0.15370859E+02		4		
CHCL2CCL2	P10/94C	2H	1CL	4	OG	300.000	5000.000
0.13634293E+02	0.42701792E-02	-0.10517723E-05	0.99582370E-10	-0.21065231E-14	2		
-0.18383386E+04	-0.35921562E+02	0.42201591E+01	0.34928415E-01	-0.36928839E-04	3		
0.17622723E-07	-0.28922901E-11	0.40294922E+03	0.11270744E+02		4		
CHCLCHCL	P10/94C	2H	2CL	2	G	300.000	5000.000
0.94631375E+01	0.51515079E-02	-0.16778675E-05	0.25891876E-09	-0.15525513E-13	2		
-0.30817402E+04	-0.21968365E+02	0.20329971E+01	0.25629377E-01	-0.22238923E-04	3		
0.91865536E-08	-0.14298341E-11	-0.98589640E+03	0.16537584E+02		4		
CHCL3	P10/94C	1H	1CL	3	G	300.000	5000.000
0.90477147E+01	0.32742733E-02	-0.95266130E-06	0.12079908E-09	-0.54755265E-14	2		
-0.15376271E+05	-0.17795726E+02	0.29015156E+01	0.23067488E-01	-0.24412111E-04	3		
0.12248021E-07	-0.23202639E-11	-0.13875711E+05	0.13133513E+02		4		
C2HCL3	P10/94C	2H	1CL	3	G	300.000	5000.000
0.12725462E+02	0.59504624E-03	0.84580747E-06	-0.30392218E-09	0.28397080E-13	2		
-0.51359782E+04	-0.35095353E+02	0.28919044E+01	0.31549887E-01	-0.34747813E-04	3		
0.17374022E-07	-0.31772109E-11	-0.26936660E+04	0.14583176E+02		4		
CHCL2	P10/94C	1H	1CL	2	G	300.000	5000.000
0.51442385E+01	0.57757862E-02	-0.22314852E-05	0.38657242E-09	-0.25288025E-13	2		
0.99970615E+04	0.28689941E+01	0.55123724E+01	0.30736563E-02	0.26132165E-05	3		
-0.28704184E-08	0.72099705E-12	0.10030083E+05	0.15048866E+01		4		
CH2CL	P10/94C	1H	2CL	1	G	300.000	5000.000
0.10520900E+01	0.11300151E-01	-0.54116678E-05	0.11070237E-08	-0.81819566E-13	2		
0.12429656E+05	0.21056787E+02	0.39551559E+01	0.37551619E-03	0.87360054E-05	3		
-0.64405083E-08	0.13396084E-11	0.11875614E+05	0.70144032E+01		4		
CCL2	P10/94C	1H	0CL	2	G	300.000	5000.000
0.48322901E+01	0.29322569E-02	-0.72355114E-06	0.48679054E-10	0.14172532E-14	2		
0.24734539E+05	-0.35843497E+01	0.33955448E+01	0.10399313E-01	-0.12406611E-04	3		
0.72168755E-08	-0.15140293E-11	0.24843151E+05	0.27042721E+01		4		
CH2CLCCL2	P10/94C	2H	2CL	3	G	300.000	5000.000
0.11493675E+02	0.58294476E-02	-0.14826589E-05	0.15237175E-09	-0.44112387E-14	2		
-0.67358464E+03	-0.26597219E+02	0.28402924E+01	0.32829150E-01	-0.32357578E-04	3		
0.15454731E-07	-0.27781701E-11	0.15007491E+04	0.17208644E+02		4		
CH3CCL2	P10/94C	2H	3CL	2	G	300.000	5000.000
0.95475152E+01	0.80575939E-02	-0.28705701E-05	0.48644217E-09	-0.31751213E-13	2		
0.14293506E+04	-0.21177335E+02	0.21520572E+01	0.27554920E-01	-0.21467310E-04	3		
0.81330422E-08	-0.11834790E-11	0.35937547E+04	0.17448789E+02		4		
CH3CHCL2	P10/94C	2H	4CL	2	G	300.000	5000.000
0.87264654E+01	0.11305046E-01	-0.37457760E-05	0.57848010E-09	-0.34321256E-13	2		
-0.18968706E+05	-0.17422107E+02	0.12377428E+01	0.34406469E-01	-0.30055752E-04	3		
0.13713478E-07	-0.24720447E-11	-0.17056908E+05	0.20592819E+02		4		
CH3CHCL	P10/94C	2H	4CL	1	G	300.000	5000.000
0.52813139E+01	0.12584294E-01	-0.44671059E-05	0.73471400E-09	-0.46150365E-13	2		
0.64316140E+04	-0.46170334E+00	0.46186697E+00	0.28107349E-01	-0.22887081E-04	3		
0.10257213E-07	-0.18522811E-11	0.76101270E+04	0.23794156E+02		4		
CCL3	P10/94C	1H	0CL	3	G	300.000	5000.000
0.93915649E+01	-0.69571490E-04	0.44058198E-06	-0.14132486E-09	0.12871309E-13	2		
0.64566461E+04	-0.18508889E+02	0.40458420E+01	0.17221369E-01	-0.20000110E-04	3		
0.10307488E-07	-0.19404665E-11	0.77489272E+04	0.83528585E+01		4		
CH2CH2CL	P10/94C	2H	4CL	1	G	300.000	5000.000
0.35908562E+01	0.15927518E-01	-0.62514355E-05	0.11087717E-08	-0.73748112E-13	2		
0.87186907E+04	0.94197430E+01	-0.79051360E+00	0.34785866E-01	-0.33958968E-04	3		
0.18005682E-07	-0.37401047E-11	0.94157743E+04	0.29964877E+02		4		
C2HCL	P10/94C	2H	1CL	1	G	300.000	5000.000
0.68356786E+01	0.25476731E-02	-0.60179017E-06	0.51957071E-10	-0.60466463E-15	2		
0.21299149E+05	-0.10826875E+02	0.39577670E+01	0.11946460E-01	-0.11796042E-04	3		
0.58054421E-08	-0.10807137E-11	0.21986735E+05	0.36035719E+01		4		
CHCL	P10/94C	1H	1CL	1	G	300.000	5000.000
0.20387190E+01	0.76359239E-02	-0.37271108E-05	0.76180645E-09	-0.56092390E-13	2		
0.34858192E+05	0.14656131E+02	0.36747739E+01	0.16110985E-02	0.39187194E-05	3		
-0.32432244E-08	0.69187865E-12	0.34537604E+05	0.67045919E+01		4		
C2H2CL3	P10/94C	2H	2CL	3	G	300.000	5000.000
0.11493675E+02	0.58294476E-02	-0.14826589E-05	0.15237175E-09	-0.44112387E-14	2		
0.56158694E+02	-0.26647546E+02	0.28402924E+01	0.32829150E-01	-0.32357578E-04	3		

0.15454731E-07-0.27781701E-11 0.22304924E+04 0.17158317E+02	4
C2CL2 P10/94C 2H 0CL 2 G 300.000 5000.000	1
0.84591307E+01 0.16889036E-02-0.48001740E-06 0.58698351E-10-0.25079088E-14	2
0.22431078E+05-0.16420815E+02 0.54659420E+01 0.11029896E-01-0.11172105E-04	3
0.53617169E-08-0.96124238E-12 0.23183792E+05-0.12675372E+01	4
CHCL2CHCL2 P10/94C 2H 2CL 4 G 300.000 5000.000	1
0.15332844E+02 0.46023135E-02-0.11284751E-05 0.11467281E-09-0.33881043E-14	2
-0.23657750E+05-0.47215947E+02 0.43612952E+01 0.37546654E-01-0.37570889E-04	3
0.17752003E-07-0.31710968E-11-0.20786692E+05 0.87625075E+01	4
CHCLCCL3 P 1/93C 2H 1CL 4 OG 300.000 3000.000	1
0.14443678E+02 0.38386676E-02-0.14789734E-05 0.34384812E-09-0.36501038E-13	2
-0.75038721E+03-0.40733475E+02 0.54832840E+01 0.30734422E-01-0.30618172E-04	3
0.13535860E-07-0.20246714E-11 0.15748201E+04 0.49362869E+01	4
CH2CLCCL3 P 1/93C 2H 2CL 4 OG 300.000 3000.000	1
0.17803976E+02 0.84718049E-03 0.31754277E-06 0.12692352E-10-0.22157909E-13	2
-0.27469547E+05-0.60004227E+02 0.32799888E+01 0.31757694E-01-0.83450514E-05	3
-0.19129333E-07 0.11395941E-10-0.23011398E+05 0.17270849E+02	4
CH2CLCH2CL P10/94C 2H 4CL 2 G 300.000 5000.000	1
0.55051266E+01 0.15831832E-01-0.55223551E-05 0.87565450E-09-0.52613788E-13	2
-0.17773551E+05 0.14876700E+01 0.23769081E+01 0.31671282E-01-0.30408645E-04	3
0.16444241E-07-0.34461413E-11-0.17483068E+05 0.15359186E+02	4
CH2CLO P10/94C 1H 2O 1CL 1G 300.000 5000.000	1
0.57528946E+01 0.65677779E-02-0.25423970E-05 0.45778564E-09-0.31229826E-13	2
-0.13287212E+04-0.34630135E+02 0.14372864E+01 0.17325994E-01-0.12065486E-04	3
0.40070549E-08-0.50001806E-12-0.11417805E+02 0.18989387E+02	4
CCL4 P01/95C 1H 0CL 4 G 300.000 5000.000	1
0.12487347E+02-0.64903288E-03 0.97642032E-06-0.28292069E-09 0.24806749E-13	2
-0.15626863E+05-0.34630135E+02 0.52484550E+01 0.22344856E-01-0.24543533E-04	3
0.10802090E-07-0.12952491E-11-0.13885509E+05 0.17754669E+01	4
C2CL P01/95C 2H 0CL 1 G 300.000 5000.000	1
0.53440723E+01 0.23043347E-02-0.65500564E-06 0.75917529E-10-0.28887580E-14	2
0.61678023E+05-0.13407097E+01 0.52041640E+01 0.12562138E-02 0.38130136E-05	3
-0.52927889E-08 0.20858291E-11 0.61777090E+05-0.29275513E+00	4
CHCLCCL P01/95C 2H 1CL 2 G 300.000 5000.000	1
0.10699759E+02 0.35750587E-02-0.76420179E-06 0.21375962E-10 0.49982953E-14	2
0.25395225E+05-0.28641571E+02 0.25131929E+01 0.28215362E-01-0.27483307E-04	3
0.12146612E-07-0.18548709E-11 0.27508666E+05 0.13051695E+02	4
C2CL3 P01/95C 2H 0CL 3 G 300.000 5000.000	1
0.13380778E+02 0.99350337E-03 0.26866530E-06-0.16591521E-09 0.17683771E-13	2
0.23802111E+05-0.38188507E+02 0.44092226E+01 0.28227594E-01-0.29645893E-04	3
0.13730973E-07-0.22271807E-11 0.26102887E+05 0.74369049E+01	4
CHCCL2 P01/95C 2H 1CL 2 G 300.000 5000.000	1
0.10699759E+02 0.35750587E-02-0.76420179E-06 0.21375962E-10 0.49982953E-14	2
0.25395225E+05-0.28641571E+02 0.25131929E+01 0.28215362E-01-0.27483307E-04	3
0.12146612E-07-0.18548709E-11 0.27508666E+05 0.13051695E+02	4
CHCHCL P01/95C 2H 2CL 1 G 300.000 5000.000	1
0.45177388E+01 0.10521499E-01-0.38629746E-05 0.62949940E-09-0.38781458E-13	2
0.28298650E+05 0.29812889E+01 0.34766102E+00 0.21647524E-01-0.12828822E-04	3
0.16028799E-08 0.99774301E-12 0.29443686E+05 0.24560469E+02	4
CH2CCL P01/95C 2H 2CL 1 G 300.000 5000.000	1
0.45177388E+01 0.10521499E-01-0.38629746E-05 0.62949940E-09-0.38781458E-13	2
0.28298650E+05 0.29812889E+01 0.34766102E+00 0.21647524E-01-0.12828822E-04	3
0.16028799E-08 0.99774301E-12 0.29443686E+05 0.24560469E+02	4
C2CL4 P01/95C 2H 0CL 4 G 300.000 5000.000	1
0.15434170E+02-0.14343550E-02 0.14496014E-05-0.38283879E-09 0.32067980E-13	2
-0.70298721E+04-0.48358032E+02 0.59464254E+01 0.24723917E-01-0.24021634E-04	3
0.95466142E-08-0.10966838E-11-0.43874663E+04 0.73069382E+00	4
CHCLCHCL2 P01/95C 2H 2CL 3 G 300.000 5000.000	1
0.11494323E+02 0.58273752E-02-0.14806018E-05 0.15166346E-09-0.43348203E-14	2
0.56023926E+02-0.26650749E+02 0.34233587E+01 0.28675772E-01-0.21952390E-04	3
0.45188262E-08 0.13228568E-11 0.21694880E+04 0.14701477E+02	4
CHCL2CCL2 P01/95C 2H 1CL 4 G 300.000 5000.000	1
0.13634293E+02 0.42701792E-02-0.10517723E-05 0.99582370E-10-0.21065231E-14	2
-0.18383386E+04-0.35921562E+02 0.42201591E+01 0.34928415E-01-0.36928839E-04	3
0.17622723E-07-0.28922901E-11 0.40294922E+03 0.11270744E+02	4
C2CL6 P06/96C 2CL 6 0 OG 300.000 5000.000	1

0.21271847E+02-0.12639830E-02 0.14274715E-05-0.38610193E-09 0.32802029E-13	2
-0.24164621E+05-0.75062607E+02 0.77888622E+01 0.40664885E-01-0.46075180E-04	3
0.22628070E-07-0.39246085E-11-0.20773922E+05-0.67850266E+01	4
C2CL5 P06/96C 2CL 5 0 OG 300.000 5000.000	1
0.17338524E+02 0.75760548E-03 0.16377437E-06-0.90971161E-10 0.92276608E-14	2
-0.21677263E+04-0.54349243E+02 0.72537951E+01 0.30117758E-01-0.30441270E-04	3
0.12969123E-07-0.17212493E-11 0.51967139E+03-0.26647606E+01	4
C2HCL5 P06/96C 2H 1CL 5 OG 300.000 5000.000	1
0.19006657E+02 0.80011255E-03 0.22282087E-06-0.99915555E-10 0.94312621E-14	2
-0.23834852E+05-0.65114525E+02 0.58341422E+01 0.38179144E-01-0.37595888E-04	3
0.15403444E-07-0.18817424E-11-0.20243217E+05 0.27133179E+01	4
CHFCL2 FC-21 g10/95C 1.H 1.F 1.CL 2.G 200.000 6000.00 1000.00	1
8.37401723E+00 4.30314499E-03-1.59217626E-06 2.62235213E-10-1.59210981E-14	2
-3.73789063E+04-1.46847225E+01 2.48413026E+00 2.08069354E-02-1.61071429E-05	3
2.49102694E-09 1.65635035E-12-3.57942445E+04 1.55938698E+01-3.42653987E+04	4
CHF2CL HCFC-22 T 6/11C 1.H 1.F 2.CL 1.G 200.000 6000.000 1000.00	1
7.76128170E+00 4.91347187E-03-1.82716472E-06 3.01909107E-10-1.83696720E-14	2
-6.10833550E+04-1.29719847E+01 2.58815578E+00 1.48447979E-02 1.50136954E-07	3
-1.39370626E-08 7.48510026E-12-5.94759437E+04 1.47131828E+01-5.80671621E+04	4
CHCLF tpis91C 1.H 1.F 1.CL 1.G 200.000 6000.000 1000.00	1
5.79907625E+00 3.87089199E-03-1.42325028E-06 2.33407383E-10-1.41278820E-14	2
-1.22754763E+04-2.86636087E+00 3.17163254E+00 4.39562862E-03 1.52334157E-05	3
-2.53605757E-08 1.10258963E-11-1.12721320E+04 1.22016293E+01-1.00414632E+04	4
CF3CL FC-13 ATcT/AC 1.F 3.CL 1. O.G 200.000 6000.000 1000.00	1
1.00910272E+01 2.97814049E-03-1.16598694E-06 1.99015814E-10-1.23754356E-14	2
-8.90715215E+04-2.52797602E+01 1.20856943E+00 3.31175441E-02-4.09170603E-05	3
2.42831659E-08-5.60239796E-12-8.69114408E+04 1.91836730E+01-8.53952909E+04	4
CF2CL tpis91C 1.F 2.CL 1. O.G 200.000 6000.000 1000.00	1
8.02826537E+00 2.01883629E-03-7.90446242E-07 1.34920166E-10-8.38987185E-15	2
-3.59242877E+04-1.26213146E+01 2.23327502E+00 2.07400983E-02-2.34004409E-05	3
1.18983365E-08-2.08808316E-12-3.44781789E+04 1.65915805E+01-3.30747092E+04	4
CFCL2 RUS 91C 1.F 1.CL 2. O.G 200.000 6000.000 1000.00	1
8.43494631E+00 1.61095820E-03-6.32734606E-07 1.08218634E-10-6.73872264E-15	2
-1.55335532E+04-1.33240848E+01 2.48480800E+00 2.32678936E-02-3.17729264E-05	3
2.09727276E-08-5.43785295E-12-1.41617230E+04 1.60941173E+01-1.26285253E+04	4
CF2CL2 FREON-12 T 6/11C 1.F 2.CL 2. O.G 200.000 6000.000 1000.00	1
1.06592482E+01 2.40830053E-03-9.45665269E-07 1.61716164E-10-1.00690307E-14	2
-6.33828537E+04-2.63364834E+01 1.43593509E+00 3.76738346E-02-5.53363470E-05	3
3.99081002E-08-1.14079923E-11-6.13190917E+04 1.89063992E+01-5.96318965E+04	4
CFCL3 FC-11 T 7/11C 1.F 1.CL 3. O.G 200.000 6000.000 1000.00	1
1.11913531E+01 1.87182223E-03-7.37586831E-07 1.26418446E-10-7.88344911E-15	2
-3.87724073E+04-2.79829261E+01 1.78320835E+00 4.15078790E-02-6.83507494E-05	3
5.43232731E-08-1.68194876E-11-3.68314630E+04 1.73140424E+01-3.49593662E+04	4
CF3CCL3 CCL3-CF3 T03/10C 2.CL 3.F 3. O.G 200.000 6000.000 1000.00	1
1.83386227E+01 3.72752259E-03-1.65550039E-06 3.01426912E-10-1.94679770E-14	2
-9.78629030E+04-6.24387417E+01 2.54280448E+00 6.08764967E-02-8.62331221E-05	3
6.07754537E-08-1.72690290E-11-9.41176258E+04 1.59691230E+01-9.13036318E+04	4
CF3CCL2H FC-123 T 5/10C 2.H 1.CL 2.F 3.G 200.000 6000.000 1000.00	1
1.56625902E+01 5.87170026E-03-2.37405900E-06 4.12118722E-10-2.58820189E-14	2
-9.70174588E+04-5.08181942E+01 2.84643751E+00 4.16333276E-02-3.58348291E-05	3
9.82621644E-09 1.07531569E-12-9.35022937E+04 1.52680777E+01-9.10998291E+04	4
CF3CCL2 OC 2F 3CL 2 G 300.000 3000.000 1000.00	1 H298=-
134.4/S298=87.0	
0.12035889E+02 0.10757107E-01-0.67932501E-05 0.19632769E-08-0.21407440E-12	2 set of vib
from Wang et al, THEOCHEM, 959, 2010, 101	
-0.72023432E+05-0.28654637E+02 0.31246545E+01 0.43582600E-01-0.51802326E-04	3
0.29149884E-07-0.63058656E-11-0.70100213E+05 0.15041777E+02	4
FCL OF 1CL 1 G 300.000 3000.000 1000.00	1
recalc., nist-chem-web, Chase, 1998	
0.35933072E+01 0.16815061E-02-0.10999110E-05 0.30178380E-09-0.24184684E-13	2
-0.71940390E+04 0.52576095E+01 0.25192378E+01 0.70816811E-02-0.10856019E-04	3
0.79097531E-08-0.22021513E-11-0.70344200E+04 0.10163399E+02	4
CFCLO T01/09C 1.O 1.F 1.CL 1.G 200.000 6000.000 1000.00	1
7.36494485E+00 2.62710462E-03-1.01273314E-06 1.71175837E-10-1.05744900E-14	2
-5.22709049E+04-1.02064249E+01 1.75554389E+00 2.23375897E-02-2.90814416E-05	3
1.93455212E-08-5.21729559E-12-5.09127525E+04 1.77760452E+01-4.96176665E+04	4

```

!
!*** C3HFx ***
!CF3CHCH2          H  3C  3F  3  0g  300.00  5000.00 1000.00      1
! 1.19726859E+01 1.25436030E-02-4.97049536E-06 8.98531469E-10-6.09049619E-14      2
!-8.09542161E+04-3.53084262E+01-1.76944260E-01 5.04272890E-02-4.98918705E-05      3
! 2.45443525E-08-4.55045979E-12-7.77960857E+04 2.64237596E+01      4
CF3CHCH2          H  3C  3F  3  0g  200.00  6000.00 1000.00      1 Burcat
! 1.22166309E+01 1.11177411E-02-4.07566929E-06 6.63454514E-10-3.98729557E-14      2
-8.08780489E+04-3.63340348E+01 1.56834820E+00 3.70715693E-02-1.66534622E-05      3
-1.15669918E-08 9.46282072E-12-7.78570098E+04 1.92579065E+01-7.59072147E+04      4
!CF3CCH2          H  2C  3F  3  0g  300.00  5000.00 1000.00      1
! 1.23019497E+01 9.51096222E-03-3.81477953E-06 6.95310445E-10-4.74033015E-14      2
!-4.99225413E+04-3.49756046E+01 8.07938725E-01 4.82284101E-02-5.55615570E-05      3
! 3.31924991E-08-8.04824987E-12-4.70705880E+04 2.27361360E+01      4
CF3CCH2          H  2C  3F  3  0g  200.00  6000.00 1000.00      1 Burcat
! 1.25859962E+01 8.12317961E-03-2.95982852E-06 4.80631726E-10-2.89086264E-14      2
-4.99277916E+04-3.65971752E+01 1.34293581E+00 4.37082126E-02-4.41291023E-05      3
! 1.98066011E-08-2.52757681E-12-4.70859152E+04 2.02494155E+01-4.50947551E+04      4
CF3CCH          H  1C  3F  3  0g  300.00  5000.00 1000.00      1
! 1.23075571E+01 6.73607631E-03-2.69300970E-06 4.89991898E-10-3.33727293E-14      2
-5.60204633E+04-3.43479861E+01 2.81616474E-01 5.25169846E-02-7.44406106E-05      3
! 5.35249568E-08-1.53175885E-11-5.33966440E+04 2.34333278E+01      4
!
!*** C2HOFx ***
CF3COCH3          H  3C  3O  1F  3g  300.00  5000.00 1000.00      1
! 1.37707128E+01 1.39114007E-02-5.56646243E-06 1.01277226E-09-6.89535233E-14      2
-1.06311755E+05-4.15671452E+01 2.31183560E+00 4.62931613E-02-3.86726491E-05      3
! 1.45780128E-08-1.48757320E-12-1.03127581E+05 1.75781936E+01      4
!
!*** CHBrx ***
!C2H3BR          H  3C  2Br 1  0g  300.00  5000.00 1000.00      1
! 6.18272332E+00 9.06458750E-03-3.48619075E-06 6.16873253E-10-4.11658974E-14      2
! 5.71731552E+03-5.39046319E+00 9.11868419E-01 2.57628448E-02-2.38745332E-05      3
! 1.17910898E-08-2.27220616E-12 7.08251435E+03 2.13419060E+01      4
!
!*** CHBrFx ***
CF3CHBRCH2       H  3C  3F  3BR 1g  300.00  5000.00 1000.00      1
! 1.55697883E+01 1.19400469E-02-4.72448387E-06 8.53282156E-10-5.78032768E-14      2
-7.03949517E+04-4.87869148E+01 1.47869208E+00 6.02024944E-02-6.99636869E-05      3
! 4.19438289E-08-1.01112486E-11-6.69599480E+04 2.17133393E+01      4
!BTP              H  2C  3F  3BR 1g  300.00  5000.00 1000.00      1 Hf -
143.7, db
! 1.46667151E+01 1.01380748E-02-4.06918919E-06 7.42198345E-10-5.06305036E-14      2
!-7.79627873E+04-4.51432754E+01 8.73900901E-01 5.74719145E-02-6.85523350E-05      3
! 4.19986296E-08-1.03943433E-11-7.45967271E+04 2.38649170E+01      4
BTP              H  2C  3F  3BR 1g  300.00  5000.00 1000.00      1 Hf -141.3, db
! 1.46667151E+01 1.01380748E-02-4.06918919E-06 7.42198345E-10-5.06305036E-14      2
-7.97462661E+04-4.51432754E+01 8.73900901E-01 5.74719145E-02-6.85523350E-05      3
! 4.19986296E-08-1.03943433E-11-7.33887771E+04 2.38649170E+01      4
CF3CBRCH         H  1C  3F  3BR 1g  300.00  5000.00 1000.00      1
! 1.51495752E+01 6.86658256E-03-2.79601807E-06 5.15042463E-10-3.53815429E-14      2
-4.66708144E+04-4.56453495E+01 1.65445273E+00 5.69985094E-02-7.77154359E-05      3
! 5.34289245E-08-1.46906054E-11-4.35725961E+04 2.09211868E+01      4
!
!*****
!*** HFO-1234yf Species ***
!*****
CH2CF3CF3        H  2C  3F  4  0g  300.00  5000.00 1000.00      1
! 1.38025152E+01 1.09423490E-02-4.38230123E-06 7.98269990E-10-5.44115721E-14      2
-1.04626748E+05-4.23589421E+01-1.40297627E-01 5.65621711E-02-6.25089680E-05      3
! 3.49176854E-08-7.75462767E-12-1.01117684E+05 2.79384422E+01      4
Z-CHCF3CF3       H  1C  3F  4  0g  300.00  5000.00 1000.00      1
! 1.43105513E+01 7.69863542E-03-3.13358295E-06 5.77166671E-10-3.96498418E-14      2
-7.21916057E+04-4.40025839E+01 2.86870469E-01 5.75830767E-02-7.40174904E-05      3
! 4.80980964E-08-1.25631262E-11-6.88652927E+04 2.57084409E+01      4
E-CHCF3CF3       H  1C  3F  4  0g  300.00  5000.00 1000.00      1

```

```

1.43305917E+01 7.67891368E-03-3.12554989E-06 5.75677977E-10-3.95468411E-14 2
-7.19438569E+04-4.40207007E+01 4.07734684E-01 5.71707819E-02-7.34031966E-05 3
4.76597961E-08-1.24406272E-11-6.86394188E+04 2.51983371E+01 4
CH3CF3 H 3C 3F 4 0g 300.00 5000.00 1000.00 1
1.40002765E+01 1.36222591E-02-5.43559860E-06 9.87263383E-10-6.71418143E-14 2
-9.78203459E+04-4.19517680E+01 2.30366232E+00 4.60562097E-02-3.66287581E-05 3
1.14678614E-08-1.26434216E-13-9.45626482E+04 1.85158056E+01 4
CH2CHF3 H 3C 3F 4 0g 300.00 5000.00 1000.00 1
1.47604910E+01 1.27071365E-02-5.02697832E-06 9.07940305E-10-6.15126187E-14 2
-9.62200064E+04-4.63478575E+01 1.20595493E+00 5.55551628E-02-5.65511018E-05 3
2.84465409E-08-5.40085009E-12-9.27416776E+04 2.23406976E+01 4
CH2OCF3 H 2C 3O 1F 4g 300.00 5000.00 1000.00 1
1.52762528E+01 1.27676333E-02-5.19710722E-06 9.56633072E-10-6.56661659E-14 2
-8.70427647E+04-4.83335154E+01 2.11292740E+00 4.95113084E-02-4.13366473E-05 3
1.41776903E-08-7.64498202E-13-8.33825341E+04 1.96744886E+01 4
CH2OCF3 H 2C 3O 1F 4g 300.00 5000.00 1000.00 1
1.55928095E+01 1.23410579E-02-4.99941576E-06 9.17684873E-10-6.28847743E-14 2
-9.13777965E+04-5.19182315E+01-2.05716188E-01 6.01344408E-02-5.84796652E-05 3
2.62383361E-08-3.93303490E-12-8.72171768E+04 2.86738951E+01 4
CHOCF3 H 1C 3O 1F 4g 300.00 5000.00 1000.00 1
1.56140203E+01 9.67087932E-03-4.00306546E-06 7.45060573E-10-5.15367334E-14 2
-1.07375545E+05-4.85831533E+01 2.64256070E+00 4.81858706E-02-4.66588830E-05 3
2.11934018E-08-3.41949252E-12-1.03891925E+05 1.78466606E+01 4
CH2COF H 2C 2O 1F 1g 300.00 5000.00 1000.00 1
7.75376004E+00 7.73264584E-03-3.00996167E-06 5.37492431E-10-3.61181564E-14 2
-3.32200786E+04-1.32815724E+01 6.64900022E-01 3.19056262E-02-3.57994882E-05 3
2.14338635E-08-5.24521787E-12-3.14753982E+04 2.22388006E+01 4
CF3CFCO C 3O 1F 4 0g 300.00 5000.00 1000.00 1
1.52017468E+01 7.18698806E-03-3.02060571E-06 5.67656920E-10-3.95204162E-14 2
-1.06844237E+05-4.63229211E+01 2.43402596E+00 5.03195764E-02-6.14439376E-05 3
3.83086790E-08-9.75004581E-12-1.03669877E+05 1.77895846E+01 4
CH3COFCF3 H 3C 3O 1F 4g 300.00 5000.00 1000.00 1
1.77036638E+01 1.24471876E-02-4.85050161E-06 8.67831752E-10-5.84327100E-14 2
-1.21367005E+05-6.13716136E+01 4.83326270E-01 7.29118287E-02-8.85136553E-05 3
5.47350862E-08-1.35377906E-11-1.17271570E+05 2.43519688E+01 4
CH3COF H 3C 2O 1F 1g 300.00 5000.00 1000.00 1
6.85691021E+00 1.14552570E-02-4.47324041E-06 8.00181950E-10-5.38228737E-14 2
-5.67055808E+04-8.42632051E+00 1.99917235E+00 2.16534404E-02-8.10218991E-06 3
-4.05220080E-09 3.06243164E-12-5.51552214E+04 1.75750981E+01 4
CH2OHCFCF3 H 3C 3O 1F 4g 300.00 5000.00 1000.00 1
1.63597683E+01 1.40264299E-02-5.54952222E-06 1.00303429E-09-6.80118648E-14 2
-1.15164874E+05-5.23627769E+01 2.39467310E+00 5.36744294E-02-4.47464036E-05 3
1.48151679E-08-4.00359510E-13-1.11356419E+05 1.95200627E+01 4
CH2COHFCF3 H 3C 3O 1F 4g 300.00 5000.00 1000.00 1
1.77036638E+01 1.24471876E-02-4.85050161E-06 8.67831752E-10-5.84327100E-14 2
-1.21367005E+05-6.13716136E+01 4.83326270E-01 7.29118287E-02-8.85136553E-05 3
5.47350862E-08-1.35377906E-11-1.17271570E+05 2.43519688E+01 4
CH2OHCFCF3 H 3C 3O 1F 4g 300.00 5000.00 1000.00 1
1.61146995E+01 1.47072157E-02-5.92769489E-06 1.08396913E-09-7.40696237E-14 2
-1.12947516E+05-5.30806522E+01 1.54612828E+00 5.56194484E-02-4.60052926E-05 3
1.51181549E-08-4.13557483E-13-1.08929774E+05 2.20728631E+01 4
CHOHCFCF3 H 3C 3O 1F 4g 300.00 5000.00 1000.00 1
1.67602347E+01 1.35203036E-02-5.31833487E-06 9.57574134E-10-6.47594099E-14 2
-1.18278762E+05-5.55735174E+01 1.91625062E+00 5.87277537E-02-5.61574645E-05 3
2.50416078E-08-3.70568753E-12-1.14395859E+05 2.00462717E+01 4
CHFCHOH H 3C 2O 1F 1g 300.00 5000.00 1000.00 1
7.65908139E+00 1.02592955E-02-3.89890440E-06 6.84992606E-10-4.55091077E-14 2
-4.05649548E+04-1.32900056E+01 5.03962241E-01 3.07679511E-02-2.40894438E-05 3
7.34117033E-09 1.16932670E-13-3.86366954E+04 2.34556762E+01 4
END

```

Transport parameters in CHEMKIN format

AR	0	136.500	3.330	0.000	0.000	0.000	
C	0	71.400	3.298	0.000	0.000	0.000	! *
CH	1	80.000	2.750	0.000	0.000	0.000	
CH2	1	144.000	3.800	0.000	0.000	0.000	
CH2*	1	144.000	3.800	0.000	0.000	0.000	
CH3	1	144.000	3.800	0.000	0.000	0.000	
CH4	2	141.400	3.746	0.000	2.600	13.000	
CO	1	98.100	3.650	0.000	1.950	1.800	
CO2	1	244.000	3.763	0.000	2.650	2.100	
HCO	2	498.000	3.590	0.000	0.000	0.000	
CH2O	2	498.000	3.590	0.000	0.000	2.000	
CH2OH	2	417.000	3.690	1.700	0.000	2.000	
CH3O	2	417.000	3.690	1.700	0.000	2.000	
CH3OH	2	481.800	3.626	0.000	0.000	1.000	! SVE
C2	1	97.530	3.621	0.000	1.760	4.000	
C2O	1	232.400	3.828	0.000	0.000	1.000	! *
C2H	1	209.000	4.100	0.000	0.000	2.500	
C2H2	1	209.000	4.100	0.000	0.000	2.500	
H2CC	2	209.000	4.100	0.000	0.000	2.500	
C2H3	2	209.000	4.100	0.000	0.000	1.000	! *
C2H4	2	280.800	3.971	0.000	0.000	1.500	
C2H5	2	252.300	4.302	0.000	0.000	1.500	
C2H6	2	252.300	4.302	0.000	0.000	1.500	
HCCO	2	150.000	2.500	0.000	0.000	1.000	! *
HCCOH	2	436.000	3.970	0.000	0.000	2.000	
CH2CO	2	436.000	3.970	0.000	0.000	2.000	
CH2CHO	2	436.000	3.970	0.000	0.000	2.000	
C2H2OH	2	224.700	4.162	0.000	0.000	1.000	! *
C3H2	2	209.000	4.100	0.000	0.000	1.000	! *
C3H3	2	252.000	4.760	0.000	0.000	1.000	! JAM
aC3H4	1	252.000	4.760	0.000	0.000	1.000	
pC3H4	1	252.000	4.760	0.000	0.000	1.000	
cC3H4	1	252.000	4.760	0.000	0.000	1.000	
CH2OCH2	1	252.000	4.760	0.000	0.000	1.000	
CH2OCH	1	252.000	4.760	0.000	0.000	1.000	
CH3CH2CHO	1	252.000	4.760	0.000	0.000	1.000	
C4H	1	357.000	5.180	0.000	0.000	1.000	
C4H2	1	357.000	5.180	0.000	0.000	1.000	
H2C4O	2	357.000	5.180	0.000	0.000	1.000	! JAM
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	! *
iC4H3	2	357.000	5.180	0.000	0.000	1.000	! JAM
nC4H3	2	357.000	5.180	0.000	0.000	1.000	! JAM
C4H4	2	357.000	5.180	0.000	0.000	1.000	! JAM
iC4H5	2	357.000	5.180	0.000	0.000	1.000	! JAM
nC4H5	2	357.000	5.180	0.000	0.000	1.000	! JAM
C4H5-2	2	357.000	5.180	0.000	0.000	1.000	!
C4H6	2	357.000	5.180	0.000	0.000	1.000	
C4H6-2	2	357.000	5.180	0.000	0.000	1.000	
C4H612	2	357.000	5.180	0.000	0.000	1.000	
CH3CHOCH2	2	357.000	5.180	0.000	0.000	1.000	
C5H2	1	357.000	5.180	0.000	0.000	1.000	
C5H3	1	357.000	5.180	0.000	0.000	1.000	
C5H5	1	357.000	5.180	0.000	0.000	1.000	
C5H6	1	357.000	5.180	0.000	0.000	1.000	
1C5H7	1	357.000	5.180	0.000	0.000	1.000	
C4H6O25	1	357.000	5.180	0.000	0.000	1.000	
C4H6O23	1	357.000	5.180	0.000	0.000	1.000	
C4H4O	1	357.000	5.180	0.000	0.000	1.000	
CH2CHCO	1	357.000	5.180	0.000	0.000	1.000	
CH3CHOCH2	1	357.000	5.180	0.000	0.000	1.000	
CH2CHCHCHO	1	357.000	5.180	0.000	0.000	1.000	
CH3CHCHCO	1	357.000	5.180	0.000	0.000	1.000	
C2H3CHOCH2	1	357.000	5.180	0.000	0.000	1.000	
CH3CHCHCHO	1	357.000	5.180	0.000	0.000	1.000	
C6H	1	357.000	5.180	0.000	0.000	1.000	
C6H2	1	357.000	5.180	0.000	0.000	1.000	



C6H3	2	357.000	5.180	0.000	0.000	1.000	!
l-C6H4	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
nC6H5	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
i-C6H5	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
l-C6H6	2	412.300	5.349	0.000	0.000	1.000	! (SVE)
n-C6H7	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
i-C6H7	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
C6H8	2	412.300	5.349	0.000	0.000	1.000	! (JAM)
HE	0	10.200	2.576	0.000	0.000	0.000	! *
H	0	145.000	2.050	0.000	0.000	0.000	
H2	1	38.000	2.920	0.000	0.790	280.000	
H2O	2	572.400	2.605	1.844	0.000	4.000	
H2O2	2	107.400	3.458	0.000	0.000	3.800	
HO2	2	107.400	3.458	0.000	0.000	1.000	! *
N2	1	97.530	3.621	0.000	1.760	4.000	
O	0	80.000	2.750	0.000	0.000	0.000	
O2	1	107.400	3.458	0.000	1.600	3.800	
OH	1	80.000	2.750	0.000	0.000	0.000	
c-C6H4	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H6	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H5	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H5CH3	2	495.3	5.68	0.43	12.30	1.000	!
C6H5C2H3	2	546.2	6.00	0.13	15.00	1.000	!
C6H5CH2	2	495.3	5.68	0.43	12.30	1.000	!
C6H5C2H	2	535.6	5.72	0.77	12.00	1.000	!
A2	2	630.4	6.18	0.00	16.50	1.000	!
c-C6H7	2	464.8	5.29	0.00	10.32	0.000	! benze
C5H4O	2	464.8	5.29	0.00	10.32	0.000	! benze
C5H5O	2	464.8	5.29	0.00	10.32	0.000	! benze
C5H4OH	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H5O	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H5OH	2	464.8	5.29	0.00	10.32	0.000	! benze
ac3H5	2	266.800	4.982	0.000	0.000	1.000	
CH3CCH2	2	266.800	4.982	0.000	0.000	1.000	
CH3CHCH	2	266.800	4.982	0.000	0.000	1.000	
C3H6	2	266.800	4.982	0.000	0.000	1.000	
C3H7	2	266.800	4.982	0.000	0.000	1.000	
C4H6	2	357.000	5.180	0.000	0.000	1.000	
iC3H7	2	266.800	4.982	0.000	0.000	1.000	
nC3H7	2	266.800	4.982	0.000	0.000	1.000	
C3H8	2	266.800	4.982	0.000	0.000	1.000	
C4H	1	357.000	5.180	0.000	0.000	1.000	
C4H2	1	357.000	5.180	0.000	0.000	1.000	
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	! *
iC4H5	2	357.000	5.176	0.000	0.000	1.000	
C4H6	2	357.000	5.176	0.000	0.000	1.000	
C4H7	2	357.000	5.176	0.000	0.000	1.000	
iC4H7	2	357.000	5.176	0.000	0.000	1.000	
C4H81	2	357.000	5.176	0.000	0.000	1.000	
C4H82	2	357.000	5.176	0.000	0.000	1.000	
iC4H8	2	357.000	5.176	0.000	0.000	1.000	
tC4H9	2	357.000	5.176	0.000	0.000	1.000	
iC4H9	2	357.000	5.176	0.000	0.000	1.000	
pC4H9	2	357.000	5.176	0.000	0.000	1.000	
sC4H9	2	357.000	5.176	0.000	0.000	1.000	
C4H10	2	357.000	5.176	0.000	0.000	1.000	
iC4H10	2	357.000	5.176	0.000	0.000	1.000	
CH3COCH3	2	357.000	5.176	0.000	0.000	1.000	
C2H3CHO	2	357.000	5.176	0.000	0.000	1.000	
iC4H7O	2	450.000	5.500	0.000	0.000	1.000	! JAM
CH3CHO	2	436.000	3.970	0.000	0.000	2.000	
CH3CO	2	436.000	3.970	0.000	0.000	2.000	
C5H5O (2, 4)	2	494	5.2	1.6	0.0	1.0	
C5H5O (1, 2)	2	494	5.2	1.6	0.0	1.0	
C5H5O (1, 3)	2	494	5.2	1.6	0.0	1.0	
C4H5	2	329	5.1	0.0	0.0	1.0	

c-C4H5	2	329	5.1	0.0	0.0	1.0	
C6H5CO	2	593	5.5	2.8	0.0	1.0	
C6H5CHO	2	593	5.47	2.8	0.0	1.0	
C6H5C2H5	2	485	5.425	0.4	0.0	1.0	
C6H4O2	2	485	5.425	0.4	0.0	1.0	
HOC6H4CH3	2	567	5.60	1.6	0.0	1.0	
C6H5CH2OH	2	572	5.82	1.7	0.0	1.0	
bi-C6H5CH2	2	620	7.24	0.0	0.0	1.0	
C5H5OH	2	464.800	5.290	0.000	10.320	0.000	! as C5H4OH, ZD99
C5H4OH	2	464.800	5.290	0.000	10.320	0.000	! benze
o-C6H4	2	464.8	5.29	0.00	10.32	0.000	! benze
C6H5C6H5	2	676.5	6.31	0.00	20.00	1.000	! biphe
OC6H4CH3	2	567	5.6	1.6	0.0	1.000	
C10H8	2	630.4	6.18	0.00	16.50	1.000	! napht
C6H4CH3	2	495.3	5.68	0.43	12.30	1.000	!
C2H5OH	2	470.600	4.410	0.000	0.000	1.500	! NMM
CH3CHOH	2	470.600	4.410	0.000	0.000	1.500	
C2H4OH	2	470.600	4.410	0.000	0.000	1.500	
CH3CH2O	2	470.600	4.410	0.000	0.000	1.500	! NMM
HOC2H4O2	2	443.200	4.120	0.000	0.000	1.000	
F	0	80.000	2.750	0.000	0.000	0.000	!
F2	1	125.700	3.301	0.000	1.600	3.800	!
HF	1	330.000	3.148	1.920	2.460	1.000	! (sv/mec)
HF0	1	352.000	2.490	1.730	0.000	5.000	!
HF1	1	352.000	2.490	1.730	0.000	5.000	!
HF2	1	352.000	2.490	1.730	0.000	5.000	!
HF3	1	352.000	2.490	1.730	0.000	5.000	!
HF4	1	352.000	2.490	1.730	0.000	5.000	!
HF5	1	352.000	2.490	1.730	0.000	5.000	!
HF6	1	352.000	2.490	1.730	0.000	5.000	!
HF7	1	352.000	2.490	1.730	0.000	5.000	!
HF8	1	352.000	2.490	1.730	0.000	5.000	!
HOF	2	107.400	3.458	0.000	0.000	0.000	! (ois)
F2O	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO	1	109.600	3.412	0.000	0.000	0.000	! (ois)
HOOF	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
F2O2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
FO2	2	107.400	3.458	0.000	0.000	0.000	!prwH2O2?
CH3F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CH2F2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF3	2	262.	4.123	1.8	0.000	0.000	!ReidPRW
CF4	2	134.0	4.662	0.000	0.000	0.000	!ReidPra
CH2F	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CHF2	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF3	2	121.000	4.320	0.000	0.000	0.000	! (ois)
CHF	2	262.	4.123	1.8	0.000	0.000	!PRW2/93
CF2	2	108.000	3.977	0.000	0.000	0.000	! (ois)
CF	1	94.200	3.635	0.000	0.000	0.000	! (Svehla)
CF3OH	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3OF	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CH2FO	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF2O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF3O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CHF:O	2	350.500	4.906	0.000	0.000	0.000	!prwCF2O?
CF2:O	2	350.500	4.906	0.000	0.000	0.000	! (ois)
CF:O	2	860.000	4.000	0.000	0.000	0.000	! (ois)
CH3-CH2F	2	312.2	4.583	2.0	0.000	0.000	!ReidPRW
CH3-CHF2	2	323.4	4.798	2.3	0.000	0.000	!ReidPRW
CH2F-CH2F	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF3	2	289.1	4.911	2.3	0.000	0.000	!ReidPRW
CH2F-CHF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF3	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CHF2-CHF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CHF2-CF3	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93

CHF2-CHF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CHF2-CF3	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CF3-CF3	2	231.8	4.969	0.0	0.000	0.000	!PRW2/93
CH3-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH2F-CH2	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CH3-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CHF	2	312.2	4.583	2.0	0.000	0.000	!PRW2/93
CHF2-CH2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CH2F-CF2	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CHF	2	323.4	4.798	2.3	0.000	0.000	!PRW2/93
CHF2-CF2	2	323.4	4.85	2.0	0.000	0.000	!PRW2/93
CF3-CH2	2	289.1	4.911	2.3	0.000	0.000	!PRW2/93
CF3-CHF	2	323.4	4.85	2.3	0.000	0.000	!PRW2/93
CF3-CF2	2	323.4	4.9	1.5	0.000	0.000	!PRW2/93
CH2:CHF	2	272.2	4.322	1.4	0.000	0.000	!ReidPRW
CH2:CF2	2	251.5	4.442	1.4	0.000	0.000	!ReidPRW
CHF:CHF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CHF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CHF[Z]	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF2	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CF2	2	254.2	4.647	0.0	0.000	0.000	!ReidPRW
CH2:CF	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-E	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH-Z	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CH[Z]	2	272.2	4.322	1.4	0.000	0.000	!PRW2/93
CHF:CF-E	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF-Z	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CHF:CF[Z]	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CH	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
CF2:CF	2	251.5	4.442	1.4	0.000	0.000	!PRW2/93
C2HF	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
C2F2	1	240.	4.4	0.	0.000	0.000	!PRW2/93
C2F	1	225.	4.25	1.0	0.000	0.000	!PRW2/93
CHF <sub>2</sub> CO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF <sub>2</sub> CO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
FCCO-E	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
FCO	2	350.500	4.906	0.000	0.000	0.000	!PRW10/93?
CF <sub>2</sub> CL <sub>2</sub>	2	253.000	5.250	0.000	0.000	0.000	!(ois)
CF <sub>2</sub> CLBR	2	253.000	5.250	0.000	0.000	0.000	!(ois)

/data included by R hynes for FM-200 species and some others^M  
/the data for these compounds is based on C2 compounds of similar structure^M  
/the data used is NIST's data; see above species. e.g. C3F7 = C2F5 etc.^M

!C3F7	2	323.4	4.9	1.5	0.00	0.00	!C2F5 data ^M
!C3F7H	2	323.4	4.9	1.5	0.000	0.00	!CF3CF2H^M
C3F7H	2	795.3	4.7	0.0	0.000	0.00	!Smith KD^M
C3F7	2	795.3	4.7	0.0	0.000	0.00	!c3f7h data^M
!C3F7H	2	730.5	6.7	0.0	0.000	0.00	!Frencklach/Wang mw- approximation^M
!C3F6	2	254.2	4.647	0.0	0.000	0.000	!C2F4 data^M
C3F6	2	795.3	4.7	0.0	0.000	0.00	!c3f7h dt^M
CF <sub>3</sub> CO	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>2</sub> O ^M
CF <sub>3</sub> CHO	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>2</sub> O data^M
CF <sub>3</sub> COF	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>2</sub> O data^M
!C3F6O	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>2</sub> O dt^M
C3F6O	2	795.3	4.7	0.0	0.000	0.00	!c3f7h-Smith KD^M
!C3F7OH	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>3</sub> O dta^M
C3F7OH	2	795.3	4.7	0.0	0.000	0.00	!c3f7h-Smith KD^M
!C3F7O	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>3</sub> O data^M
C3F7O	2	795.3	4.7	0.0	0.000	0.00	!c3f7h-Smith KD^M
C3F7O <sub>2</sub>	2	350.500	4.906	0.000	0.000	0.000	!CF <sub>3</sub> O data^M
C2F <sub>5</sub> COC3F7	2	1045.0	8.2	0.000	0.000	0.000	!Frencklach/Wang-mw- correlation^M
!C2F <sub>5</sub> COC3F7	2	385.0	6.64	0.000	0.000	0.000	!Pc-Tc-
correlation,reid et al,p.29,^M							
C3F7CO	2	398.4	6.16	0.000	0.000	0.000	!setokuchi et al, chem.phys.let.,2006,429,p.360^M

C2F5CO	2	376.4	5.59	0.000	0.000	0.000	!setokuchi et al,
chem.phys.let.,2006,429,p.360^M							
C3F7CHO	2	398.4	6.16	0.000	0.000	0.000	!c3f7co-setokuchi et
al, chem.phys.let.,2006,429,p.360^M							
C2F5CHO	2	376.4	5.59	0.000	0.000	0.000	!c2f5co-setokuchi et
al, chem.phys.let.,2006,429,p.360^M							
!							
CL	0	151.000	3.339	0.000	2.300	1.0	
HCL	1	344.700	3.339	1.100	2.640	1.0	
CL2	1	316.000	4.217	0.200	4.600	1.0	
CLO	1	211.350	3.842	1.700	2.990	1.0	
HOCL	2	453.970	3.968	1.930	3.390	1.0	
COCL2	1	376.000	4.700	1.100	6.790	1.0	
CHCLO	2	361.000	4.340	1.500	4.890	1.0	
CHCL	1	224.700	4.163	1.570	3.730	1.0	
CCL2	1	348.000	4.644	0.000	5.630	1.0	
CCL3	2	444.360	5.031	0.000	7.930	1.0	
CHCL2	2	420.850	4.694	1.570	6.030	1.0	
CH2CL	2	340.280	4.305	0.800	3.830	1.0	
CH3CL	2	350.000	4.182	1.900	4.230	1.0	
CH2CL2	2	356.300	4.898	1.800	6.430	1.0	
CHCL3	2	340.200	5.389	1.100	8.330	1.0	
CCL4	2	322.700	5.947	0.000	10.530	1.0	
C2HCL	1	332.620	4.335	0.440	5.540	1.0	
C2CL2	1	442.700	4.958	0.000	7.440	1.0	
CH2CCL	1	345.170	4.738	1.500	5.740	1.0	
CHCHCL	1	345.170	4.738	1.500	5.740	1.0	
CHCLCCL	1	426.190	5.140	0.900	7.640	1.0	
CHCCL2	1	426.190	5.140	0.900	7.640	1.0	
C2CL3	1	473.360	5.247	0.900	9.540	1.0	
C2H3CL	1	349.000	4.644	1.500	6.140	1.0	
CH2CCL2	1	412.180	5.013	1.340	8.040	1.0	
CHCLCHCL	1	426.190	5.140	0.900	8.040	1.0	
CH2CHCL2	1	426.190	5.140	0.900	8.040	1.0	
C2HCL3	1	472.500	5.316	0.900	9.940	1.0	
CHCLCHCL2	1	472.500	5.316	0.900	9.940	1.0	
CH2CCL3	1	472.500	5.316	0.900	9.940	1.0	
C2CL4	1	514.900	5.640	0.000	11.840	1.0	
CHCLCCL3	1	514.900	5.640	0.000	11.840	1.0	
CH2CH2CL	2	379.290	4.816	2.000	5.960	1.0	
CH3CHCL	2	379.290	4.816	2.000	5.960	1.0	
CH2CLCHCL	2	471.190	5.116	1.800	7.860	1.0	
CH3CCL2	2	435.910	5.103	2.000	7.860	1.0	
CHCL2CH2	2	435.910	5.103	2.000	7.860	1.0	
CH2CLCCL2	2	498.910	5.379	1.700	9.760	1.0	
CHCL2CCL2	2	525.050	5.872	1.320	11.660	1.0	
C2CL5	2	556.000	6.142	0.910	13.560	1.0	
C2H5CL	2	300.000	4.898	2.000	6.360	1.0	
CH3CHCL2	2	435.900	5.102	2.000	8.260	1.0	
CH2CLCH2CL	2	471.200	5.116	1.800	8.260	1.0	
CH2CLCHCL2	2	498.900	5.397	1.700	10.160	1.0	
CH3CCL3	2	454.000	5.406	1.770	10.160	1.0	
CHCL2CHCL2	2	540.700	5.868	1.320	12.060	1.0	
CH2CLCCL3	2	520.600	5.841	1.390	12.060	1.0	
C2HCL5	2	556.000	6.142	0.920	13.960	1.0	
C2CL6	2	581.780	6.457	0.000	15.860	1.0	
CH2CLO	2	535.00	4.610	1.800	4.820	1.0	
CCLO	1	388.530	4.730	1.800	4.490	1.0	
!							
CF3CCL2H	2	221.75	4.053	3.100	0.000	1.0	!2003,Stoll
etal, J.Chem.Phys.,119,11396,cor.dip.mom.							
CF3CCL2	2	221.75	4.053	3.100	0.000	1.0	
!CF3CCL2H,cor.dip.mom.							
CF3CCL3	2	221.75	4.053	3.100	0.000	1.0	
!CF3CCL2H,cor.dip.mom.							
CFCL2	2	220.69	3.652	2.630	0.000	1.0	!CHFCL2,cor.dip.mom.

CF2CL	2	177.43	3.468	2.100	0.000	1.0	!CHF2CL,cor.dip.mom.
CF3CL	2	149.95	3.618	1.826	0.000	1.0	!2003,Stoll
etal,J.Chem.Phys.,119,11396							
CF2CL2	2	185.66	3.829	2.322	0.000	1.0	!2003,Stoll
etal,J.Chem.Phys.,119,11396							
CFCL3	2	224.15	4.021	2.701	0.000	1.0	!2003,Stoll
etal,J.Chem.Phys.,119,11396							
CHF2CL	2	177.43	3.468	2.100	0.000	1.0	!2003,Stoll
etal,J.Chem.Phys.,119,11396,cor.dip.mom.							
CHFCL2	2	220.69	3.652	2.630	0.000	1.0	!2003,Stoll
etal,J.Chem.Phys.,119,11396,cor.dip.mom.							
FCL	1	211.350	3.842	1.700	2.990	1.0	!CLO
!							
BR2	1	507.9	4.296	0.2	7.02	0.0	!Reid-
!BR2		520.	4.268				!Hirsh
HBR	1	449.	3.353	0.8	3.61	0.0	!Reid-
BR	0	230.	3.7	0.0	0.00	0.0	
BRO	1	360.	3.8	1.76	0.0	0.0	
BROH	2	440.	3.95	0.0	0.0	0.0	
CH3BR	2	449.2	4.118	1.8	5.87	0.0	!Reid-
CH2BR	2	449.	4.1	0.0	0.0	0.0	
C2H5BR	2	470.	4.85	2.0	8.05	0.0	
C2H3BR	2	460.	4.6	1.42	7.59	0.0	
CF3BR	2	270.	4.1	0.0	0.0	0.0	
!							
CF3CHCH2	2	335.	4.7	0.0	0.0	0.0	!btp-species,weight
correlation with "empirical-average"							
CF3CCH2	2	333.	4.7	2.444	6.006	0.0	!correction for br-f-
species							
CF3CCH	2	331.	4.7	0.0	0.0	0.0	
CF3COCH3	2	367.	5.0	0.0	0.0	0.0	
CF3CHBRCH2	2	477.	5.8	0.0	0.0	0.0	
CF3CBRCH2	2	475.	5.8	0.0	0.0	0.0	
BTP	2	475.	5.8	0.0	0.0	0.0	
CF3CBRCH	2	473.	5.7	0.0	0.0	0.0	
!							
CH2CF3	2	281.140	5.328	2.684	4.863	1.000	
Z-CHCF3	2	335.000	4.700	2.722	4.631	1.000	
E-CHCF3	2	335.000	4.700	2.451	4.636	1.000	
CH3CF3	2	281.140	5.328	2.751	4.992	1.000	
CH2CHF3	2	281.140	5.328	2.689	4.884	1.000	
CH2OCF3	2	300.000	5.500	1.969	5.356	1.000	
CH2COF3	2	300.000	5.500	2.490	5.356	1.000	
CHOCF3	2	300.000	5.500	2.284	5.238	1.000	
CH2COF	2	312.200	4.583	3.302	3.442	1.000	
CF3CFCO	2	300.000	5.500	1.087	5.012	1.000	
CH3COF3	2	300.000	5.500	2.571	5.356	1.000	
CH3COF	2	350.500	4.906	3.375	3.605	1.000	
CH2OHCF3	2	300.000	5.500	1.739	5.532	1.000	
CH2COHF3	2	300.000	5.500	1.266	5.337	1.000	
CH2OCHF3	2	300.000	5.500	1.653	5.492	1.000	
CHOHCF3	2	300.000	5.500	2.369	5.541	1.000	
CHFCHOH	2	350.500	4.906	3.580	3.882	1.000	

## Kinetic parameters in CHEMKIN format

REACTIONS			
H+O2<=>O+OH	2.203E+16	-0.671	17041.00
O+H2<=>H+OH	4.589E+04	2.700	6260.00
OH+H2<=>H+H2O	1.734E+08	1.510	3430.00
2OH<=>O+H2O	3.973E+04	2.400	-2110.00

2H+M<=>H2+M	1.780E+18	-1.000	0.00
H2/0.00/ H2O/0.00/ CO2/0.00/ AR/0.63/			
2H+H2<=>2H2	9.000E+16	-0.600	0.00
2H+H2O<=>H2+H2O	5.624E+19	-1.250	0.00
2H+CO2<=>H2+CO2	5.500E+20	-2.000	0.00
H+OH+M<=>H2O+M	1.100E+22	-2.000	0.00
H2/2.00/ H2O/6.30/ CO/1.75/ CO2/3.60/ AR/0.38/			
O+H+M<=>OH+M	9.428E+18	-1.000	0.00
H2/ 2.00/ H2O/12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/			
2O+M<=>O2+M	1.200E+17	-1.000	0.00
H2/ 2.40/ H2O/15.40/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.83/			
H+O2 (+M) <=>HO2 (+M)	6.139E+12	0.440	0.00
LOW / 7.594E+19 -1.400 0.00/			
TROE/ 0.5000 0.10E-29 0.10E+31 0.00E+00 /			
H2O/11.89/ O2/ 0.85/ CO/ 1.09/ CO2/ 2.18/ AR/ 0.40/			
H2+O2<=>HO2+H	5.916E+05	2.433	53502.00
2OH (+M) <=>H2O2 (+M)	1.110E+14	-0.370	0.00
LOW / 2.010E+17 -0.584 -2293.00/			
TROE/ 0.7346 94.00 1756.00 5182.00 /			
H2/2.00/ H2O/6.00/ CO/1.75/ CO2/3.60/ AR/0.70/			
HO2+H<=>O+H2O	3.970E+12	0.000	671.00
HO2+H<=>2OH	3.743E+13	0.000	295.00
HO2+O<=>OH+O2	4.000E+13	0.000	0.00
2HO2<=>O2+H2O2	1.300E+11	0.000	-1630.00
DUPLICATE			
2HO2<=>O2+H2O2	3.658E+14	0.000	12000.00
DUPLICATE			
OH+HO2<=>H2O+O2	1.410E+18	-1.760	60.00
DUPLICATE			
OH+HO2<=>H2O+O2	1.120E+85	-22.300	26900.00
DUPLICATE			
DUPLICATE			
OH+HO2<=>H2O+O2	1.074E+71	-16.720	32900.00
DUPLICATE			
DUPLICATE			
OH+HO2<=>H2O+O2	2.510E+12	2.000	40000.00
DUPLICATE			
DUPLICATE			
OH+HO2<=>H2O+O2	1.000+136	-40.000	34800.00
DUPLICATE			
H2O2+H<=>HO2+H2	6.050E+06	2.000	5200.00
H2O2+H<=>OH+H2O	2.410E+13	0.000	3970.00
H2O2+O<=>OH+HO2	9.630E+06	2.000	3970.00
H2O2+OH<=>HO2+H2O	2.000E+12	0.000	427.00
DUPLICATE			
H2O2+OH<=>HO2+H2O	2.670E+41	-7.000	37600.00
DUPLICATE			
CO+O (+M) <=>CO2 (+M)	1.362E+10	0.000	2384.00
LOW / 1.173E+24 -2.790 4191.00/			
H2/ 2.00/ H2O/12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/			
CO+OH<=>CO2+H	5.872E+04	2.053	-355.67
DUPLICATE			
CO+OH<=>CO2+H	5.757E+12	-0.664	331.83
DUPLICATE			
CO+O2<=>CO2+O	1.119E+12	0.000	47700.00
CO+HO2<=>CO2+OH	1.570E+05	2.180	17942.61
HCO+H<=>CO+H2	8.592E+13	0.000	0.00
HCO+O<=>CO+OH	3.000E+13	0.000	0.00
HCO+O<=>CO2+H	3.000E+13	0.000	0.00
HCO+OH<=>CO+H2O	3.020E+13	0.000	0.00
HCO+M<=>CO+H+M	3.740E+17	-1.000	17000.00
H2/2.00/ H2O/0.00/ CO/1.75/ CO2/3.60/			
HCO+H2O<=>CO+H+H2O	1.122E+18	-1.000	17000.00
HCO+O2<=>CO+HO2	2.408E+10	0.807	-727.00
CO+H2 (+M) <=>CH2O (+M)	4.300E+07	1.500	79600.00
LOW / 5.070E+27 -3.420 84350.00/			

```

TROE/ 0.9320 197.00 1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
C+OH<=>CO+H 5.000E+13 0.000 0.00
C+O2<=>CO+O 5.800E+13 0.000 576.00
CH+H<=>C+H2 1.100E+14 0.000 0.00
CH+O<=>CO+H 5.700E+13 0.000 0.00
CH+OH<=>HCO+H 3.000E+13 0.000 0.00
CH+H2<=>CH2+H 1.107E+08 1.790 1670.00
CH+H2O<=>CH2O+H 5.710E+12 0.000 -755.00
CH+O2<=>HCO+O 3.300E+13 0.000 0.00
CH+CO (+M) <=>HCCO (+M) 5.000E+13 0.000 0.00
LOW / 2.690E+28 -3.740 1936.00/
TROE/ 0.5757 237.00 1652.00 5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH+CO2<=>HCO+CO 3.400E+12 0.000 690.00
HCO+H (+M) <=>CH2O (+M) 1.090E+12 0.480 -260.00
LOW / 1.350E+24 -2.570 1425.00/
TROE/ 0.7824 271.00 2755.00 6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH2+H (+M) <=>CH3 (+M) 2.500E+16 -0.800 0.00
LOW / 3.200E+27 -3.140 1230.00/
TROE/ 0.6800 78.00 1995.00 5590.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH2+O<=>HCO+H 8.000E+13 0.000 0.00
CH2+OH<=>CH2O+H 2.000E+13 0.000 0.00
CH2+OH<=>CH+H2O 1.130E+07 2.000 3000.00
CH2+H2<=>H+CH3 5.000E+05 2.000 7230.00
CH2+O2<=>HCO+OH 1.060E+13 0.000 1500.00
CH2+O2<=>CO2+2H 2.640E+12 0.000 1500.00
CH2+HO2<=>CH2O+OH 2.000E+13 0.000 0.00
CH2+C<=>C2H+H 5.000E+13 0.000 0.00
CH2+CO (+M) <=>CH2CO (+M) 8.100E+11 0.500 4510.00
LOW / 2.690E+33 -5.110 7095.00/
TROE/ 0.5907 275.00 1226.00 5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH2+CH<=>C2H2+H 4.000E+13 0.000 0.00
2CH2<=>C2H2+H2 3.200E+13 0.000 0.00
CH2*+N2<=>CH2+N2 1.500E+13 0.000 600.00
CH2*+AR<=>CH2+AR 9.000E+12 0.000 600.00
CH2*+H<=>CH+H2 3.000E+13 0.000 0.00
CH2*+O<=>CO+H2 1.500E+13 0.000 0.00
CH2*+O<=>HCO+H 1.500E+13 0.000 0.00
CH2*+OH<=>CH2O+H 3.000E+13 0.000 0.00
CH2*+H2<=>CH3+H 7.000E+13 0.000 0.00
CH2*+O2<=>H+OH+CO 2.800E+13 0.000 0.00
CH2*+O2<=>CO+H2O 1.200E+13 0.000 0.00
CH2*+H2O (+M) <=>CH3OH (+M) 2.000E+13 0.000 0.00
LOW / 2.700E+38 -6.300 3100.00/
TROE/ 0.1507 134.00 2383.00 7265.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2*+H2O<=>CH2+H2O 3.000E+13 0.000 0.00
CH2*+CO<=>CH2+CO 9.000E+12 0.000 0.00
CH2*+CO2<=>CH2+CO2 7.000E+12 0.000 0.00
CH2*+CO2<=>CH2O+CO 1.400E+13 0.000 0.00
CH2O+H (+M) <=>CH2OH (+M) 5.400E+11 0.454 3600.00
LOW / 1.270E+32 -4.820 6530.00/
TROE/ 0.7187 103.00 1291.00 4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2O+H (+M) <=>CH3O (+M) 5.400E+11 0.454 2600.00
LOW / 2.200E+30 -4.800 5560.00/
TROE/ 0.7580 94.00 1555.00 4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2O+H<=>HCO+H2 2.300E+10 1.050 3275.00
CH2O+O<=>HCO+OH 3.900E+13 0.000 3540.00
CH2O+OH<=>HCO+H2O 6.860E+09 1.180 -447.00
CH2O+O2<=>HCO+HO2 1.000E+14 0.000 40000.00

```

CH2O+HO2<=>HCO+H2O2	4.110E+04	2.500	10205.00
CH2O+CH<=>CH2CO+H	9.460E+13	0.000	-515.00
CH3+H (+M) <=>CH4 (+M)	3.175E+15	-0.630	383.00
LOW / 6.193E+32 -4.760 2440.00/			
TROE/ 0.7830 74.00 2941.00 6964.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
CH3+O<=>CH2O+H	8.430E+13	0.000	0.00
CH3+OH (+M) <=>CH3OH (+M)	6.300E+13	0.000	0.00
LOW / 2.700E+38 -6.300 3100.00/			
TROE/ 0.2105 83.50 5398.00 8370.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH3+OH<=>CH2+H2O	5.600E+07	1.600	5420.00
CH3+OH<=>CH2*+H2O	1.250E+14	0.000	0.00
CH3+O2<=>O+CH3O	3.083E+13	0.000	28800.00
CH3+O2<=>OH+CH2O	3.600E+10	0.000	8940.00
CH3+HO2<=>CH4+O2	1.000E+12	0.000	0.00
CH3+HO2<=>CH3O+OH	2.411E+13	0.000	0.00
CH3+H2O2<=>CH4+HO2	2.450E+04	2.470	5180.00
CH3+C<=>C2H2+H	5.000E+13	0.000	0.00
CH3+CH<=>C2H3+H	3.000E+13	0.000	0.00
CH3+HCO<=>CH4+CO	8.480E+12	0.000	0.00
CH3+CH2O<=>CH4+HCO	3.320E+03	2.810	5860.00
CH3+CH2<=>C2H4+H	4.000E+13	0.000	0.00
CH3+CH2* <=>C2H4+H	1.200E+13	0.000	-570.00
2CH3 (+M) <=>C2H6 (+M)	4.240E+16	-0.970	620.00
LOW / 3.540E+50 -9.670 6220.00/			
TROE/ 0.5325 151.00 1038.00 4970.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
2CH3<=>H+C2H5	1.408E+13	0.100	10600.00
CH3+HCCO<=>C2H4+CO	5.000E+13	0.000	0.00
CH3+C2H<=>C3H3+H	2.410E+13	0.000	0.00
CH3O+H (+M) <=>CH3OH (+M)	5.000E+13	0.000	0.00
LOW / 8.600E+28 -4.000 3025.00/			
TROE/ 0.8902 144.00 2838.00 45569.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH3O+H<=>CH2OH+H	3.400E+06	1.600	0.00
CH3O+H<=>CH2O+H2	2.000E+13	0.000	0.00
CH3O+H<=>CH3+OH	3.200E+13	0.000	0.00
CH3O+H<=>CH2*+H2O	1.600E+13	0.000	0.00
CH3O+O<=>CH2O+OH	1.000E+13	0.000	0.00
CH3O+OH<=>CH2O+H2O	5.000E+12	0.000	0.00
CH3O+O2<=>CH2O+HO2	4.280E-13	7.600	-3530.00
CH2OH+H (+M) <=>CH3OH (+M)	1.800E+13	0.000	0.00
LOW / 3.000E+31 -4.800 3300.00/			
TROE/ 0.7679 338.00 1812.00 5081.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH2OH+H<=>CH2O+H2	2.000E+13	0.000	0.00
CH2OH+H<=>CH3+OH	1.200E+13	0.000	0.00
CH2OH+H<=>CH2*+H2O	6.000E+12	0.000	0.00
CH2OH+O<=>CH2O+OH	1.000E+13	0.000	0.00
CH2OH+OH<=>CH2O+H2O	5.000E+12	0.000	0.00
CH2OH+O2<=>CH2O+HO2	1.800E+13	0.000	900.00
CH4+H<=>CH3+H2	6.600E+08	1.620	10840.00
CH4+O<=>CH3+OH	1.020E+09	1.500	8600.00
CH4+OH<=>CH3+H2O	1.000E+08	1.600	3120.00
CH4+CH<=>C2H4+H	6.000E+13	0.000	0.00
CH4+CH2<=>2CH3	2.460E+06	2.000	8270.00
CH4+CH2* <=>2CH3	1.600E+13	0.000	-570.00
CH4+C2H<=>C2H2+CH3	1.810E+12	0.000	500.00
CH3OH+H<=>CH2OH+H2	1.700E+07	2.100	4870.00
CH3OH+H<=>CH3O+H2	4.200E+06	2.100	4870.00
CH3OH+O<=>CH2OH+OH	3.880E+05	2.500	3100.00
CH3OH+O<=>CH3O+OH	1.300E+05	2.500	5000.00
CH3OH+OH<=>CH2OH+H2O	1.440E+06	2.000	-840.00
CH3OH+OH<=>CH3O+H2O	6.300E+06	2.000	1500.00
CH3OH+CH3<=>CH2OH+CH4	3.000E+07	1.500	9940.00



CH3OH+CH3<=>CH3O+CH4	1.000E+07	1.500	9940.00
C2H+H(+M)<=>C2H2(+M)	1.000E+17	-1.000	0.00
LOW / 3.750E+33 -4.800 1900.00/			
TROE/ 0.6464 132.00 1315.00 5566.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H+O<=>CH+CO	5.000E+13	0.000	0.00
C2H+OH<=>H+HCCO	2.000E+13	0.000	0.00
C2H+O2<=>HCO+CO	5.000E+13	0.000	1500.00
C2H+H2<=>H+C2H2	4.900E+05	2.500	560.00
C2O+H<=>CH+CO	5.000E+13	0.000	0.00
C2O+O<=>2CO	5.000E+13	0.000	0.00
C2O+OH<=>2CO+H	2.000E+13	0.000	0.00
C2O+O2<=>2CO+O	2.000E+13	0.000	0.00
HCCO+H<=>CH2*+CO	1.000E+14	0.000	0.00
HCCO+O<=>H+2CO	1.000E+14	0.000	0.00
HCCO+O2<=>OH+2CO	1.600E+12	0.000	854.00
HCCO+CH<=>C2H2+CO	5.000E+13	0.000	0.00
HCCO+CH2<=>C2H3+CO	3.000E+13	0.000	0.00
2HCCO<=>C2H2+2CO	1.000E+13	0.000	0.00
HCCO+OH<=>C2O+H2O	3.000E+13	0.000	0.00
C2H2(+M)<=>H2CC(+M)	1.091E+15	-0.520	50750.00
LOW / 3.341E+15 -0.640 49700.00/			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H4/2.50/ C2H6/3.00/			
C2H3(+M)<=>C2H2+H(+M)	2.573E+08	1.620	37048.20
LOW / 1.710E+27 -3.400 35798.72/			
TROE/ 1.9816 5383.70 4.29 -0.08 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/ AR/0.70/			
C2H2+O<=>C2H+OH	4.600E+19	-1.410	28950.00
C2H2+O<=>CH2+CO	4.080E+06	2.000	1900.00
C2H2+O<=>HCCO+H	1.632E+07	2.000	1900.00
C2H2+OH<=>CH2CO+H	2.180E-04	4.500	-1000.00
C2H2+OH<=>HCCOH+H	5.040E+05	2.300	13500.00
C2H2+OH<=>C2H+H2O	3.370E+07	2.000	14000.00
C2H2+OH<=>CH3+CO	4.830E-04	4.000	-2000.00
C2H2+HCO<=>C2H3+CO	1.000E+07	2.000	6000.00
C2H2+CH2<=>C3H3+H	1.200E+13	0.000	6620.00
C2H2+CH2*+<=>C3H3+H	2.000E+13	0.000	0.00
C2H2+C2H<=>C4H2+H	9.600E+13	0.000	0.00
C2H2+C2H(+M)<=>nC4H3(+M)	8.300E+10	0.899	-363.00
LOW / 1.240E+31 -4.718 1871.00/			
TROE/ 1.0000 100.00 5613.00 13387.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/2.50/ C2H4/2.50/ C2H6/3.00/			
C2H2+C2H(+M)<=>iC4H3(+M)	8.300E+10	0.899	-363.00
LOW / 1.240E+31 -4.718 1871.00/			
TROE/ 1.0000 100.00 5613.00 13387.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/2.50/ C2H4/2.50/ C2H6/3.00/			
C2H2+HCCO<=>C3H3+CO	1.000E+11	0.000	3000.00
C2H2+CH3<=>pC3H4+H	2.560E+09	1.100	13644.00
C2H2+CH3<=>aC3H4+H	5.140E+09	0.860	22153.00
C2H2+CH3<=>CH3CCH2	4.990E+22	-4.390	18850.00
C2H2+CH3<=>CH3CHCH	3.200E+35	-7.760	13300.00
C2H2+CH3<=>aC3H5	2.680E+53	-12.820	35730.00
H2CC+H<=>C2H2+H	1.000E+14	0.000	0.00
H2CC+OH<=>CH2CO+H	2.000E+13	0.000	0.00
H2CC+O2<=>2HCO	8.947E+12	0.000	0.00
H2CC+C2H2(+M)<=>C4H4(+M)	3.500E+05	2.055	-2400.00
LOW / 1.400E+60 -12.599 7417.00/			
TROE/ 0.9800 56.00 580.00 4164.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/			
H2CC+C2H4<=>C4H6	1.000E+12	0.000	0.00
CH2CO+H(+M)<=>CH2CHO(+M)	3.300E+14	-0.060	8500.00
LOW / 3.800E+41 -7.640 11900.00/			
TROE/ 0.3370 1707.00 3200.00 4131.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/ AR/0.70/			
CH2CO+H<=>HCCO+H2	5.000E+13	0.000	8000.00
CH2CO+H<=>CH3+CO	1.500E+09	1.430	2690.00

CH2CO+O<=>HCCO+OH	1.000E+13	0.000	8000.00
CH2CO+O<=>CH2+CO2	1.750E+12	0.000	1350.00
CH2CO+OH<=>HCCO+H2O	7.500E+12	0.000	2000.00
HCCOH+H<=>CH2CO+H	1.000E+13	0.000	0.00
C2H3+H (+M) <=>C2H4 (+M)	6.080E+12	0.270	280.00
LOW / 1.400E+30 -3.860 3320.00/			
TROE/ 0.7820 207.50 2663.00 6095.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/ AR/0.70/			
C2H3+H<=>C2H2+H2	7.928E+13	0.000	0.00
C2H3+H<=>H2CC+H2	6.000E+13	0.000	0.00
C2H3+O<=>CH2CO+H	4.800E+13	0.000	0.00
C2H3+O<=>CH3+CO	4.800E+13	0.000	0.00
C2H3+OH<=>C2H2+H2O	3.011E+13	0.000	0.00
C2H3+O2<=>C2H2+HO2	1.340E+06	1.610	-383.40
C2H3+O2<=>CH2CHO+O	8.803E+10	0.290	11.00
C2H3+O2<=>HCO+CH2O	1.031E+17	-1.390	1010.00
C2H3+HO2<=>CH2CHO+OH	1.000E+13	0.000	0.00
C2H3+H2O2<=>C2H4+HO2	1.210E+10	0.000	-596.00
C2H3+HCO<=>C2H4+CO	9.033E+13	0.000	0.00
C2H3+HCO<=>C2H3CHO	1.800E+13	0.000	0.00
C2H3+CH3<=>C2H2+CH4	3.920E+11	0.000	0.00
C2H3+CH3 (+M) <=>C3H6 (+M)	2.500E+13	0.000	0.00
LOW / 4.270E+58 -11.940 9769.80/			
TROE/ 0.1750 1340.60 60000.00 10139.80 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H4/3.00/ C2H6/3.00/ AR/0.70/			
C2H3+CH3<=>aC3H5+H	1.500E+24	-2.830	18618.00
C2H3+C2H2<=>nC4H4+H	2.000E+18	-1.680	10600.00
C2H3+C2H2<=>nC4H5	9.300E+38	-8.760	12000.00
C2H3+C2H2<=>iC4H5	1.600E+46	-10.980	18600.00
2C2H3<=>C4H6	1.500E+42	-8.840	12483.00
2C2H3<=>iC4H5+H	1.200E+22	-2.440	13654.00
2C2H3<=>nC4H5+H	2.400E+20	-2.040	15361.00
2C2H3<=>C2H2+C2H4	9.600E+11	0.000	0.00
CH2CHO<=>CH3+CO	7.800E+41	-9.147	46900.00
CH2CHO+H (+M) <=>CH3CHO (+M)	1.000E+14	0.000	0.00
LOW / 5.200E+39 -7.297 4700.00/			
TROE/ 0.5500 8900.00 4350.00 7244.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/			
CH2CHO+H<=>CH3CO+H	5.000E+12	0.000	0.00
CH2CHO+H<=>CH3+HCO	9.000E+13	0.000	0.00
CH2CHO+H<=>CH2CO+H2	2.000E+13	0.000	4000.00
CH2CHO+O<=>CH2CO+OH	2.000E+13	0.000	4000.00
CH2CHO+OH<=>CH2CO+H2O	1.000E+13	0.000	2000.00
CH2CHO+O2<=>CH2CO+HO2	1.400E+11	0.000	0.00
CH2CHO+O2<=>CH2O+CO+OH	1.800E+10	0.000	0.00
CH3+CO (+M) <=>CH3CO (+M)	4.850E+07	1.650	6150.00
LOW / 7.800E+30 -5.395 8600.00/			
TROE/ 0.2580 598.00 21002.00 1773.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/ AR/0.70/			
CH3CO+H (+M) <=>CH3CHO (+M)	9.600E+13	0.000	0.00
LOW / 3.850E+44 -8.569 5500.00/			
TROE/ 1.0000 2900.00 2900.00 5132.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/			
CH3CO+H<=>CH3+HCO	9.600E+13	0.000	0.00
CH3CO+O<=>CH2CO+OH	3.900E+13	0.000	0.00
CH3CO+O<=>CH3+CO2	1.500E+14	0.000	0.00
CH3CO+OH<=>CH2CO+H2O	1.200E+13	0.000	0.00
CH3CO+OH<=>CH3+CO+OH	3.000E+13	0.000	0.00
CH3CO+HO2<=>CH3+CO2+OH	3.000E+13	0.000	0.00
CH3CO+H2O2<=>CH3CHO+HO2	1.800E+11	0.000	8226.00
CH3+HCO (+M) <=>CH3CHO (+M)	1.800E+13	0.000	0.00
LOW / 2.200E+48 -9.588 5100.00/			
TROE/ 0.6173 13.08 2078.00 5093.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H2/3.00/ C2H4/3.00/ C2H6/3.00/			
CH3CHO+H<=>CH3CO+H2	4.100E+09	1.160	2400.00
CH3CHO+H<=>CH4+HCO	5.000E+10	0.000	0.00

CH3CHO+O<=>CH3CO+OH	5.800E+12	0.000	1800.00
CH3CHO+OH<=>CH3CO+H2O	2.350E+10	0.730	-1110.00
CH3CHO+CH3<=>CH3CO+CH4	2.000E-06	5.600	2460.00
CH3CHO+HCO<=>CO+HCO+CH4	8.000E+12	0.000	10400.00
CH3CHO+O2<=>CH3CO+HO2	3.000E+13	0.000	39100.00
CH2OCH2<=>CH3+HCO	3.630E+13	0.000	57200.00
CH2OCH2<=>CH3CHO	7.260E+13	0.000	57200.00
CH2OCH2<=>CH4+CO	1.210E+13	0.000	57200.00
CH2OCH2+H<=>CH2OCH+H2	2.000E+13	0.000	8300.00
CH2OCH2+H<=>C2H3+H2O	5.000E+09	0.000	5000.00
CH2OCH2+H<=>C2H4+OH	9.510E+10	0.000	5000.00
CH2OCH2+O<=>CH2OCH+OH	1.910E+12	0.000	5250.00
CH2OCH2+OH<=>CH2OCH+H2O	1.780E+13	0.000	3610.00
CH2OCH2+CH3<=>CH2OCH+CH4	1.070E+12	0.000	11830.00
CH2OCH+M<=>CH3+CO+M	3.160E+14	0.000	12000.00
CH2OCH+M<=>CH2CHO+M	5.000E+09	0.000	0.00
CH2OCH+M<=>CH2CO+H+M	3.000E+13	0.000	8000.00
C2H4 (+M) <=>H2+H2CC (+M)	3.200E+13	0.440	88770.00
LOW / 2.800E+51	-9.310	99860.00/	
TROE/ 0.7345	180.00	1035.00	5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H4+H (+M) <=>C2H5 (+M)	1.367E+09	1.463	1355.00
LOW / 2.027E+39	-6.642	5769.00/	
TROE/ -0.5690	299.00	9147.00	-152.40 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H4+H<=>C2H3+H2	5.070E+07	1.900	12950.00
C2H4+O<=>C2H3+OH	4.158E+07	1.900	3740.00
C2H4+O<=>CH3+HCO	4.800E+06	1.830	220.00
C2H4+O<=>CH2+CH2O	3.840E+05	1.830	220.00
C2H4+OH<=>C2H3+H2O	1.335E+07	2.000	2500.00
C2H4+HCO<=>C2H5+CO	1.000E+07	2.000	8000.00
C2H4+CH<=>aC3H4+H	3.000E+13	0.000	0.00
C2H4+CH<=>pC3H4+H	3.000E+13	0.000	0.00
C2H4+CH2<=>aC3H5+H	2.000E+13	0.000	6000.00
C2H4+CH2* <=>H2CC+CH4	5.000E+13	0.000	0.00
C2H4+CH2* <=>aC3H5+H	5.000E+13	0.000	0.00
C2H4+CH3<=>C2H3+CH4	2.270E+05	2.000	9200.00
C2H4+CH3<=>nC3H7	3.300E+11	0.000	7700.00
C2H4+C2H<=>C4H4+H	1.200E+13	0.000	0.00
C2H4+O2<=>C2H3+HO2	4.220E+13	0.000	60800.00
C2H4+C2H3<=>C4H7	7.930E+38	-8.470	14220.00
C2H4+HO2<=>CH2OCH2+OH	2.820E+12	0.000	17100.00
C2H5+H (+M) <=>C2H6 (+M)	5.210E+17	-0.990	1580.00
LOW / 1.990E+41	-7.080	6685.00/	
TROE/ 0.8422	125.00	2219.00	6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H5+H<=>C2H4+H2	2.000E+12	0.000	0.00
C2H5+O<=>CH3+CH2O	1.604E+13	0.000	0.00
C2H5+O<=>CH3CHO+H	8.020E+13	0.000	0.00
C2H5+O2<=>C2H4+HO2	2.000E+10	0.000	0.00
C2H5+HO2<=>C2H6+O2	3.000E+11	0.000	0.00
C2H5+HO2<=>C2H4+H2O2	3.000E+11	0.000	0.00
C2H5+HO2<=>CH3+CH2O+OH	2.400E+13	0.000	0.00
C2H5+H2O2<=>C2H6+HO2	8.700E+09	0.000	974.00
C2H5+CH3 (+M) <=>C3H8 (+M)	4.900E+14	-0.500	0.00
LOW / 6.800E+61	-13.420	6000.00/	
TROE/ 1.0000	1000.00	1433.90	5328.80 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H5+C2H3 (+M) <=>C4H8 (+M)	1.500E+13	0.000	0.00
LOW / 1.550E+56	-11.790	8984.50/	
TROE/ 0.1980	2277.90	60000.00	5723.20 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C2H5+C2H3<=>aC3H5+CH3	3.900E+32	-5.220	19747.00
C2H6+H<=>C2H5+H2	1.150E+08	1.900	7530.00
C2H6+O<=>C2H5+OH	8.980E+07	1.920	5690.00
C2H6+OH<=>C2H5+H2O	3.540E+06	2.120	870.00

C2H6+CH2*=>C2H5+CH3	4.000E+13	0.000	-550.00
C2H6+CH3=>C2H5+CH4	6.140E+06	1.740	10450.00
C3H3+H<=>pC3H4	1.500E+13	0.000	0.00
C3H3+H<=>aC3H4	2.500E+12	0.000	0.00
C3H3+O<=>CH2O+C2H	2.000E+13	0.000	0.00
C3H3+O2<=>CH2CO+HCO	3.000E+10	0.000	2868.00
C3H3+HO2<=>OH+CO+C2H3	8.000E+11	0.000	0.00
C3H3+HO2<=>aC3H4+O2	3.000E+11	0.000	0.00
C3H3+HO2<=>pC3H4+O2	2.500E+12	0.000	0.00
C3H3+HCO<=>aC3H4+CO	2.500E+13	0.000	0.00
C3H3+HCO<=>pC3H4+CO	2.500E+13	0.000	0.00
C3H3+HCCO<=>C4H4+CO	2.500E+13	0.000	0.00
C3H3+CH<=>iC4H3+H	5.000E+13	0.000	0.00
C3H3+CH2<=>C4H4+H	5.000E+13	0.000	0.00
C3H3+CH3 (+M) <=>C4H612 (+M)	1.500E+12	0.000	0.00
LOW /	2.600E+57	-11.940	9770.00/
TROE/	0.1750	1340.60	60000.00 9769.80 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C3H3+C2H2<=>C5H5	6.870E+55	-12.500	42025.00
2C3H3=>C6H5+H	5.000E+12	0.000	0.00
2C3H3=>C6H6	2.000E+12	0.000	0.00
C3H3+C4H4<=>C6H5CH2	6.530E+05	1.280	-4611.00
C3H3+C4H6<=>C6H5CH3+H	6.530E+05	1.280	-4611.00
aC3H4+H<=>C3H3+H2	1.300E+06	2.000	5500.00
aC3H4+H<=>CH3CHCH	5.400E+29	-6.090	16300.00
aC3H4+H<=>CH3CCH2	9.460E+42	-9.430	11190.00
aC3H4+H<=>aC3H5	1.520E+59	-13.540	26949.00
aC3H4+O<=>C2H4+CO	2.000E+07	1.800	1000.00
aC3H4+OH<=>C3H3+H2O	5.300E+06	2.000	2000.00
aC3H4+CH3<=>C3H3+CH4	1.300E+12	0.000	7700.00
aC3H4+CH3<=>iC4H7	2.000E+11	0.000	7500.00
aC3H4+C2H<=>C2H2+C3H3	1.000E+13	0.000	0.00
pC3H4<=>cC3H4	1.200E+44	-9.920	69250.00
pC3H4<=>aC3H4	5.150E+60	-13.930	91117.00
pC3H4+H<=>aC3H4+H	6.270E+17	-0.910	10079.00
pC3H4+H<=>CH3CCH2	1.660E+47	-10.580	13690.00
pC3H4+H<=>CH3CHCH	5.500E+28	-5.740	4300.00
pC3H4+H<=>aC3H5	4.910E+60	-14.370	31644.00
pC3H4+H<=>C3H3+H2	1.300E+06	2.000	5500.00
pC3H4+C3H3<=>aC3H4+C3H3	6.140E+06	1.740	10450.00
pC3H4+O<=>HCCO+CH3	7.300E+12	0.000	2250.00
pC3H4+O<=>C2H4+CO	1.000E+13	0.000	2250.00
pC3H4+OH<=>C3H3+H2O	1.000E+06	2.000	100.00
pC3H4+C2H<=>C2H2+C3H3	1.000E+13	0.000	0.00
pC3H4+CH3<=>C3H3+CH4	1.800E+12	0.000	7700.00
cC3H4<=>aC3H4	4.890E+41	-9.170	49594.00
aC3H5+H (+M) <=>C3H6 (+M)	2.000E+14	0.000	0.00
LOW /	1.330E+60	-12.000	5967.80/
TROE/	0.0200	1096.60	1096.60 6859.50 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
aC3H5+H<=>aC3H4+H2	1.800E+13	0.000	0.00
aC3H5+O<=>C2H3CHO+H	6.000E+13	0.000	0.00
aC3H5+OH<=>C2H3CHO+2H	4.200E+32	-5.160	30126.00
aC3H5+OH<=>aC3H4+H2O	6.000E+12	0.000	0.00
aC3H5+O2<=>aC3H4+HO2	4.990E+15	-1.400	22428.00
aC3H5+O2<=>CH3CO+CH2O	1.190E+15	-1.010	20128.00
aC3H5+O2<=>C2H3CHO+OH	1.820E+13	-0.410	22859.00
aC3H5+HO2<=>C3H6+O2	2.660E+12	0.000	0.00
aC3H5+HO2<=>OH+C2H3+CH2O	6.600E+12	0.000	0.00
aC3H5+HCO<=>C3H6+CO	6.000E+13	0.000	0.00
aC3H5+CH3 (+M) <=>C4H81 (+M)	1.000E+14	-0.320	-262.30
LOW /	3.910E+60	-12.810	6250.00/
TROE/	0.1040	1606.00	60000.00 6118.40 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
aC3H5+CH3<=>aC3H4+CH4	3.000E+12	-0.320	-131.00
aC3H5<=>CH3CCH2	7.060E+56	-14.080	75868.00

aC3H5<=>CH3CHCH	5.000E+51	-13.020	73300.00
aC3H5+C2H2<=>1C5H7	8.380E+30	-6.242	12824.00
CH3CCH2<=>CH3CHCH	1.500E+48	-12.710	53900.00
CH3CCH2+H<=>pC3H4+H2	3.340E+12	0.000	0.00
CH3CCH2+O<=>CH3+CH2CO	6.000E+13	0.000	0.00
CH3CCH2+OH<=>CH3+CH2CO+H	5.000E+12	0.000	0.00
CH3CCH2+O2<=>CH3CO+CH2O	1.000E+11	0.000	0.00
CH3CCH2+HO2<=>CH3+CH2CO+OH	2.000E+13	0.000	0.00
CH3CCH2+HCO<=>C3H6+CO	9.000E+13	0.000	0.00
CH3CCH2+CH3<=>pC3H4+CH4	1.000E+11	0.000	0.00
CH3CCH2+CH3<=>iC4H8	2.000E+13	0.000	0.00
CH3CHCH+H<=>pC3H4+H2	3.340E+12	0.000	0.00
CH3CHCH+O<=>C2H4+HCO	6.000E+13	0.000	0.00
CH3CHCH+OH<=>C2H4+HCO+H	5.000E+12	0.000	0.00
CH3CHCH+O2<=>CH3CHO+HCO	1.000E+11	0.000	0.00
CH3CHCH+HO2<=>C2H4+HCO+OH	2.000E+13	0.000	0.00
CH3CHCH+HCO<=>C3H6+CO	9.000E+13	0.000	0.00
CH3CHCH+CH3<=>pC3H4+CH4	1.000E+11	0.000	0.00
C3H6+H (+M) <=>nC3H7 (+M)	1.330E+13	0.000	3260.70
LOW /	6.260E+38	-6.660	7000.00/
TROE/	1.0000	1000.00	1310.00 48097.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C3H6+H (+M) <=>iC3H7 (+M)	1.330E+13	0.000	1559.80
LOW /	8.700E+42	-7.500	4721.80/
TROE/	1.0000	1000.00	645.40 6844.30 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C3H6+H<=>C2H4+CH3	8.000E+21	-2.390	11180.00
C3H6+H<=>aC3H5+H2	1.730E+05	2.500	2490.00
C3H6+H<=>CH3CCH2+H2	4.000E+05	2.500	9790.00
C3H6+H<=>CH3CHCH+H2	8.040E+05	2.500	12283.00
C3H6+O<=>CH2CO+CH3+H	8.000E+07	1.650	327.00
C3H6+O<=>C2H3CHO+2H	4.000E+07	1.650	327.00
C3H6+O<=>C2H5+HCO	3.500E+07	1.650	-972.00
C3H6+O<=>aC3H5+OH	1.800E+11	0.700	5880.00
C3H6+O<=>CH3CCH2+OH	6.000E+10	0.700	7630.00
C3H6+O<=>CH3CHCH+OH	1.210E+11	0.700	8960.00
C3H6+OH<=>aC3H5+H2O	3.100E+06	2.000	-298.00
C3H6+OH<=>CH3CCH2+H2O	1.100E+06	2.000	1450.00
C3H6+OH<=>CH3CHCH+H2O	2.140E+06	2.000	2778.00
C3H6+HO2<=>aC3H5+H2O2	9.600E+03	2.600	13910.00
C3H6+CH3<=>aC3H5+CH4	2.200E+00	3.500	5675.00
C3H6+CH3<=>CH3CCH2+CH4	8.400E-01	3.500	11660.00
C3H6+CH3<=>CH3CHCH+CH4	1.350E+00	3.500	12848.00
C3H6+C2H3<=>C4H6+CH3	7.230E+11	0.000	5000.00
C3H6+HO2<=>CH3CHOCH2+OH	1.090E+12	0.000	14200.00
C2H3CHO+H<=>C2H4+HCO	1.080E+11	0.454	5820.00
C2H3CHO+O<=>C2H3+OH+CO	3.000E+13	0.000	3540.00
C2H3CHO+O<=>CH2O+CH2CO	1.900E+07	1.800	220.00
C2H3CHO+OH<=>C2H3+H2O+CO	3.430E+09	1.180	-447.00
C2H3CHO+CH3<=>CH2CHCO+CH4	2.000E+13	0.000	11000.00
C2H3CHO+C2H3<=>C4H6+HCO	2.800E+21	-2.440	14720.00
CH2CHCO<=>C2H3+CO	1.000E+14	0.000	27000.00
CH2CHCO+H<=>C2H3CHO	1.000E+14	0.000	0.00
CH3CHOCH2<=>CH3CH2CHO	1.840E+14	0.000	58500.00
CH3CHOCH2<=>C2H5+HCO	2.450E+13	0.000	58500.00
CH3CHOCH2<=>CH3+CH2CHO	2.450E+13	0.000	58800.00
CH3CHOCH2<=>CH3COCH3	1.010E+14	0.000	59900.00
CH3CHOCH2<=>CH3+CH3CO	4.540E+13	0.000	59900.00
iC3H7+H (+M) <=>C3H8 (+M)	2.400E+13	0.000	0.00
LOW /	1.700E+58	-12.080	11263.70/
TROE/	0.6490	1213.10	1213.10 13369.70 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
iC3H7+H<=>CH3+C2H5	1.400E+28	-3.940	15916.00
iC3H7+H<=>C3H6+H2	3.200E+12	0.000	0.00
iC3H7+O<=>CH3CHO+CH3	9.600E+13	0.000	0.00
iC3H7+OH<=>C3H6+H2O	2.400E+13	0.000	0.00

iC3H7+O2<=>C3H6+HO2	1.300E+11	0.000	0.00
iC3H7+HO2<=>CH3CHO+CH3+OH	2.400E+13	0.000	0.00
iC3H7+HCO<=>C3H8+CO	1.200E+14	0.000	0.00
iC3H7+CH3<=>CH4+C3H6	2.200E+14	-0.680	0.00
nC3H7+H(+M)<=>C3H8(+M)	3.600E+13	0.000	0.00
LOW /	3.010E+48	-9.320	5833.60/
TROE/	0.4980	1314.00	1314.00 50000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
nC3H7+H<=>C2H5+CH3	3.700E+24	-2.920	12505.00
nC3H7+H<=>C3H6+H2	1.800E+12	0.000	0.00
nC3H7+O<=>C2H5+CH2O	9.600E+13	0.000	0.00
nC3H7+OH<=>C3H6+H2O	2.400E+13	0.000	0.00
nC3H7+O2<=>C3H6+HO2	9.000E+10	0.000	0.00
nC3H7+HO2<=>C2H5+OH+CH2O	2.400E+13	0.000	0.00
nC3H7+HCO<=>C3H8+CO	6.000E+13	0.000	0.00
nC3H7+CH3<=>CH4+C3H6	1.100E+13	0.000	0.00
C3H8+H<=>H2+nC3H7	1.300E+06	2.540	6756.00
C3H8+H<=>H2+iC3H7	1.300E+06	2.400	4471.00
C3H8+O<=>nC3H7+OH	1.900E+05	2.680	3716.00
C3H8+O<=>iC3H7+OH	4.760E+04	2.710	2106.00
C3H8+OH<=>nC3H7+H2O	1.400E+03	2.660	527.00
C3H8+OH<=>iC3H7+H2O	2.700E+04	2.390	393.00
C3H8+O2<=>nC3H7+HO2	4.000E+13	0.000	50930.00
C3H8+O2<=>iC3H7+HO2	4.000E+13	0.000	47590.00
C3H8+HO2<=>nC3H7+H2O2	4.760E+04	2.550	16490.00
C3H8+HO2<=>iC3H7+H2O2	9.640E+03	2.600	13910.00
C3H8+CH3<=>CH4+nC3H7	9.030E-01	3.650	7153.00
C3H8+CH3<=>CH4+iC3H7	1.510E+00	3.460	5480.00
C4H2+H<=>nC4H3	1.100E+42	-8.720	15300.00
C4H2+H<=>iC4H3	1.100E+30	-4.920	10800.00
C4H2+OH<=>H2C4O+H	6.600E+12	0.000	-410.00
C4H2+C2H<=>C6H2+H	9.600E+13	0.000	0.00
C4H2+C2H<=>C6H3	4.500E+37	-7.680	7100.00
H2C4O+H<=>C2H2+HCCO	5.000E+13	0.000	3000.00
H2C4O+OH<=>CH2CO+HCCO	1.000E+07	2.000	2000.00
nC4H3<=>iC4H3	4.100E+43	-9.490	53000.00
nC4H3+H<=>iC4H3+H	2.500E+20	-1.670	10800.00
nC4H3+H<=>C2H2+H2CC	6.300E+25	-3.340	10014.00
nC4H3+H<=>C4H4	2.000E+47	-10.260	13070.00
nC4H3+H<=>C4H2+H2	3.000E+13	0.000	0.00
nC4H3+OH<=>C4H2+H2O	2.000E+12	0.000	0.00
nC4H3+C2H2<=>1-C6H4+H	2.500E+14	-0.560	10600.00
nC4H3+C2H2<=>C6H5	9.600E+70	-17.770	31300.00
nC4H3+C2H2<=>o-C6H4+H	6.900E+46	-10.010	30100.00
iC4H3+H<=>C2H2+H2CC	2.800E+23	-2.550	10780.00
iC4H3+H<=>C4H4	3.400E+43	-9.010	12120.00
iC4H3+H<=>C4H2+H2	6.000E+13	0.000	0.00
iC4H3+OH<=>C4H2+H2O	4.000E+12	0.000	0.00
iC4H3+O2<=>HCCO+CH2CO	7.860E+16	-1.800	0.00
C4H4+H<=>nC4H5	1.300E+51	-11.920	16500.00
C4H4+H<=>iC4H5	4.900E+51	-11.920	17700.00
C4H4+H<=>nC4H3+H2	6.650E+05	2.530	12240.00
C4H4+H<=>iC4H3+H2	3.330E+05	2.530	9240.00
C4H4+OH<=>nC4H3+H2O	3.100E+07	2.000	3430.00
C4H4+OH<=>iC4H3+H2O	1.550E+07	2.000	430.00
C4H4+O<=>C3H3+HCO	6.000E+08	1.450	-860.00
C4H4+C2H<=>1-C6H4+H	1.200E+13	0.000	0.00
nC4H5<=>iC4H5	1.500E+67	-16.890	59100.00
nC4H5+H<=>iC4H5+H	3.100E+26	-3.350	17423.00
nC4H5+H<=>C4H4+H2	1.500E+13	0.000	0.00
nC4H5+OH<=>C4H4+H2O	2.000E+12	0.000	0.00
nC4H5+HCO<=>C4H6+CO	5.000E+12	0.000	0.00
nC4H5+HO2<=>C2H3+CH2CO+OH	6.600E+12	0.000	0.00
nC4H5+H2O2<=>C4H6+HO2	1.210E+10	0.000	-596.00
nC4H5+HO2<=>C4H6+O2	6.000E+11	0.000	0.00
nC4H5+O2<=>CH2CHCHCHO+O	3.000E+11	0.290	11.00

nC4H5+O2<=>HCO+C2H3CHO	9.200E+16	-1.390	1010.00
nC4H5+C2H2<=>C6H6+H	1.600E+16	-1.330	5400.00
nC4H5+C2H3<=>C6H6+H2	1.840E-13	7.070	-3611.00
iC4H5+H<=>C4H4+H2	3.000E+13	0.000	0.00
iC4H5+H<=>C3H3+CH3	2.000E+13	0.000	2000.00
iC4H5+OH<=>C4H4+H2O	4.000E+12	0.000	0.00
iC4H5+HCO<=>C4H6+CO	5.000E+12	0.000	0.00
iC4H5+HO2<=>C4H6+O2	6.000E+11	0.000	0.00
iC4H5+HO2<=>C2H3+CH2CO+OH	6.600E+12	0.000	0.00
iC4H5+H2O2<=>C4H6+H2O	1.210E+10	0.000	-596.00
iC4H5+O2<=>CH2CO+CH2CHO	2.160E+10	0.000	2500.00
C4H5-2<=>iC4H5	1.500E+67	-16.890	59100.00
iC4H5+H<=>C4H5-2+H	3.100E+26	-3.350	17423.00
C4H5-2+HO2<=>OH+C2H2+CH3CO	8.000E+11	0.000	0.00
C4H5-2+O2<=>CH3CO+CH2CO	2.160E+10	0.000	2500.00
C4H5-2+C2H2<=>C6H6+H	5.000E+14	0.000	25000.00
C4H5-2+C2H4<=>C5H6+CH3	5.000E+14	0.000	25000.00
C4H6<=>iC4H5+H	5.700E+36	-6.270	112353.00
C4H6<=>nC4H5+H	5.300E+44	-8.620	123608.00
C4H6<=>C4H4+H2	2.500E+15	0.000	94700.00
C4H6+H<=>nC4H5+H2	1.330E+06	2.530	12240.00
C4H6+H<=>iC4H5+H2	6.650E+05	2.530	9240.00
C4H6+H<=>C2H4+C2H3	1.460E+30	-4.340	21647.00
C4H6+H<=>pC3H4+CH3	2.000E+12	0.000	7000.00
C4H6+H<=>aC3H4+CH3	2.000E+12	0.000	7000.00
C4H6+O<=>nC4H5+OH	7.500E+06	1.900	3740.00
C4H6+O<=>iC4H5+OH	7.500E+06	1.900	3740.00
C4H6+O<=>CH3CHCHCO+H	1.500E+08	1.450	-860.00
C4H6+O<=>CH2CHCHCHO+H	4.500E+08	1.450	-860.00
C4H6+OH<=>nC4H5+H2O	6.200E+06	2.000	3430.00
C4H6+OH<=>iC4H5+H2O	3.100E+06	2.000	430.00
C4H6+HO2<=>C4H6O25+OH	1.200E+12	0.000	14000.00
C4H6+HO2<=>C2H3CHOCH2+OH	4.800E+12	0.000	14000.00
C4H6+CH3<=>nC4H5+CH4	2.000E+14	0.000	22800.00
C4H6+CH3<=>iC4H5+CH4	1.000E+14	0.000	19800.00
C4H6+C2H3<=>nC4H5+C2H4	5.000E+13	0.000	22800.00
C4H6+C2H3<=>iC4H5+C2H4	2.500E+13	0.000	19800.00
C4H6+C3H3<=>nC4H5+aC3H4	1.000E+13	0.000	22500.00
C4H6+C3H3<=>iC4H5+aC3H4	5.000E+12	0.000	19500.00
C4H6+aC3H5<=>nC4H5+C3H6	1.000E+13	0.000	22500.00
C4H6+aC3H5<=>iC4H5+C3H6	5.000E+12	0.000	19500.00
C4H6+C2H3<=>C6H6+H2+H	5.620E+11	0.000	3240.00
C4H612<=>iC4H5+H	4.200E+15	0.000	92600.00
C4H612+H<=>C4H6+H	2.000E+13	0.000	4000.00
C4H612+H<=>iC4H5+H2	1.700E+05	2.500	2490.00
C4H612+H<=>aC3H4+CH3	2.000E+13	0.000	2000.00
C4H612+H<=>pC3H4+CH3	2.000E+13	0.000	2000.00
C4H612+CH3<=>iC4H5+CH4	7.000E+13	0.000	18500.00
C4H612+O<=>CH2CO+C2H4	1.200E+08	1.650	327.00
C4H612+O<=>iC4H5+OH	1.800E+11	0.700	5880.00
C4H612+OH<=>iC4H5+H2O	3.100E+06	2.000	-298.00
C4H612<=>C4H6	3.000E+13	0.000	65000.00
C4H6-2<=>C4H6	3.000E+13	0.000	65000.00
C4H6-2<=>C4H612	3.000E+13	0.000	67000.00
C4H6-2+H<=>C4H612+H	2.000E+13	0.000	4000.00
C4H6-2+H<=>C4H5-2+H2	3.400E+05	2.500	2490.00
C4H6-2+H<=>CH3+pC3H4	2.600E+05	2.500	1000.00
C4H6-2<=>H+C4H5-2	5.000E+15	0.000	87300.00
C4H6-2+CH3<=>C4H5-2+CH4	1.400E+14	0.000	18500.00
C2H3CHOCH2<=>C4H6O23	2.000E+14	0.000	50600.00
C4H6O23<=>CH3CHCHCHO	1.950E+13	0.000	49400.00
C4H6O23<=>C2H4+CH2CO	5.750E+15	0.000	69300.00
C4H6O23<=>C2H2+CH2OCH2	1.000E+16	0.000	75800.00
C4H6O25<=>C4H4O+H2	5.300E+12	0.000	48500.00
C4H4O<=>CO+pC3H4	1.780E+15	0.000	77500.00
C4H4O<=>C2H2+CH2CO	5.010E+14	0.000	77500.00

CH3CHCHCHO<=>C3H6+CO	3.900E+14	0.000	69000.00
CH3CHCHCHO+H<=>CH2CHCHCHO+H2	1.700E+05	2.500	2490.00
CH3CHCHCHO+H<=>CH3CHCHCO+H2	1.000E+05	2.500	2490.00
CH3CHCHCHO+H<=>CH3+C2H3CHO	4.000E+21	-2.390	11180.00
CH3CHCHCHO+H<=>C3H6+HCO	4.000E+21	-2.390	11180.00
CH3CHCHCHO+CH3<=>CH2CHCHCHO+CH4	2.100E+00	3.500	5675.00
CH3CHCHCHO+CH3<=>CH3CHCHCO+CH4	1.100E+00	3.500	5675.00
CH3CHCHCHO+C2H3<=>CH2CHCHCHO+C2H4	2.210E+00	3.500	4682.00
CH3CHCHCHO+C2H3<=>CH3CHCHCO+C2H4	1.110E+00	3.500	4682.00
CH3CHCHCO<=>CH3CHCH+CO	1.000E+14	0.000	30000.00
CH3CHCHCO+H<=>CH3CHCHCHO	1.000E+14	0.000	0.00
CH2CHCHCHO<=>aC3H5+CO	1.000E+14	0.000	25000.00
CH2CHCHCHO+H<=>CH3CHCHCHO	1.000E+14	0.000	0.00
C4H7<=>C4H6+H	2.480E+53	-12.300	52000.00
C4H7+H (+M) <=>C4H81 (+M)	3.600E+13	0.000	0.00
LOW / 3.010E+48 -9.320 5833.60/			
TROE/ 0.4980 1314.00 1314.00 50000.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C4H7+H<=>CH3+aC3H5	2.000E+21	-2.000	11000.00
C4H7+H<=>C4H6+H2	1.800E+12	0.000	0.00
C4H7+O2<=>C4H6+HO2	1.000E+11	0.000	0.00
C4H7+HO2<=>CH2O+OH+aC3H5	2.400E+13	0.000	0.00
C4H7+HCO<=>C4H81+CO	6.000E+13	0.000	0.00
C4H7+CH3<=>C4H6+CH4	1.100E+13	0.000	0.00
iC4H7+H (+M) <=>iC4H8 (+M)	2.000E+14	0.000	0.00
LOW / 1.330E+60 -12.000 5967.80/			
TROE/ 0.0200 1096.60 1096.60 6859.50 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
iC4H7+H<=>CH3CCH2+CH3	2.600E+45	-8.190	37890.00
iC4H7+O<=>CH2O+CH3CCH2	9.000E+13	0.000	0.00
iC4H7+HO2<=>CH3CCH2+CH2O+OH	4.000E+12	0.000	0.00
C4H81+H (+M) <=>pC4H9 (+M)	1.330E+13	0.000	3260.70
LOW / 6.260E+38 -6.660 7000.00/			
TROE/ 1.0000 1000.00 1310.00 48097.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C4H81+H (+M) <=>sC4H9 (+M)	1.330E+13	0.000	1559.80
LOW / 8.700E+42 -7.500 4721.80/			
TROE/ 1.0000 1000.00 645.40 6844.30 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C4H81+H<=>C2H4+C2H5	1.600E+22	-2.390	11180.00
C4H81+H<=>C3H6+CH3	3.200E+22	-2.390	11180.00
C4H81+H<=>C4H7+H2	6.500E+05	2.540	6756.00
C4H81+O<=>nC3H7+HCO	3.300E+08	1.450	-402.00
C4H81+O<=>C4H7+OH	1.500E+13	0.000	5760.00
DUPLICATE			
C4H81+O<=>C4H7+OH	2.600E+13	0.000	4470.00
DUPLICATE			
C4H81+OH<=>C4H7+H2O	7.000E+02	2.660	527.00
C4H81+O2<=>C4H7+HO2	2.000E+13	0.000	50930.00
C4H81+HO2<=>C4H7+H2O2	1.000E+12	0.000	14340.00
C4H81+CH3<=>C4H7+CH4	4.500E-01	3.650	7153.00
C4H82+H (+M) <=>sC4H9 (+M)	1.330E+13	0.000	1559.80
LOW / 8.700E+42 -7.500 4721.80/			
TROE/ 1.0000 1000.00 645.40 6844.30 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C4H82+H<=>C4H7+H2	3.400E+05	2.500	2490.00
C4H82+O<=>C2H4+CH3CHO	2.400E+08	1.650	327.00
C4H82+OH<=>C4H7+H2O	6.200E+06	2.000	-298.00
C4H82+O2<=>C4H7+HO2	5.000E+13	0.000	53300.00
C4H82+HO2<=>C4H7+H2O2	1.900E+04	2.600	13910.00
C4H82+CH3<=>C4H7+CH4	4.400E+00	3.500	5675.00
iC4H8+H (+M) <=>iC4H9 (+M)	1.330E+13	0.000	3260.70
LOW / 6.260E+38 -6.660 7000.00/			
TROE/ 1.0000 1000.00 1310.00 48097.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
iC4H8+H<=>iC4H7+H2	1.200E+06	2.540	6760.00



ic4H8+H<=>C3H6+CH3	8.000E+21	-2.390	11180.00
ic4H8+O<=>2CH3+CH2CO	1.200E+08	1.650	327.00
ic4H8+O<=>ic3H7+HCO	3.500E+07	1.650	-972.00
ic4H8+O<=>ic4H7+OH	2.900E+05	2.500	3640.00
ic4H8+OH<=>ic4H7+H2O	1.500E+08	1.530	775.00
ic4H8+HO2<=>ic4H7+H2O2	2.000E+04	2.550	15500.00
ic4H8+O2<=>ic4H7+HO2	2.700E+13	0.000	50900.00
ic4H8+CH3<=>ic4H7+CH4	9.100E-01	3.650	7150.00
C2H4+C2H5<=>pC4H9	1.500E+11	0.000	7300.00
pC4H9+H (+M) <=>C4H10 (+M)	3.600E+13	0.000	0.00
LOW /	3.010E+48	-9.320	5833.60/
TROE/	0.4980	1314.00	1314.00 50000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
pC4H9+H<=>2C2H5	3.700E+24	-2.920	12505.00
pC4H9+H<=>C4H81+H2	1.800E+12	0.000	0.00
pC4H9+O<=>nC3H7+CH2O	9.600E+13	0.000	0.00
pC4H9+OH<=>C4H81+H2O	2.400E+13	0.000	0.00
pC4H9+O2<=>C4H81+HO2	2.700E+11	0.000	0.00
pC4H9+HO2<=>nC3H7+OH+CH2O	2.400E+13	0.000	0.00
pC4H9+HCO<=>C4H10+CO	9.000E+13	0.000	0.00
pC4H9+CH3<=>C4H81+CH4	1.100E+13	0.000	0.00
C3H6+CH3 (+M) <=>sC4H9 (+M)	1.700E+11	0.000	7403.60
LOW /	2.310E+28	-4.270	1831.00/
TROE/	0.56506000000	534.20	3007.20 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
sC4H9+H (+M) <=>C4H10 (+M)	2.400E+13	0.000	0.00
LOW /	1.700E+58	-12.080	11263.70/
TROE/	0.6490	1213.10	1213.10 13369.70 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
sC4H9+H<=>2C2H5	1.400E+28	-3.940	15916.00
sC4H9+H<=>C4H81+H2	3.200E+12	0.000	0.00
sC4H9+H<=>C4H82+H2	2.100E+12	0.000	0.00
sC4H9+O<=>CH3CHO+C2H5	9.600E+13	0.000	0.00
sC4H9+OH<=>C4H81+H2O	2.400E+13	0.000	0.00
sC4H9+OH<=>C4H82+H2O	1.600E+13	0.000	0.00
sC4H9+O2<=>C4H81+HO2	5.100E+10	0.000	0.00
sC4H9+O2<=>C4H82+HO2	1.200E+11	0.000	0.00
sC4H9+HO2<=>CH3CHO+C2H5+OH	2.400E+13	0.000	0.00
sC4H9+HCO<=>C4H10+CO	1.200E+14	0.000	0.00
sC4H9+CH3<=>CH4+C4H81	2.200E+14	-0.680	0.00
sC4H9+CH3<=>CH4+C4H82	1.500E+14	-0.680	0.00
C3H6+CH3 (+M) <=>ic4H9 (+M)	9.600E+10	0.000	8003.60
LOW /	1.300E+28	-4.270	2431.10/
TROE/	0.56506000000	534.20	3007.20 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
ic4H9+H (+M) <=>ic4H10 (+M)	3.600E+13	0.000	0.00
LOW /	3.270E+56	-11.740	6430.80/
TROE/	0.5060	1266.60	1266.60 50000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
ic4H9+H<=>ic3H7+CH3	1.900E+35	-5.830	22470.00
ic4H9+H<=>ic4H8+H2	9.000E+11	0.000	0.00
ic4H9+O<=>ic3H7+CH2O	9.600E+13	0.000	0.00
ic4H9+OH<=>ic4H8+H2O	1.200E+13	0.000	0.00
ic4H9+O2<=>ic4H8+HO2	2.400E+10	0.000	0.00
ic4H9+HO2<=>ic3H7+CH2O+OH	2.410E+13	0.000	0.00
ic4H9+HCO<=>ic4H10+CO	3.600E+13	0.000	0.00
ic4H9+CH3<=>ic4H8+CH4	6.000E+12	-0.320	0.00
tC4H9 (+M) <=>ic4H8+H (+M)	8.300E+13	0.000	38150.40
LOW /	1.900E+41	-7.360	36631.70/
TROE/	0.2930	649.00	60000.00 3425.90 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
tC4H9+H (+M) <=>ic4H10 (+M)	2.400E+13	0.000	0.00
LOW /	1.470E+61	-12.940	8000.00/
TROE/	0.0000	1456.40	1000.00 10000.50 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
tC4H9+H<=>ic3H7+CH3	2.600E+36	-6.120	25640.00

tC4H9+H<=>iC4H8+H2	5.420E+12	0.000	0.00
tC4H9+O<=>iC4H8+OH	1.800E+14	0.000	0.00
tC4H9+O<=>CH3COCH3+CH3	1.800E+14	0.000	0.00
tC4H9+OH<=>iC4H8+H2O	1.800E+13	0.000	0.00
tC4H9+O2<=>iC4H8+HO2	4.800E+11	0.000	0.00
tC4H9+HO2<=>CH3+CH3COCH3+OH	1.800E+13	0.000	0.00
tC4H9+HCO<=>iC4H10+CO	6.000E+13	0.000	0.00
tC4H9+CH3<=>iC4H8+CH4	3.800E+15	-1.000	0.00
CH3COCH3+H<=>H2+CH2CO+CH3	1.300E+06	2.540	6756.00
CH3COCH3+O<=>OH+CH2CO+CH3	1.900E+05	2.680	3716.00
CH3COCH3+OH<=>H2O+CH2CO+CH3	3.200E+07	1.800	934.00
CH3+CH3CO<=>CH3COCH3	4.000E+15	-0.800	0.00
nC3H7+CH3 (+M) <=>C4H10 (+M)	1.930E+14	-0.320	0.00
LOW / 2.680E+61 -13.240 6000.00/			
TROE/ 1.0000 1000.00 1433.90 5328.80 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
2C2H5 (+M) <=>C4H10 (+M)	1.880E+14	-0.500	0.00
LOW / 2.610E+61 -13.420 6000.00/			
TROE/ 1.0000 1000.00 1433.90 5328.80 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
C4H10+H<=>pC4H9+H2	9.200E+05	2.540	6756.00
C4H10+H<=>sC4H9+H2	2.400E+06	2.400	4471.00
C4H10+O<=>pC4H9+OH	4.900E+06	2.400	5500.00
C4H10+O<=>sC4H9+OH	4.300E+05	2.600	2580.00
C4H10+OH<=>pC4H9+H2O	3.300E+07	1.800	954.00
C4H10+OH<=>sC4H9+H2O	5.400E+06	2.000	-596.00
C4H10+O2<=>pC4H9+HO2	4.000E+13	0.000	50930.00
C4H10+O2<=>sC4H9+HO2	8.000E+13	0.000	47590.00
C4H10+HO2<=>pC4H9+H2O2	4.760E+04	2.550	16490.00
C4H10+HO2<=>sC4H9+H2O2	1.900E+04	2.600	13910.00
C4H10+CH3<=>pC4H9+CH4	9.030E-01	3.650	7153.00
C4H10+CH3<=>sC4H9+CH4	3.000E+00	3.460	5480.00
iC3H7+CH3 (+M) <=>iC4H10 (+M)	1.400E+15	-0.680	0.00
LOW / 4.160E+61 -13.330 3903.40/			
TROE/ 0.93106000000 1265.30 5469.80 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/			
iC4H10+H<=>iC4H9+H2	1.800E+06	2.540	6760.00
iC4H10+H<=>tC4H9+H2	6.000E+05	2.400	2580.00
iC4H10+O<=>iC4H9+OH	4.300E+05	2.500	3640.00
iC4H10+O<=>tC4H9+OH	1.570E+05	2.500	1110.00
iC4H10+OH<=>iC4H9+H2O	2.300E+08	1.530	775.00
iC4H10+OH<=>tC4H9+H2O	5.730E+10	0.510	64.00
iC4H10+HO2<=>iC4H9+H2O2	3.000E+04	2.550	15500.00
iC4H10+HO2<=>tC4H9+H2O2	3.600E+03	2.550	10500.00
iC4H10+O2<=>iC4H9+HO2	4.000E+13	0.000	50900.00
iC4H10+O2<=>tC4H9+HO2	4.000E+13	0.000	44000.00
iC4H10+CH3<=>iC4H9+CH4	1.360E+00	3.650	7150.00
iC4H10+CH3<=>tC4H9+CH4	9.000E-01	3.460	4600.00
C6H2+H<=>C6H3	1.100E+30	-4.920	10800.00
C6H3+H<=>C4H2+C2H2	2.800E+23	-2.550	10780.00
C6H3+H<=>1-C6H4	3.400E+43	-9.010	12120.00
C6H3+H<=>C6H2+H2	3.000E+13	0.000	0.00
C6H3+OH<=>C6H2+H2O	4.000E+12	0.000	0.00
1-C6H4+H<=>C6H5	1.700E+78	-19.720	31400.00
1-C6H4+H<=>o-C6H4+H	1.400E+54	-11.700	34500.00
1-C6H4+H<=>C6H3+H2	1.330E+06	2.530	9240.00
1-C6H4+OH<=>C6H3+H2O	3.100E+06	2.000	430.00
C4H2+C2H2<=>o-C6H4	5.000E+78	-19.310	67920.00
o-C6H4+OH<=>CO+C5H5	1.000E+13	0.000	0.00
C6H5+CH3<=>C6H5CH3	1.380E+13	0.000	46.00
C6H5CH3+O2<=>C6H5CH2+HO2	3.000E+14	0.000	42992.00
C6H5CH3+OH<=>C6H5CH2+H2O	1.620E+13	0.000	2770.00
C6H5CH3+OH<=>C6H4CH3+H2O	1.333E+08	1.420	1450.00
C6H5CH3+H<=>C6H5CH2+H2	1.259E+14	0.000	8359.00
C6H5CH3+H<=>C6H6+CH3	1.930E+06	2.170	4163.00
C6H5CH3+O<=>OC6H4CH3+H	2.600E+13	0.000	3795.00

C6H5CH3+CH3<=>C6H5CH2+CH4	3.160E+11	0.000	9500.00
C6H5CH3+C6H5<=>C6H5CH2+C6H6	2.103E+12	0.000	4400.00
C6H5CH3+HO2<=>C6H5CH2+H2O2	3.975E+11	0.000	14069.00
C6H5CH3+HO2<=>C6H4CH3+H2O2	5.420E+12	0.000	28810.00
C6H5CH2+H (+M) <=>C6H5CH3 (+M)	1.000E+14	0.000	0.00
LOW / 1.100+103 -24.630 14590.00/			
TROE/ 0.4310 383.00 152.00 4730.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
C6H5CH2+H<=>C6H5+CH3	1.500E+66	-13.940	64580.00
C6H5CH2+O<=>C6H5CHO+H	4.000E+14	0.000	0.00
C6H5CH2+OH<=>C6H5CH2OH	2.000E+13	0.000	0.00
C6H5CH2+HO2<=>C6H5CHO+H+OH	5.000E+12	0.000	0.00
C6H5CH2+C6H5OH<=>C6H5CH3+C6H5O	1.050E+11	0.000	9500.00
C6H5CH2+HOC6H4CH3<=>C6H5CH3+OC6H4CH3	1.050E+11	0.000	9500.00
C6H5CH2OH+OH<=>C6H5CHO+H2O+H	5.000E+12	0.000	0.00
C6H5CH2OH+H<=>C6H5CHO+H2+H	8.000E+13	0.000	8235.00
C6H5CH2OH+H<=>C6H6+CH2OH	1.200E+13	0.000	5148.00
C6H5CH2OH+C6H5<=>C6H5CHO+C6H6+H	1.400E+12	0.000	4400.00
C6H5+HCO<=>C6H5CHO	1.000E+13	0.000	0.00
C6H5CHO<=>C6H5CO+H	3.980E+15	0.000	86900.00
C6H5CHO+O2<=>C6H5CO+HO2	1.020E+13	0.000	38950.00
C6H5CHO+OH<=>C6H5CO+H2O	2.350E+10	0.730	-1110.00
C6H5CHO+H<=>C6H5CO+H2	4.100E+09	1.160	2400.00
C6H5CHO+H<=>C6H6+HCO	1.930E+06	2.170	4163.00
C6H5CHO+O<=>C6H5CO+OH	5.800E+12	0.000	1800.00
C6H5CHO+C6H5CH2<=>C6H5CO+C6H5CH3	2.000E-06	5.600	2460.00
C6H5CHO+CH3<=>C6H5CO+CH4	2.000E-06	5.600	2460.00
C6H5CHO+C6H5<=>C6H5CO+C6H6	2.103E+12	0.000	4400.00
C6H5CO+H2O2<=>C6H5CHO+HO2	1.800E+11	0.000	8226.00
OC6H4CH3+H (+M) <=>HOC6H4CH3 (+M)	1.000E+14	0.000	0.00
LOW / 4.000E+93 -21.840 13880.00/			
TROE/ 0.0430 304.20 60000.00 5896.40 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/			
OC6H4CH3+H<=>C6H5O+CH3	1.930E+06	2.170	4163.00
OC6H4CH3+O<=>C6H4O2+CH3	8.000E+13	0.000	0.00
HOC6H4CH3+OH<=>OC6H4CH3+H2O	6.000E+12	0.000	0.00
HOC6H4CH3+H<=>OC6H4CH3+H2	1.150E+14	0.000	12400.00
HOC6H4CH3+H<=>C6H5CH3+OH	2.210E+13	0.000	7910.00
HOC6H4CH3+H<=>C6H5OH+CH3	1.200E+13	0.000	5148.00
C6H5CO<=>C6H5+CO	5.270E+14	0.000	29013.00
C6H5+H (+M) <=>C6H6 (+M)	1.000E+14	0.000	0.00
LOW / 6.600E+75 -16.300 7000.00/			
TROE/ 1.0000 0.10 584.90 6113.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/			
C6H6+OH<=>C6H5+H2O	3.985E+05	2.286	1058.00
C6H6+OH<=>C6H5OH+H	1.300E+13	0.000	10600.00
C6H6+O<=>C6H5O+H	1.390E+13	0.000	4910.00
C6H6+O<=>C5H5+HCO	1.390E+13	0.000	4530.00
C6H5+H2<=>C6H6+H	5.707E+04	2.430	6273.00
C6H5 (+M) <=>C6H4+H (+M)	4.300E+12	0.616	77313.00
LOW / 1.000E+84 -18.866 90064.00/			
TROE/ 0.9020 696.00 358.00 3856.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/			
C6H5+H<=>C6H4+H2	2.000E+11	1.100	24500.00
C6H5+O2<=>C6H5O+O	2.600E+13	0.000	6120.00
C6H5+O2<=>C6H4O2+H	3.000E+13	0.000	8980.00
C6H5+O<=>C5H5+CO	1.000E+14	0.000	0.00
C6H5+OH<=>C6H5O+H	3.000E+13	0.000	0.00
C6H5+HO2<=>C6H5O+OH	3.000E+13	0.000	0.00
C6H5+HO2<=>C6H6+O2	1.000E+12	0.000	0.00
C6H5+CH4<=>C6H6+CH3	3.890E-03	4.570	5256.00
C6H5+C2H6<=>C6H6+C2H5	2.100E+11	0.000	4443.00
C6H5+CH2O<=>C6H6+HCO	8.550E+04	2.190	38.00
C6H4O2<=>C5H4O+CO	7.400E+11	0.000	59000.00
C6H4O2+H<=>CO+C5H5O (1,3)	4.300E+09	1.450	3900.00
C6H4O2+O<=>2CO+C2H2+CH2CO	3.000E+13	0.000	5000.00

C6H5O+H<=>C5H5+HCO	1.000E+13	0.000	12000.00
C6H5O+H<=>C5H6+CO	5.000E+13	0.000	0.00
C6H5O<=>CO+C5H5	3.760E+54	-12.060	72800.00
C6H5O+O<=>C6H4O2+H	2.600E+10	0.470	795.00
C6H5OH<=>C5H6+CO	1.000E+12	0.000	60808.00
C6H5OH+OH<=>C6H5O+H2O	2.950E+06	2.000	-1312.00
C6H5OH+H<=>C6H5O+H2	1.150E+14	0.000	12398.00
C6H5OH+O<=>C6H5O+OH	2.810E+13	0.000	7352.00
C6H5OH+C2H3<=>C6H5O+C2H4	6.000E+12	0.000	0.00
C6H5OH+nC4H5<=>C6H5O+C4H6	6.000E+12	0.000	0.00
C6H5OH+C6H5<=>C6H5O+C6H6	4.910E+12	0.000	4400.00
C5H6+H<=>C2H2+aC3H5	7.740E+36	-6.180	32890.00
C5H6+H<=>1C5H7	8.270+126	-32.300	82348.00
C5H6+H<=>C5H5+H2	3.030E+08	1.710	5590.00
C5H6+O<=>C5H5+OH	4.770E+04	2.710	1106.00
C5H6+O<=>C5H5O(1,3)+H DUPLICATE	8.910E+12	-0.150	590.00
C5H6+O<=>C5H5O(1,3)+H DUPLICATE	5.600E+12	-0.060	200.00
C5H6+O<=>nC4H5+CO+H	8.700E+51	-11.090	33240.00
C5H6+OH<=>C5H5+H2O	3.080E+06	2.000	0.00
C5H6+HO2<=>C5H5+H2O2	1.100E+04	2.600	12900.00
C5H6+O2<=>C5H5+HO2	4.000E+13	0.000	37150.00
C5H6+HCO<=>C5H5+CH2O	1.080E+08	1.900	16000.00
C5H6+CH3<=>C5H5+CH4	1.800E-01	4.000	0.00
C5H5+H(+M)<=>C5H6(+M)	1.000E+14	0.000	0.00
LOW /	4.400E+80	-18.280	12994.00/
TROE/	0.0680	400.70	4135.80 5501.90 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/			
C5H5+O2<=>C5H5O(2,4)+O	7.780E+15	-0.730	48740.00
C5H5+O<=>C5H5O(2,4)	1.120E-12	5.870	-17310.00
C5H5+O<=>C5H4O+H	5.810E+13	-0.020	20.00
C5H5+O<=>nC4H5+CO	3.200E+13	-0.170	440.00
C5H5+OH<=>C5H4OH+H	3.510E+57	-12.180	48350.00
C5H5+OH<=>C5H5O(2,4)+H	1.360E+51	-10.460	57100.00
C5H5+HO2<=>C5H5O(2,4)+OH	6.270E+29	-4.690	11650.00
C5H5+OH<=>C5H5OH DUPLICATE	6.490E+14	-0.850	-2730.00
C5H5+OH<=>C5H5OH DUPLICATE	1.150E+43	-8.760	18730.00
C5H5+OH<=>C5H5OH DUPLICATE	1.060E+59	-13.080	33450.00
C5H5+O2<=>C5H4O+OH	1.800E+12	0.080	18000.00
C5H5OH+H<=>C5H5O(2,4)+H2	1.150E+14	0.000	15400.00
C5H5OH+H<=>C5H4OH+H2	1.200E+05	2.500	1492.00
C5H5OH+OH<=>C5H5O(2,4)+H2O	6.000E+12	0.000	0.00
C5H5OH+OH<=>C5H4OH+H2O	3.080E+06	2.000	0.00
C5H5O(2,4)+H<=>C5H5OH	1.000E+14	0.000	0.00
C5H5O(2,4)<=>C5H4O+H	2.000E+13	0.000	30000.00
C5H5O(2,4)+O2<=>C5H4O+HO2	1.000E+11	0.000	0.00
C5H4O+H<=>C5H5O(1,3)	2.000E+13	0.000	2000.00
C5H5O(1,3)<=>c-C4H5+CO	1.000E+12	0.000	36000.00
C5H5O(1,3)+O2<=>C5H4O+HO2	1.000E+11	0.000	0.00
C5H4OH<=>C5H4O+H	2.100E+13	0.000	48000.00
C5H4O<=>2C2H2+CO	6.200E+41	-7.870	98700.00
C5H4O+H<=>CO+c-C4H5	4.300E+09	1.450	3900.00
C5H4O+O<=>CO+HCO+C3H3	6.200E+08	1.450	-858.00
c-C4H5+H<=>C4H6	1.000E+13	0.000	0.00
c-C4H5+H<=>C2H4+C2H2	1.000E+13	0.000	0.00
c-C4H5+O<=>CH2CHO+C2H2	1.000E+14	0.000	0.00
c-C4H5+O2<=>CH2CHO+CH2CO	4.800E+11	0.000	19000.00
c-C4H5<=>C4H4+H	3.000E+12	0.000	52000.00
c-C4H5<=>C2H3+C2H2	2.000E+12	0.000	58000.00
aC3H5+C2H3<=>1C5H7+H	1.000E+13	0.000	0.00
1C5H7+O<=>C2H3CHO+C2H3	5.000E+13	0.000	0.00

1C5H7+OH<=>C2H3CHO+C2H4 2.000E+13 0.000 0.00

!\*\*\*\*\* C2H5OH Reactions \*\*\*\*\*

!-----

! Just for high pressure flame speed calcs purposes

!Ref: Saxena and Williams, PCI 2007

!-----

C2H5OH(+M)=CH3+CH2OH(+M) 5E15 0.0 82000  
LOW /3E16 0.0 58000/  
TROE/ 0.5 1E-30 1E+30 /  
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ CH4/2.00/ AR/ .70/  
C2H5OH(+M)<=>C2H4+H2O(+M) 8E13 0.0 65000  
LOW /1E17 0.0 54000/  
TROE/ 0.5 1E-30 1E+30 /  
H2/2.00/ H2O/6.00/ CO/1.50/ CO2/2.00/ CH4/2.00/ AR/ .70/

!-----

! J. Li, PhD thesis

C2H5OH+OH = C2H4OH+H2O 1.810E+11 0.39 7.165E+02  
C2H5OH+OH = CH3CHOH+H2O 3.090E+10 0.49 -3.798E+02  
C2H5OH+OH = CH3CH2O+H2O 1.050E+10 0.79 7.169E+02

! Marinov, IJCK 31:183 (1999)

C2H5OH+H = C2H4OH+H2 1.900E+07 1.80 5.098E+03 ! \*1.5  
C2H5OH+H = CH3CHOH+H2 2.580E+07 1.65 2.827E+03  
C2H5OH+H = CH3CH2O+H2 1.500E+07 1.60 3.038E+03  
C2H5OH+O = C2H4OH+OH 9.410E+07 1.70 5.459E+03  
C2H5OH+O = CH3CHOH+OH 1.880E+07 1.85 1.824E+03  
C2H5OH+O = CH3CH2O+OH 1.580E+07 2.00 4.448E+03  
C2H5OH+CH3 = C2H4OH+CH4 2.190E+02 3.18 9.622E+03  
C2H5OH+CH3 = CH3CHOH+CH4 7.280E+02 2.99 7.948E+03  
C2H5OH+CH3 = CH3CH2O+CH4 1.450E+02 2.99 7.649E+03

!

!TESTING - MC

!C2H5OH+CH3 = C2H4OH+CH4 4.380E+02 3.18 9.622E+03  
!C2H5OH+CH3 = CH3CHOH+CH4 1.456E+03 2.99 7.948E+03  
!C2H5OH+CH3 = CH3CH2O+CH4 2.900E+02 2.99 7.649E+03

!

C2H5OH+HO2 = CH3CHOH+H2O2 8.200E+03 2.55 1.075E+04  
C2H5OH+HO2 = C2H4OH+H2O2 2.430E+04 2.55 1.575E+04 ! \*2.0  
C2H5OH+HO2 = CH3CH2O+H2O2 3.800E+12 0.00 2.400E+04 ! \*1.5

!

CH3CH2O+M = CH3CHO+H+M 5.600E+34 -5.89 2.5274E+04 ! \*0.5  
CH3CH2O+M = CH3+CH2O+M 5.350E+37 -6.96 2.380E+04 ! \*0.4  
CH3CH2O+O2 = CH3CHO+HO2 4.000E+10 0.00 1.100E+03  
CH3CH2O+CO = C2H5+CO2 4.680E+02 3.16 5.380E+03  
CH3CH2O+H = CH3+CH2OH 3.000E+13 0.00 0.000E+00  
CH3CH2O+H = C2H4+H2O 3.000E+13 0.00 0.000E+00  
CH3CH2O+OH = CH3CHO+H2O 1.000E+13 0.00 0.000E+00  
CH3CHOH+O2 = CH3CHO+HO2 4.820E+13 0.00 5.017E+03 ! \*0.1  
DUPLICATE  
CH3CHOH+O2 = CH3CHO+HO2 8.430E+14 -1.20 0.000E+00  
DUPLICATE  
CH3CHOH+O = CH3CHO+OH 1.000E+14 0.00 0.000E+00  
CH3CHOH+H = C2H4+H2O 3.000E+13 0.00 0.000E+00  
CH3CHOH+H = CH3+CH2OH 3.000E+13 0.00 0.000E+00  
CH3CHOH+HO2 = CH3CHO+OH+OH 4.000E+13 0.00 0.000E+00  
CH3CHOH+OH = CH3CHO+H2O 5.000E+12 0.00 0.000E+00  
CH3CHOH+M = CH3CHO+H+M 1.000E+14 0.00 2.500E+04  
C2H4OH+O2 = HOC2H4O2 1.000E+12 0.00 -1.100E+03  
HOC2H4O2 = CH2O+CH2O+OH 1.800E+11 0.00 2.450E+04 ! \*3.0

! Diau and Lee, J. Phys. Chem. 96:377 (1992)

C2H4+OH = C2H4OH 2.410E+11 0.00 -2.385E+03

```

! Tsang and Hampson, JPC Ref. Data, 15:1087 (1986)
C2H5+HO2 = CH3CH2O+OH 4.000E+13 0.00 0.000E+00 ! *1.3

! BAW added from Hynes shock tube study
! gtl removed C3F7H thrid body info C3F7H/12.00/
CF3-CHF (+M)=CHF:CF2 + F (+M) 6.30E14 0.0 62000.0
LOW /5.51E19 0.0 62000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
!!!*****
! stuff being adjusted here
!CHF3 (+M) = HF + CF2 (+M) 1.29E14 0.0 72118 !SCH/WAG
!LOW /2.06E35 -5.75 58400/ !MOD/LAG
CH2F+H<=>CH2*+HF 11.000E+13 0.0 0.0
CH2F+H<=>CHF+H2 5.000E+13 .000 .00
!CHF2 +H <=>CF2+H2 1.250E+13 .000 .00

!CHF3 + H = CF3 + H2 3.76E13 0.0 13100 ! Saso change
CHF3 + H = CF3 + H2 7.83E06 2.06 12300. !2004LOU/GON10586-10593/vb,08/12
CHF3 + H = CH2F2 + F 4.32e08 1.60 62990. !1997BER/EHL107-116

CHF + H = CH + HF 0.65E14 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT)

CHF + H = CF + H2 2.30E14 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT)
CH + HF = CF + H2 2.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CO + F + M = CF:O + M 3.09E19 -1.40 -487.
H2/2.00/ H2O/18.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
!<A HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM) Saso change

CF:O + H = CO + HF 2.50E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CHO Saso change
!*****
CH2F + O = CHF:O + H 5.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3)
CHF2 + O = CF2:O + H 3.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3)
!CF3 + O = CF2:O + F 1.90E13 0.00 0. !<A
HREF=#89TSA/BEL>89TSA/BEL</A> (EXPT)
!gt1 change
CF3 + O = CF2:O + F 1.54E13 0.00 0. !<A HREF=#98TAK/SEK> (EXPT)

!*****
CH2F + OH = CH2O + HF 2.50E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3+O)
CHF2 + OH = CHF:O + HF 1.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3+O)
!CF3 + OH = CF2:O + HF 2.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (O)
CF3 + OH = CF2:O + HF 1.46E13 -0.06 -266. !2007SRI/SU6822-6831 /vb,08-12
!*****
CH2F + CF2 = CHF:CF2 + H 2.00E12 0.00 3500. !BAW 4E12=>2E12
CF:O + CHF2 = CF2CO + HF 2.70E13 0.00 20000. !BAW change, C&F 113:164 (1998)
CF2CO + H = CHF2 + CO 1.13E13 0.00 3428. !<A HREF=#96BUR/ZAC

!*****
!***** HYDROGEN/OXYGEN/FLUORINE *****
!*****

!*****
!*** HF, F, F2: Combination, decomposition ***
!*****

```

```

HF      + M      = H      + F + M      3.12E13  0.00  99320.  !<A
HREF=#81BAU/DUX>81BAU/DUX</A> (EXPT)
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
AR/0.70/ CHF3/2.00/

!*****
!*** HF, F, F2: Atom transfer ***
!*****
H2      + F      = H      + HF      2.56E12  0.50  650.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89STE/BRU>89STE/BRU</A> (FIT)
OH      + F      = O      + HF      2.00E13  0.00  0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (H+HNO3)
HO2     + F      = O2     + HF      2.89E12  0.50  0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#83WAL/WAG>83WAL/WAG</A> (FIT)
H2O     + F      = OH     + HF      1.30E09  1.50  0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#83WAL/WAG>83WAL/WAG</A> (FIT)
H2O2    + F      = HO2    + HF      1.73E12  0.50  0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#83WAL/WAG>83WAL/WAG</A> (FIT)

!*****
!***** C1 FLUOROCARBONS *****
!*****

!*****
!*** <A name=ch4d>FLUOROMETHANES: THERMAL DECOMPOSITIONS</A> ***
!*****
!CH2* + HF = CH3F 1.91E23 -3.62 1780. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#73SCH/WAG>73SCH/WAG</A> (FIT)
!BAW change
CH3F (+M) = CH2* + HF (+M) 1.00E14 0.0 85000.! 73 SCH/WAG
LOW /1.50E16 0.0 67499./ !73 SCH/WAG
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
CHF      + H2     = CH3F      2.25E17  -2.85  13000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F     + H      = CH3F     3.03E21  -3.38  3460.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
! BAW converted to low pressure limit, added 3rd body efficiencies
CHF      + HF +M = CH2F2 +M 3.04E26 -3.26 4060.
!<A HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

CF2      + H2     = CH2F2     1.70E06  -0.71  40900.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2     + H      = CH2F2     2.75E06  -0.32  7690.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CHF3     + M      = CF2     + HF +M 3.41E30  -4.00  69050.
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ CHF3/6.00/
CH2F2/6.00/ CH3F/6.00/ HF /2.00/
!<A HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#91HID/NAK>91HID/NAK</A> (FIT)
!BAW change
!CHF3 = HF + CF2 1.29E14 0.0 72118 !SCH/WAG
!LOW /2.06E35 -5.75 58400/ !MOD/LAG
!*****
!CF3     + F      = CF4     1.60E38  -7.90  8950.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86PLU/R YA>86PLU/R YA</A> (RRKM)
!BAW change convert to low pressure limit, 3rd body efficiency
CF4 + M = CF3 + F + M 9.0E34 -4.64 122400
H2/2.00/ H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ CF4 /6.00/

```

```

!*****
!*** FLUOROMETHANES: ACTIVATED DECOMPOSITIONS ***
!*****
CH2* + HF = CHF + H2 2.08E07 1.27 8330. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(RRKM)
!CH2F + H = CH2* + HF 8.19E15 -0.63 505. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(RRKM)
!CH2F + H = CHF + H2 5.21E08 1.16 1000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!BAW change
!CH2F+H<=>CH2*+HF 4.000E+13 0.0 0.0
!CH2F+H<=>CHF+H2 1.200E+14 .000 .00

CH3 + F = CH2* + HF 1.62E16 -0.88 -981. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(RRKM)
CH3 + F = CH2F + H 1.36E12 -0.39 -265. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CHF + HF = CF2 + H2 5.77E06 1.35 17900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2 + H = CHF + HF 1.49E14 -0.11 101. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2 + H = CF2 + H2 5.50E03 2.42 -420. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!BAW change
!CHF2 +H <=>CF2+H2 5.000E+13 .000 .00

CH2F + F = CHF + HF 5.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
!CF3 + H = CF2 + HF 5.50E13 0.00 0. !<A
HREF=#89TSA/MCF>89TSA/MCF</A> (EXPT)
!gt1 change
CF3 + H = CF2 + HF 5.33E13 0.00 0. !<A HREF=#98TAK/SEK> (EXPT)
CHF2 + F = CF2 + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

!*****
!*** <A name=ch4a>FLUOROMETHANES: ABSTRACTION TO METHYLS</A> ***
!*****

!*****
!*** Fluoromethanes: Reactions with H ***
!*****
CH3F + H = CH2F + H2 2.70E03 3.00 5300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#75WES/DEH>75WES/DEH</A> (FIT)
CH2F2 + H = CHF2 + H2 1.65E03 3.00 5600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#72RID/DAV>72RID/DAV</A> (FIT)
!CF3 + H2 = CHF3 + H 6.30E01 3.00 5300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#72BER/MAR>72BER/MAR</A> (FIT) (NEW)
!BAW change
!CHF3 + H = CF3 + H2 3.76E13 0.0 13100 ! Saso change
!*****
CH3F + H = CH3 + HF 2.75E14 0.00 31400. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CH2F2 + H = CH2F + HF 5.50E13 0.00 34100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
!CHF3 + H = CHF2 + HF 8.00E13 0.00 40300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CHF3 + H = CHF2 + HF 2.11E08 1.77 39800. !2004LOU/GON10586-10593/vb;08-12
!CF4 + H = CF3 + HF 1.10E15 0.00 44600. !<A
HREF=#71KOC/MOI>71KOC/MOI</A> (EXPT)
CF4 + H = CF3 + HF 3.07e09 1.58 41330. !1997BER/EHL107-116/vb;08-12
CF4 + H = CHF3 + F 9.15e08 1.45 63590. !1997BER/EHL107-116/vb;08-12
!*****

```



```

!*** Fluoromethanes: Reactions with O, OH, HO2 ***
!*****
CH3F + O = CH2F + OH 6.50E07 1.50 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#67PAR/AZA>67PAR/AZA</A> (FIT)
CH2F2 + O = CHF2 + OH 2.25E07 1.50 6100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#68PAR/NAL>68PAR/NAL</A> (FIT)
!CHF3 + O = CF3 + OH 1.00E08 1.50 9250. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78JOU/LEB>78JOU/LEB</A> (FIT)
!gt1 change
CHF3 + O = CF3 + OH 3.07E14 0.00 18950. !reference 2001FER/FON
JPhysChem105,8196-8199

!*****
CH3F + OH = CH2F + H2O 2.60E08 1.50 2940. !<A
HREF=#91COH/WES>91COH/WES</A> <A HREF=#82JEO/KAU>82JEO/KAU</A> (FIT)
CH2F2 + OH = CHF2 + H2O 2.80E07 1.70 2540. !<A
HREF=#91COH/WES>91COH/WES</A> <A HREF=#82JEO/KAU>82JEO/KAU</A> (FIT)
!CHF3 + OH = CF3 + H2O 5.77E06 1.80 4292. !<A
HREF=#87COH/BEN>87COH/BEN</A> <A HREF=#82JEO/KAU>82JEO/KAU</A> (FIT)
CHF3 + OH = CF3 + H2O 1.25E07 1.55 3670. !2007SRI/SU6822-6831/vb;08-12
!*****
CH2F + H2O2 = CH3F + HO2 1.20E10 0.00 -600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CHF2 + H2O2 = CHF2 + HO2 1.20E10 0.00 -600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CF3 + H2O2 = CHF3 + HO2 1.20E10 0.00 -600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)

!*****
!*** Fluoromethanes: Reactions with CH3, C2H3 ***
!*****
CH3F + CH3 = CH2F + CH4 1.50E11 0.00 11400. !<A
HREF=#65PRI/BRY>65PRI/BRY</A> (EXPT)
CH2F2 + CH3 = CHF2 + CH4 8.70E10 0.00 10200. !<A
HREF=#65PRI/BRY>65PRI/BRY</A> (EXPT)
CF3 + CH4 = CHF3 + CH3 8.34E11 0.00 10920. !<A
HREF=#78ART/BEL>78ART/BEL</A> (EXPT)
!*****
CH3F + C2H3 = CH2F + C2H4 1.50E11 0.00 10300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#65PRI/BRY>65PRI/BRY</A> (CH3)
CH2F2 + C2H3 = CHF2 + C2H4 9.00E10 0.00 9200. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#65PRI/BRY>65PRI/BRY</A> (CH3)
CF3 + C2H4 = CHF3 + C2H3 8.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78ART/BEL>78ART/BEL</A> (CH3)

!*****
!*** Fluoromethyls: Reactions with Fluoromethanes ***
!*****
!CH3F + CF3 = CH2F + CHF3 1.35E12 0.00 11200. !<A
HREF=#67GIL/QUI>67GIL/QUI</A> (EXPT)
CH3F + CF3 = CH2F + CHF3 5.75E11 0.00 11210. !2002OLL/LAN3341-3349, 448-
636K/vb,08-12
CH2F2 + CH2F = CHF2 + CH3F 9.00E10 0.00 14000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#65PRI/BRY>65PRI/BRY</A> (CH3)
!CH2F2 + CF3 = CHF2 + CHF3 7.20E11 0.00 11200. !<A
HREF=#67GIL/QUI>67GIL/QUI</A> (EXPT)
CH2F2 + CF3 = CHF2 + CHF3 4.27E11 0.00 11300. !2002OLL/LAN3341-3349/vb;08-12
!*****
!*** Fluoromethyls: Reactions with CH3O, CH2O, HCO ***
!*****
CH3OH + CH2F = CH3O + CH3F 1.44E01 3.10 9800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CH3OH + CHF2 = CH3O + CH2F2 1.44E01 3.10 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CH3OH + CF3 = CH3O + CHF3 1.44E01 3.10 5500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)

```

```

!*****
CH3OH + CH2F = CH2OH + CH3F 3.20E01 3.20 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87TSA>87TSA</A> (CH3)
CH3OH + CHF2 = CH2OH + CH2F2 3.20E01 3.20 9300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87TSA>87TSA</A> (CH3)
CH3OH + CF3 = CH2OH + CHF3 3.20E01 3.20 5700. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87TSA>87TSA</A> (CH3)
!*****
CH2O + CH2F = HCO + CH3F 5.54E03 2.81 8300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CH2O + CHF2 = HCO + CH2F2 5.54E03 2.81 7800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CH2O + CF3 = HCO + CHF3 5.54E03 2.81 4600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
!*****
HCO + CH2F = CO + CH3F 9.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
HCO + CHF2 = CO + CH2F2 9.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
HCO + CF3 = CO + CHF3 9.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
!*****
HCO + CH2F = CH2CO + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
HCO + CHF2 = CHF2O + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
HCO + CF3 = CF2CO + HF 2.70E13 0.00 0. !BAW change C&F 113:164 (1998)

!*****
!*** <A name=ch3>FLUOROMETHYLS</A>
!*****

!*****
!*** Fluoromethyls: Reaction with O2, O, OH, HO2 ***
!*****
CH2F + O2 => CHF:O + O + H 2.26E09 1.14 28500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF3)
CHF2 + O2 => CF2:O + O + H 2.26E09 1.14 16500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF3)
CF3 + O2 = CF3O + O 2.26E09 1.14 21500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
!CH2F + O = CHF:O + H 5.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3)
!CHF2 + O = CF2:O + H 3.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3)
!CF3 + O = CF2:O + F 1.90E13 0.00 0. !<A
HREF=#89TSA/BEL>89TSA/BEL</A> (EXPT)
!*****
!BAW change these three A factors from 2E13 to 5E13
!CH2F + OH = CH2O + HF 5.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3+O)
!CHF2 + OH = CHF:O + HF 5.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (CF3+O)
!CF3 + OH = CF2:O + HF 5.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/BEL>89TSA/BEL</A> (O)
!*****
CH2F + HO2 => CHF:O + OH + H 1.50E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH3)
CHF2 + HO2 => CF2:O + OH + H 1.50E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH3)
CF3 + HO2 = CF3O + OH 1.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH3)
!*****

```

```

CH2F + HO2 = CH3F + O2 3.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CHF2 + HO2 = CH2F2 + O2 3.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)
CF3 + HO2 = CHF3 + O2 2.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH3)

!*****
!*** CF3O ***
!*****
CF3O + M = CF2:O + F + M 9.03E26 -3.42 21700. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
AR/0.70/ CHF3/2.00/
CF3O + H = CF2:O + HF 1.00E14 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + H2 => CF2:O+HF + H 1.00E13 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + H2O => CF2:O+HF + OH 1.00E13 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + CH4 => CF2:O+HF + CH3 8.00E12 0.00 2300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92CHE/ZHU>92CHE/ZHU</A> (C2H6)
CF3O + C2H6 => CF2:O+HF + C2H5 1.20E13 0.00 2300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92CHE/ZHU>92CHE/ZHU</A> (FIT)
CF3O + C2H4 => CF2:O+HF + C2H3 1.00E13 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + C2H2 => CF2:O + CH2:CF 1.00E13 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + CH2O => CF2:O+HF + HCO 5.00E12 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3O + HCO => CF2:O+HF + CO 5.00E12 0.00 2000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!*****
!*** <A name=ch2>FLUOROCARBENES: (CH2SING,) CHF, CF2</A>
!*****
!*****
!*** Fluorocarbenes: Reaction with O2, O, OH, H2O ***
!*****
CHF + O2 = CHF:O + O 2.00E13 0.00 16500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#77KEA/MAT>77KEA/MAT</A> (CF2)
CF2 + O2 = CF2:O + O 2.00E13 0.00 26500. !<A
HREF=#77KEA/MAT>77KEA/MAT</A> (EXPT)
!*****
CHF + O = CO + HF 9.00E13 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT) (CHECK)
!CF2 + O = CF:O + F 1.20E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90TSA/MCF>90TSA/MCF</A> (FIT)
!gt1 change
CF2 + O = CF:O + F 2.45E13 0.00 0. !<A HREF=#99YAM/TAK> (EXPT)

!*****
CHF + OH = CHF:O + H 2.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (CF2)
!BAW change
!CF2 + OH = CF2:O + H 2.00E13 0.00 3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (FIT)
CF2 + OH = CF2:O + H 4.00E13 0.00 0.
CHF + OH = HCO + HF 4.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (H-Elimination)
CF2 + OH = CF:O + HF 1.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (H-Elimination)
!*****

```

```

CHF + HO2 = CHF:O + OH 1.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (OH)
CF2 + HO2 = CF2:O + OH 1.00E13 0.00 3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (OH)
CHF + HO2 = CH2F + O2 2.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (OH)
CF2 + HO2 = CHF2 + O2 2.00E12 0.00 3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78BIO/LAZ>78BIO/LAZ</A> (OH)
!*****
CHF + H2O = CH2O + HF 5.00E12 0.00 6500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CF2 + H2O = CHF:O + HF 5.00E12 0.00 25000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)

!*****
!*** Fluorocarbenes: Reaction with F ***
!*****
!CF + F = CF2 6.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
!BAW change converted to low pressure limit, 3rd body efficiencies
!CF2 + M = CF + F + M 6.0E26 -2.85 106000
!H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
!CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ CF4 /6.00/ HF /2.00/

CF2 (+ M) = CF + F (+ M) 5.3E14 0.0 118300. !ar=>n2;2900-3800K;Cobos
etal.J.PhysChem,A,2010,114,4755-4761/vb,08-12
LOW / 2.29e15 0.0 95470. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ CF4 /6.00/ HF /2.00/

!*****
!*** Fluorocarbenes: Reaction with H ***
!*****
!BAW change
!CHF + H = CH + HF 2.95E14 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT)
!CHF + H = CH + HF 1.35E14 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT)

!CHF + H = CF + H2 1.60E14 0.00 0. !<A
HREF=#90TSA/MCF>90TSA/MCF</A> (EXPT)

!CF2 + H = CF + HF 2.35E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/MCF>89TSA/MCF</A> (FIT)
!gt1 change
CF2 + H = CF + HF 3.98E13 0.00 4540. !<A HREF=#99YAM/TAK> (EXPT)

!*****
!*** Fluorocarbenes: Reaction with RH ***
!*****
CH2O + CHF = HCO + CH2F 1.00E13 0.00 15000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH2O + CHF = CH2CO + HF 1.00E13 0.00 15000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!*****
CH2O + CF2 = HCO + CHF2 1.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH2O + CF2 = CHF:CO + HF 1.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!*****
HCO + CHF = CO + CH2F 2.00E13 0.00 15000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
HCO + CF2 = CO + CHF2 2.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)

```

```

!*****
!*** CF ***
!*****
!CH      + HF      = CF      + H2      3.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
!CF      + O2      = CF:O     + O       2.00E13  0.00   1800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92PEE/VAN>92PEE/VAN</A> (FIT)
!gt1 change
CF      + O2      = CF:O     + O       6.62E12  0.00   1690. !<A HREF=#09VET/DIL> (EXPT)

CF      + H2O     = CHF:O    + H       2.00E13  0.00  17000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (H2O+C1)
!BAW adjust
CF      + H       = C       + HF      8.00E13  0.00   1160.
!CF      + H       =>C       + HF      4.00E13  0.00   750.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89TSA/MCF>89TSA/MCF</A> (FIT)
!USE REACTION BELOW INSTEAD IF C IS NOT IN MECHANISM
!CF      + H       =>CH      + F       4.00E13  0.00   750.    !96BUR/ZAC 89TSA/MCF (FIT)
(NOTE)
!BAW adjust
CF      + O       = CO + F     8.00E13  0.00   1410.
!CF      + O       = CO + F     4.00E13  0.00  1000.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90TSA/MCF>90TSA/MCF</A> (FIT)
!BAW adjust
CF      + OH      = CO       + HF      8.00E13  0.00   1410.
!CF      + OH      = CO       + HF      3.00E13  0.00  1000.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90TSA/MCF>90TSA/MCF</A> (OH)
CF      + HO2     =>CF:O    + OH      3.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + CH3     =>CH2:CF  + H       3.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + C2H3    =>C2HF    + CH2     3.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + CH2     =>C2HF    + H       3.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + CH2*    =>C2HF    + H       3.00E13  0.00    0.    !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(upper-limit)
CF      + CH4     =>CH2:CHF  + H       5.00E12  0.00  10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + C2H4    =>C2H2    + CH2F    1.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + CH2O    =>CHF     + HCO     1.00E13  0.00   8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF      + HCO     =>CHF     + CO      1.00E13  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!*****
!*** <A name=cfo>Oxidized C1 Fluorocarbons</A> ***
!*****

!*****
!*** CHF:O & CF2:O: Decompositions ***
!*****
CHF:O   + M       = CO       + HF + M   2.48E25 -3.00  43000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#85SAI/KUR>85SAI/KUR</A> (FIT)
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
AR/0.70/ CHF3/2.00/
CF:O    + F       = CF2:O    1.00E12  0.00    0.    !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!*****
!*** CHF:O & CF2:O: Reactions with H ***
!*****
CHF:O   + H       = CF:O     + H2     1.10E08  1.77  3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH2O)

```

```

!*****
CF2:O + H = CF:O + HF 2.40E07 1.88 35900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
DUP
CF2:O + H = CF:O + HF 1.20E10 0.83 22300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
DUP
CF2:O + H = CF:O + HF 5.50E08 1.42 18900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
DUP

!*****
!*** CHF:O & CF2:O: Reactions with H2O, O, OH, HO2 ***
!*****
CF2:O + H2O => CO2 + HF + HF 7.40E-3 3.84 25100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CHF:O + O = CF:O + OH 9.00E12 0.00 3080. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#80KLE/SKO>80KLE/SKO</A> (CH2O)
CHF:O + OH = CF:O + H2O 1.72E09 1.18 -447. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH2O)
CF2:O + OH => CO2 + F + HF 2.70E03 2.38 21000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (BACMP4)
CF:O + H2O2 = CHF:O + HO2 1.00E11 0.00 3900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CH2O)

!*****
!*** CHF:O & CF2:O: Reactions with Methyls ***
!*****
CHF:O + CH3 = CF:O + CH4 2.00E12 0.00 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH2O)
CHF:O + CH2F = CF:O + CH3F 2.00E12 0.00 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH2O)
CHF:O + CHF2 = CF:O + CH2F2 2.00E12 0.00 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH2O)
CHF:O + CF3 = CF:O + CHF3 2.00E12 0.00 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH2O)
CHF:O + C2H3 = CF:O + C2H4 2.00E12 0.00 5000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CH2O)

!*****
!*** CF:O Reactions ***
!*****
!CO + F + M = CF:O + M 3.09E19 -1.40 -487.
!H2O /18.0/
!<A HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM) Saso change
!CF:O + H = CO + HF 2.50E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CHO) Saso change
CF:O + O = CO2 + F 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CHO)
CF:O + OH = CO2 + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (CHO)
CF:O + HO2 => CO2 + F + OH 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CHO)
CF:O + CH3 = CH2CO + HF 2.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (CHO)
CF:O + CH2F = CHF3 + HF 2.70E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CF:O + CF:O = CO + CF2:O 2.23E13 0.00 318. !<A
HREF=#92MAR/SZE>92MAR/SZE</A> (EXPT)

!*****
!*** C2 FLUOROCARBONS ***
!*****

!*****
!*** Fluoroethanes: (C2H6,) CH3F, CH2F2, CHF3, CF4 ***

```

```

!*****
!*****
!*** Fluoroethane <A name=c2h6d>decompositions (HF elimination)</A> ***
!*****
CH3-CH2F      = C2H4      + HF      2.63E13   0.00   59900.  !<A
HREF=#70CAD/DAY>70CAD/DAY</A> (EXPT)
CH3-CHF2      = CH2:CHF   + HF      7.94E13   0.00   61900.  !<A
HREF=#70TSC/QUI>70TSC/QUI</A> (EXPT)
CH3-CF3       = CH2:CF2   + HF      1.00E14   0.00   68700.  !<A
HREF=#71TSC/QUI>71TSC/QUI</A> (EXPT)
CH2F-CH2F     = CH2:CHF   + HF      2.50E13   0.00   62900.  !<A
HREF=#71KER/TIM>71KER/TIM</A> (EXPT)
CH2F-CHF2     = CHF:CHF[Z]+HF  1.26E14   0.00   69100.  !<A
HREF=#74SEK/TSC>74SEK/TSC</A> (EXPT)
CH2F-CHF2     = CH2:CF2   + HF      1.00E13   0.00   65400.  !<A
HREF=#74SEK/TSC>74SEK/TSC</A> (EXPT)
CH2F-CF3      = CHF:CF2   + HF      2.63E13   0.00   70700.  !<A
HREF=#72MIL/TSC>72MIL/TSC</A> (EXPT)
CHF2-CHF2     = CHF:CF2   + HF      2.00E13   0.00   69400.  !<A
HREF=#71MIL/HAR>71MIL/HAR</A> (EXPT)
CHF2-CF3      = CF2:CF2   + HF      4.00E13   0.00   71600.  !<A
HREF=#71TSC/MIL>71TSC/MIL</A> (EXPT)

!*****
!*** Fluoroethane decompositions (C-C) *****
!*** Fluoromethyl association/stabilizations *****
!*** Fluoromethyl assocn/decompns via fluoroethanes ***
!*****

!*****
!*** Ethyl + Hydrogen with HF elimination ***
!*****
CH2F-CH2 + H   = C2H4      + HF      1.44E20  -2.12   1730.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3-CHF + H    = C2H4      + HF      2.27E20  -2.21   1950.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CHF + H   = CH2:CHF   + HF      2.06E23  -3.23   2280.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CHF2-CH2 + H   = CH2:CHF   + HF      5.24E16  -0.933   880.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3-CF2 + H    = CH2:CHF   + HF      2.09E16  -0.854   848.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CHF + H   = CHF:CHF[Z]+HF  1.86E20  -2.29   1750.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CHF + H   = CH2:CF2   + HF      9.95E19  -2.34   1780.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CF2 + H   = CHF:CHF[Z]+HF  6.32E19  -2.21   1630.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CF2 + H   = CH2:CF2   + HF      3.36E19  -2.26   1660.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CH2 + H    = CH2:CF2   + HF      1.12E21  -2.27   2240.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CHF + H    = CHF:CF2   + HF      6.56E24  -3.57   4225  ! BAW addition; C&F 113:164
(1998)
CHF2-CF2 + H   = CHF:CF2   + HF      1.81E22  -2.92   3070.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CF2 + H    = CF2:CF2   + HF      1.41E21  -2.40   3630.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

!*****
!*** Ethyl + Hydrogen with C-C breakage ***
!*****
CH2F-CH2 + H   = CH3      + CH2F    3.80E11   0.635   633.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

```

```

CH3-CHF + H = CH3 + CH2F 3.47E10 0.90 1370. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CHF + H = CH2F + CHF2 1.79E14 -0.105 1320. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CHF2-CH2 + H = CH3 + CHF2 2.02E06 2.16 451. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3-CF2 + H = CH3 + CHF2 1.62E05 2.50 1370. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CHF + H = CH2F + CHF2 6.36E12 0.318 1460. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CF2 + H = CH2F + CHF2 3.64E12 0.329 1180. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CH2 + H = CH3 + CF3 2.48E11 0.816 2870. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CHF + H = CF3 + CH2F 4.28E16 -0.74 4750 ! BAW addition, C&F 113:164
(1998)
CHF2-CF2 + H = CHF2 + CHF2 3.25E15 -0.524 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CF2 + H = CHF2 + CF3 4.37E16 -0.746 4360. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

!*****
!*** Ethyl + Hydrogen with stablized product ***
!*****
CH2F-CH2 + H = CH3-CH2F 1.19E35 -8.51 8140. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3-CHF + H = CH3-CH2F 9.57E38 -9.24 7360. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CHF + H = CH2F-CH2F 1.56E45 -10.80 8070. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CH2 + H = CH3-CHF2 2.96E37 -9.05 7160. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3-CF2 + H = CH3-CHF2 3.11E40 -9.59 7190. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CHF + H = CH2F-CHF2 1.20E44 -10.60 7520. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CF2 + H = CH2F-CHF2 2.74E43 -10.50 7670. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CH2 + H = CH3-CF3 7.27E42 -9.86 7360. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CF2 + H = CHF2-CHF2 3.77E46 -10.80 8980. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3-CF2 + H = CHF2-CF3 1.12E47 -10.80 4100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

!*****
!*** Methyl + Methyl combination with HF elimination ***
!*****
!BAW change
CH3 + CH2F = C2H4 + HF 1.85E19 -1.86 1870.
!CH3 + CH2F = C2H4 + HF 2.35E19 -1.86 1870. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F + CH2F = CH2:CHF + HF 7.56E21 -2.79 2590. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
! BAW change
CH3 + CHF2 = CH2:CHF + HF 1.30E15 -0.586 634.
!CH3 + CHF2 = CH2:CHF + HF 1.90E15 -0.586 634. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F + CHF2 = CHF:CHF[Z]+HF 3.88E20 -2.35 2888. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F + CHF2 = CH2:CF2 + HF 2.23E20 -2.41 2910. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3 + CF3 = CH2:CF2 + HF 5.53E19 -1.94 2440. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

```



```

CHF2      + CHF2 = CHF:CF2 + HF      2.20E19  -1.95   4100.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2      + CF3  = CF2:CF2 + HF      7.00E16  -1.17   4330.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)

!*****
!*** Methyl + Methyl with product stabilization ***
!*****
CH3       + CH2F = CH3-CH2F          1.57E31  -6.27   4440.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F     + CH2F = CH2F-CH2F          2.37E24  -3.79   2290.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3       + CHF2 = CH3-CHF2          1.93E35  -7.69   5760.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F     + CHF2 = CH2F-CHF2          9.61E38  -8.36   6940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH3       + CF3  = CH3-CF3           1.78E33  -6.64   5020.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2     + CHF2 = CHF2-CHF2          2.26E24  -3.50   3360.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2     + CF3  = CHF2-CF3           2.61E26  -4.16   4100.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!CF3     + CF3  = CF3-CF3           1.63E36  -7.26   7050.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CF3 + CF3 (+M) = CF3-CF3 (+M)       9.69e10   0.77     0.0  !Ar=>N2,Cobos
etal,J.PhysChem,2010,114:4748-4754/vb,08-12
      LOW / 2.12e60  -12.51  5910. /
      TROE / 0.069  260. 880. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
!*****
!*** Ethyl + Hydrogen with H atom disprop. ***
!*****
CH2F-CH2 + H   = CH3-CHF + H         1.87E01   3.10    137.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CHF2-CH2 + H   = CH3-CF2 + H         1.59E-3   4.35    157.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
CH2F-CF2 + H   = CHF2-CHF + H        0.64E00   3.53   1830.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CF3-CF3 + H    = CF3-CF2 + HF        1.00E15   0.00  30000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF4)
!*****
!*** Methane + Methylene combination with HF elimination ***
!*****

!*****
!*** Fluorocarbenes: Reaction with Fluoromethanes ***
!*****
CH3F +CH2* = C2H4 + HF              3.00E13   0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A> <A
HREF=#89MIL/BOW>89MIL/BOW</A> (CH4)
CH2F2+CH2* = CH2:CHF + HF           2.00E13   0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A> <A
HREF=#89MIL/BOW>89MIL/BOW</A> (CH4)
CHF3 +CH2* = CH2:CF2 + HF           1.00E13   0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A> <A
HREF=#89MIL/BOW>89MIL/BOW</A> (CH4)
CF4 +CH2* = CHF:CF2 + HF            4.00E13   0.00  31000.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A> <A
HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
!*****
CH4      + CHF = C2H4 + HF           4.00E13   0.00  15000.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CH3F    + CHF = CH2:CHF + HF         3.00E13   0.00  15000.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH2F2   + CHF = CH2:CF2 + HF         1.00E13   0.00  15000.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH2F2   + CHF = CHF:CHF[Z]+HF        1.00E13   0.00  15000.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)

```

```

CHF3 + CHF = CHF:CF2 + HF 1.00E13 0.00 15000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CF4 + CHF = CF2:CF2 + HF 4.00E13 0.00 31000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!*****
CH4 + CF2 = CH2:CHF + HF 4.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CH3F + CF2 = CH2:CF2 + HF 1.50E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH3F + CF2 = CHF:CHF[Z]+HF 1.50E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CH2F2 + CF2 = CHF:CF2 + HF 2.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CHF3 + CF2 = CF2:CF2 + HF 1.00E13 0.00 41000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
CF4 + CF2 => CF3-CF3 4.00E13 0.00 51000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!*****
CH3 + CH2F = CH4 + CHF 3.00E13 0.00 3400. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#96ZAC/WES>96ZAC/WES</A> (BACMP4)
CH2F + CH2F = CH3F + CHF 3.00E13 0.00 4800. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!BAW change
CHF2 + CH2F = CH2F2 + CHF 1.00E13 0.00 4400.
!CHF2 + CH2F = CH2F2 + CHF 3.00E13 0.00 4400. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH4)
CF3 + CH2F = CHF3 + CHF 3.00E13 0.00 4600. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH4)
!*****
! BAW change
CH3 + CHF2 = CH4 + CF2 2.50E13 0.00 800. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#67BRY/PRI>67BRY/PRI</A> (FIT)
!CH3 + CHF2 = CH4 + CF2 1.80E13 0.00 800.
CH2F + CHF2 = CH3F + CF2 3.00E13 0.00 2200. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#74FOL/PRI>74FOL/PRI</A> (FIT)
CHF2 + CHF2 = CH2F2 + CF2 3.00E13 0.00 1600. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#84PRI/NIL>84PRI/NIL</A> (FIT)
CF3 + CHF2 = CHF3 + CF2 3.00E13 0.00 2000. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
<A HREF=#69PRI/FOL>69PRI/FOL</A> (FIT)
!*****

!*****
!*** <A name=c2h6a>FLUOROETHANES: ABSTRACTION REACTIONS</A> ***
!*****

!*****
!*** CH3-CH2F: Reactions with H,O,OH ***
!*****
CH3-CH2F + H = CH2F-CH2 + H2 5.50E08 1.60 9100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CH2F + O = CH2F-CH2 + OH 2.90E08 1.60 6100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CH2F + OH = CH2F-CH2 + H2O 5.50E07 1.60 1093. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)
!*****
CH3-CH2F + H = CH3-CHF + H2 3.30E08 1.60 9100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CH2F + O = CH3-CHF + OH 1.60E08 1.60 6100. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CH2F + OH = CH3-CHF + H2O 3.30E07 1.60 1093. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)

!*****
!*** CH3-CHF2: Reactions with H,O,OH ***
!*****

```

```

CH3-CHF2 + H = CHF2-CH2 + H2 1.50E08 1.60 9600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CHF2 + O = CHF2-CH2 + OH 7.50E08 1.60 6600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CHF2 + OH = CHF2-CH2 + H2O 1.54E07 1.60 1132. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)
!*****
CH3-CHF2 + H = CH3-CF2 + H2 0.44E08 1.60 9300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CHF2 + O = CH3-CF2 + OH 2.20E07 1.60 6300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CHF2 + OH = CH3-CF2 + H2O 0.44E07 1.60 1332. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)

!*****
!*** CH3-CF3: Reactions with H,O,OH ***
!*****
CH3-CF3 + H = CF3-CH2 + H2 4.00E10 1.10 12700. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CF3 + O = CF3-CH2 + OH 2.00E10 1.10 9700. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH3-CF3 + OH = CF3-CH2 + H2O 4.08E09 1.10 4670. !<A
HREF=#87COH/BEN>87COH/BEN</A> (NEED) (FIT)

!*****
!*** CH2F-CH2F: Reactions with H,O,OH ***
!*****
CH2F-CH2F + H = CH2F-CHF + H2 6.00E08 1.70 9600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CH2F + O = CH2F-CHF + OH 3.00E08 1.70 6600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CH2F + OH = CH2F-CHF + H2O 6.16E07 1.70 1610. !<A
HREF=#87COH/BEN>87COH/BEN</A> (NEED) (FIT)

!*****
!*** CH2F-CHF2: Reactions with H,O,OH ***
!*****
CH2F-CHF2 + H = CHF2-CHF + H2 2.00E08 1.70 9800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CHF2 + O = CHF2-CHF + OH 1.00E08 1.70 6800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CHF2 + OH = CHF2-CHF + H2O 2.05E07 1.70 1800. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)
!*****
CH2F-CHF2 + H = CH2F-CF2 + H2 1.00E08 1.70 11000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CHF2 + O = CH2F-CF2 + OH 5.00E07 1.70 8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CHF2 + OH = CH2F-CF2 + H2O 1.06E07 1.70 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87COH/BEN>87COH/BEN</A> (FIT)

!*****
!*** CH2F-CF3: Reactions with H,O,OH ***
!*****
CH2F-CF3 + H = CF3-CHF + H2 2.00E08 1.70 10500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CF3 + O = CF3-CHF + OH 1.00E08 1.70 7500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CH2F-CF3 + OH = CF3-CHF + H2O 2.10E07 1.70 2524. !<A
HREF=#87COH/BEN>87COH/BEN</A> (NEED) (FIT)

!*****
!*** CHF2-CHF2: Reactions with H,O,OH ***
!*****
CHF2-CHF2 + H = CHF2-CF2 + H2 1.60E07 1.70 10600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)

```

```

CHF2-CHF2 + O      = CHF2-CF2 + OH      8.00E07   1.70   7600.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CHF2-CHF2 + OH     = CHF2-CF2 + H2O     1.60E07   1.70   2643.  !<A
HREF=#87COH/BEN>87COH/BEN</A> (NEED) (FIT)

!*****
!*** CHF2-CF3: Reactions with H,O,OH ***
!*****
CHF2-CF3 + H       = CF3-CF2 + H2       1.40E07   1.60   10200. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CHF2-CF3 + O       = CF3-CF2 + OH       7.00E07   1.60   7200.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (OH)
CHF2-CF3 + OH      = CF3-CF2 + H2O     1.40E07   1.60   2246.  !<A
HREF=#87COH/BEN>87COH/BEN</A> (NEED) (FIT)

!*****
!*** Abstraction from fluoroethanes: By HO2 ***
!*****
CH3-CHF  + H2O2 = CH3-CH2F + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CH3-CF2  + H2O2 = CH3-CHF2 + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CH2F-CH2 + H2O2 = CH3-CH2F + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CH2F-CHF + H2O2 = CH2F-CH2F+ HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CH2F-CF2 + H2O2 = CH2F-CHF2+ HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CHF2-CH2 + H2O2 = CH3-CHF2 + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CHF2-CHF + H2O2 = CH2F-CHF2+ HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CHF2-CF2 + H2O2 = CHF2-CHF2+ HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CF3-CH2  + H2O2 = CH3-CF3  + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CF3-CHF  + H2O2 = CH2F-CF3 + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)
CF3-CF2  + H2O2 = CHF2-CF3 + HO2  9.00E09   0.00   1000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H6)

!*****
!*** CH3-CH2F: Abstraction by CH3,C2H3 ***
!*****
CH3-CH2F + CH3    = CH2F-CH2 + CH4    2.00E11   0.00   13400. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#65PRI/BRY>65PRI/BRY</A> (CH3F)
CH3-CH2F + C2H3  = CH2F-CH2 + C2H4    2.00E11   0.00   10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
!*****
CH3-CH2F + CH3    = CH3-CHF  + CH4    1.50E11   0.00   10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#65PRI/BRY>65PRI/BRY</A> (CH3F)
CH3-CH2F + C2H3  = CH3-CHF  + C2H4    1.50E11   0.00   7000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CH3-CHF2: Abstraction by CH3,C2H3 ***
!*****
CH3-CHF2 + CH3    = CHF2-CH2 + CH4    2.00E11   0.00   12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH3-CHF2 + C2H3  = CHF2-CH2 + C2H4    2.00E11   0.00   9000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
!*****
CH3-CHF2 + CH3    = CH3-CF2  + CH4    8.00E10   0.00   10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH3-CHF2 + C2H3  = CH3-CF2  + C2H4    8.00E10   0.00   7000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

```

```

!*****
!*** CH3-CF3: Abstraction by CH3,C2H3 ***
!*****
CH3-CF3 + CH3 = CF3-CH2 + CH4 2.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH3-CF3 + C2H3 = CF3-CH2 + C2H4 2.00E11 0.00 9000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CH2F-CH2F: Abstraction by CH3,C2H3 ***
!*****
CH2F-CH2F + CH3 = CH2F-CHF + CH4 3.00E11 0.00 10400. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH2F-CH2F + C2H3 = CH2F-CHF + C2H4 3.00E11 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CH2F-CHF2: Abstraction by CH3,C2H3 ***
!*****
CH2F-CHF2 + CH3 = CHF2-CHF + CH4 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH2F-CHF2 + C2H3 = CHF2-CHF + C2H4 2.00E11 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
!*****
CH2F-CHF2 + CH3 = CH2F-CF2 + CH4 1.00E11 0.00 9600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH2F-CHF2 + C2H3 = CH2F-CF2 + C2H4 1.00E11 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CH2F-CF3: Abstraction by CH3,C2H3 ***
!*****
CH2F-CF3 + CH3 = CF3-CHF + CH4 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CH2F-CF3 + C2H3 = CF3-CHF + C2H4 2.00E11 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CHF2-CHF2: Abstraction by CH3,C2H3 ***
!*****
CHF2-CHF2 + CH3 = CHF2-CF2 + CH4 3.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3-CH2F)
CHF2-CHF2 + C2H3 = CHF2-CF2 + C2H4 3.00E11 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

!*****
!*** CH2F-CF3: Abstraction by CH3,C2H3 ***
!*****
CHF2-CF3 + CH3 = CF3-CF2 + CH4 5.70E10 0.00 9500. !<A
HREF=#64PRI/THO>64PRI/THO</A> (EXPT)
CHF2-CF3 + C2H3 = CF3-CF2 + C2H4 6.00E10 0.00 7000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
!gtl changes 10-30-09 from new rates provided by Don Burgess email
!*****
!*** CH2F-CF3: Abstraction by CH3CH2 etc.
!*****

!rxns provided by don burgess to gtl in fall 2009
!CHF2-CF3 + CH3CH2* = CF3-CF2 + C2H6 5.7E10 0.0 11800.
!CHF2-CF3 + CH3CH2CH2* = CF3-CF2 + C3H8 5.7E10 0.0 10300.
!CHF2-CF3 + CH3CH*CH3 = CF3-CF2 + C3H8 5.7E10 0.0 13500.
!CHF2-CF3 + *CH2CH2OH = CF3-CF2 + C2H5OH 5.7E10 0.0 10600.
!CHF2-CF3 + CH3CH*OH = CF3-CF2 + C2H5OH 5.7E10 0.0 15900.
!CHF2-CF3 + CH3CH2O* = CF3-CF2 + C2H5OH 5.7E10 0.0 8900.

```

```

!species names made consistent with mech of fldryer
CHF2-CF3 + C2H5 = CF3-CF2 + C2H6 5.7E10 0.0 11800.
!vb CHF2-CF3 + nC3H7 = CF3-CF2 + C3H8 5.7E10 0.0 10300.
!vb CHF2-CF3 + iC3H7 = CF3-CF2 + C3H8 5.7E10 0.0 13500.
CHF2-CF3 + C2H4OH = CF3-CF2 + C2H5OH 5.7E10 0.0 10600.
CHF2-CF3 + CH3CHOH = CF3-CF2 + C2H5OH 5.7E10 0.0 15900.
CHF2-CF3 + CH3CH2O = CF3-CF2 + C2H5OH 5.7E10 0.0 8900.

```

```

!*****
!*** Fluoroethanes: CH2SING insertion & CH3 elimination ***
!*****

```

```

!*****
!*** Abstraction from fluoroethanes: By CH2F ***
!*****
CH3-CH2F + CH2F = CH2F-CH2 + CH3F 2.00E11 0.00 13000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CH2F + CH2F = CH3-CHF + CH3F 1.50E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CHF2 + CH2F = CHF2-CH2 + CH3F 2.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CHF2 + CH2F = CH3-CF2 + CH3F 8.00E10 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CF3 + CH2F = CF3-CH2 + CH3F 2.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CH2F + CH2F = CH2F-CHF + CH3F 3.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CHF2 + CH2F = CHF2-CHF + CH3F 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CHF2 + CH2F = CH2F-CF2 + CH3F 1.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CF3 + CH2F = CF3-CHF + CH3F 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CHF2-CHF2 + CH2F = CHF2-CF2 + CH3F 3.00E11 0.00 11000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CHF2-CF3 + CH2F = CF3-CF2 + CH3F 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

```

```

!*****
!*** Abstraction from fluoroethanes: By CHF2 ***
!*****
CH3-CH2F + CHF2 = CH2F-CH2 + CH2F2 2.00E11 0.00 13000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CH2F + CHF2 = CH3-CHF + CH2F2 1.50E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CHF2 + CHF2 = CHF2-CH2 + CH2F2 2.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CHF2 + CHF2 = CH3-CF2 + CH2F2 8.00E10 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH3-CF3 + CHF2 = CF3-CH2 + CH2F2 2.00E11 0.00 12000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CH2F + CHF2 = CH2F-CHF + CH2F2 3.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CHF2 + CHF2 = CHF2-CHF + CH2F2 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CHF2 + CHF2 = CH2F-CF2 + CH2F2 1.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CH2F-CF3 + CHF2 = CF3-CHF + CH2F2 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CHF2-CHF2 + CHF2 = CHF2-CF2 + CH2F2 3.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)
CHF2-CF3 + CHF2 = CF3-CF2 + CH2F2 2.00E11 0.00 10000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH3)

```

```

!*****
!*** Abstraction from fluoroethanes: By CF3 ***
!*****
CH3-CH2F + CF3 = CH2F-CH2 + CHF3 9.50E11 0.00 8200. !<A
HREF=#71QUI/WHI>71QUI/WHI</A> (EXPT)
CH3-CH2F + CF3 = CH3-CHF + CHF3 9.50E11 0.00 8200. !<A
HREF=#71QUI/WHI>71QUI/WHI</A> (EXPT)
CH3-CHF2 + CF3 = CHF2-CH2 + CHF3 3.10E10 0.00 7100. !<A
HREF=#66OKS/PRA>66OKS/PRA</A> (EXPT)
CH3-CHF2 + CF3 = CH3-CF2 + CHF3 3.10E10 0.00 7100. !<A
HREF=#66OKS/PRA>66OKS/PRA</A> (EXPT)
CH3-CF3 + CF3 = CF3-CH2 + CHF3 1.45E12 0.00 13500. !<A
HREF=#67GIL/QUI>67GIL/QUI</A> (EXPT)
CH2F-CH2F + CF3 = CH2F-CHF + CHF3 5.00E11 0.00 7600. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#71QUI/WHI>71QUI/WHI</A> (CH3-CH2F)
CH2F-CHF2 + CF3 = CHF2-CHF + CHF3 3.00E11 0.00 7200. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#71QUI/WHI>71QUI/WHI</A> (CH3-CH2F)
CH2F-CHF2 + CF3 = CH2F-CF2 + CHF3 2.00E11 0.00 8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#71QUI/WHI>71QUI/WHI</A> (CH3-CH2F)
CH2F-CF3 + CF3 = CF3-CHF + CHF3 3.00E11 0.00 6400. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#71QUI/WHI>71QUI/WHI</A> (CH3-CH2F)
CHF2-CHF2 + CF3 = CHF2-CF2 + CHF3 5.70E11 0.00 11900. !<A
HREF=#67GIL/QUI>67GIL/QUI</A> (EXPT)
CHF2-CF3 + CF3 = CF3-CF2 + CHF3 1.40E11 0.00 10100. !<A
HREF=#67GIL/QUI>67GIL/QUI</A> (EXPT)

!*****
!*** <A name=c2h5>FLUOROETHYLS</A> ***
!*****

!*****
!*** Fluoroethyl decompositions (see H + fluoroethene) ***
!*****

!*****
!*** Fluoroethyl associations: + O2 ***
!*****
CH3-CHF + O2 = CH2:CHF + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
CH3-CF2 + O2 = CH2:CF2 + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
!*****
CH2F-CH2 + O2 = CH2:CHF + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
CH2F-CHF + O2 = CHF:CHF[Z]+HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
CH2F-CF2 + O2 = CHF:CF2 + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
!*****
CHF2-CH2 + O2 = CH2:CF2 + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
CHF2-CHF + O2 = CHF:CF2 + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
CHF2-CF2 + O2 = CF2:CF2 + HO2 2.56E19 -2.77 1977. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#90BOZ/DEA>90BOZ/DEA</A> (C2H5)
!*****
CF3-CH2 + O2 => CF3 + CH2O + O 1.30E13 0.00 44000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF3)
CF3-CHF + O2 => CF3 + CHF:O+ O 1.30E13 0.00 23000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF3)
CF3-CF2 + O2 => CF3 + CF2:O+ O 1.30E13 0.00 23000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CF3)

!*****
!*** Fluoroethyl associations: + O ***
!*****

```

```

!*****
CH2F-CH2 + O = CH2CO+HF + H 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CH2 + O = CHF2CO+HF + H 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CH2 + O = CF2CO+HF + H 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
!*****
CH3-CHF + O = CH2CO+HF + H 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CH2F-CHF + O = CHF2CO+HF + H 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CHF + O = CF2CO+HF + H 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CHF + O =>CF3+CF:O + H 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
!*****
CH3-CF2 + O = CH2CO+HF + F 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CH2F-CF2 + O = CHF2CO+HF + F 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CF2 + O = CF2CO+HF + F 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CF2 + O =>CF3+CF:O + F 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
!*****
CH2F-CH2 + O = CH2O + CH2F 3.30E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CH2 + O = CH2O + CHF2 3.30E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CH2 + O = CH2O + CF3 3.30E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
!*****
CH3-CHF + O = CHF:O + CH3 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CH2F-CHF + O = CHF:O + CH2F 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CHF + O = CHF:O + CHF2 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CHF + O = CHF:O + CF3 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
!*****
CH3-CF2 + O = CF2:O + CH3 1.10E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CH2F-CF2 + O = CF2:O + CH2F 1.10E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CHF2-CF2 + O = CF2:O + CHF2 1.10E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)
CF3-CF2 + O = CF2:O + CF3 1.10E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5)

!*****
!*** Fluoroethyl associations: + OH ***
!*****
CH2F-CH2 + OH =>CH2CO+HF + H2 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CHF2-CH2 + OH =>CHF2CO+HF + H2 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CF3-CH2 + OH =>CF2CO+HF + H2 6.60E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
!*****
CH3-CHF + OH =>CH2CO+H2 + HF 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CH2F-CHF + OH =>CH2CO+HF + HF 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)

```



```

CHF2-CHF + OH =>CHFCO+HF + HF 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CF3-CHF + OH =>CF2CO+HF + HF 4.40E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
!*****
CH3-CF2 + OH =>CH2CO+HF + HF 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CH2F-CF2 + OH =>CHFCO+HF + HF 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CHF2-CF2 + OH =>CF2CO+HF + HF 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
CF3-CF2 + OH =>CF3+CF:O + HF 2.20E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92BAU/COB>92BAU/COB</A> (C2H5+O)
!*****
CH2F-CH2 + OH = CH2:CHF + H2O 6.60E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
CHF2-CH2 + OH = CH2:CF2 + H2O 4.40E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
!*****
CH3-CHF + OH = CH2:CHF + H2O 6.60E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
CH2F-CHF + OH = CHF:CHF[Z]+H2O 4.40E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
CHF2-CHF + OH = CHF:CF2 + H2O 2.20E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
!*****
CH3-CF2 + OH = CH2:CF2 + H2O 6.60E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
CH2F-CF2 + OH = CHF:CF2 + H2O 4.40E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)
CHF2-CF2 + OH = CF2:CF2 + H2O 2.20E13 0. 3000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (HF-Elimination)

!*****
!*** Disproportionation with CH3 ****
!*****
CH2F-CH2 + CH3 = CH2:CHF + CH4 1.30E13 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
CHF2-CH2 + CH3 = CH2:CF2 + CH4 6.50E12 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
!*****
CH3-CHF + CH3 = CH2:CHF + CH4 1.95E13 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
CH2F-CHF + CH3 = CHF:CHF[Z]+CH4 1.30E13 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
CHF2-CHF + CH3 = CHF:CF2 + CH4 6.50E12 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
!*****
CH3-CF2 + CH3 = CH2:CF2 + CH4 1.95E13 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
CH2F-CF2 + CH3 = CHF:CF2 + CH4 1.30E13 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)
CHF2-CF2 + CH3 = CF2:CF2 + CH4 6.50E12 -0.5 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (NEED) (C2H5)

!*****
!*** Fluoroethyls reaction with HO2 ***
!*****
CH3-CHF + HO2 =>CH3+CHF:O+ OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH3-CF2 + HO2 =>CH3+CF2:O+ OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CH2 + HO2 =>CH2F+CH2O+ OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CHF + HO2 =>CH2F+CHF:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

```

```

CH2F-CF2 + HO2 =>CH2F+CF2:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CH2 + HO2 =>CHF2+CH2O+ OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CHF + HO2 =>CHF2+CHF:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CF2 + HO2 =>CHF2+CF2:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CH2 + HO2 =>CF3 +CH2O+ OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CHF + HO2 =>CF3 +CHF:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CF2 + HO2 =>CF3 +CF2:O+OH 3.00E13 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
!*****
CH3-CHF + HO2 = CH2:CHF + H2O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH3-CF2 + HO2 = CH2:CF2 + H2O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CH2 + HO2 = CH2:CHF + H2O2 2.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CHF + HO2 = CHF:CHF[Z]+H2O2 4.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CF2 + HO2 = CHF:CF2 + H2O2 2.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CH2 + HO2 = CH2:CF2 + H2O2 1.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CHF + HO2 = CHF:CF2 + H2O2 1.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CF2 + HO2 = CF2:CF2 + H2O2 1.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
!*****
CH3-CHF + HO2 = CH3-CH2F + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH3-CF2 + HO2 = CH3-CHF2 + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CH2 + HO2 = CH3-CH2F + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CHF + HO2 = CH2F-CH2F+ O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2F-CF2 + HO2 = CH2F-CHF2+ O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CH2 + HO2 = CH3-CHF2 + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CHF + HO2 = CH2F-CHF2+ O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF2-CF2 + HO2 = CHF2-CHF2+ O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CH2 + HO2 = CH3-CF3 + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CHF + HO2 = CH2F-CF3 + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF3-CF2 + HO2 = CHF2-CF3 + O2 3.00E11 0. 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
!*****
CH3-CHF + CH2O = CH3-CH2F + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CH3-CF2 + CH2O = CH3-CHF2 + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CH2F-CH2 + CH2O = CH3-CH2F + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CH2F-CHF + CH2O = CH2F-CH2F+ HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CH2F-CF2 + CH2O = CH2F-CHF2+ HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)

```

```

CHF2-CH2 + CH2O = CH3-CHF2 + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CHF2-CHF + CH2O = CH2F-CHF2+ HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CHF2-CF2 + CH2O = CHF2-CHF2+ HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CF3-CH2 + CH2O = CH3-CF3 + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CF3-CHF + CH2O = CH2F-CF3 + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)
CF3-CF2 + CH2O = CHF2-CF3 + HCO 5.50E03 2.80 5900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H5)

!*****
!*** <a name=c2h4>FLUOROETHYLENES</a> ***
!*****

!*****
!*** Fluoroethylenes: Isomerization ***
!*****

!*****
!*** Fluoroethylenes: HF elimination (kINF) ***
!*****
!BAW change these to falloff, add 3rd body efficiencies
!CH2:CHF = C2H2 + HF 1.00E14 0.00 70800. !<A
HREF=#70SIM/QUI>70SIM/QUI</A> (EXPT)
CH2:CHF (+M) = C2H2 + HF (+M) 1.00E14 0.00 70800.
LOW / 4.20E15 1.00 70800./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

!CH2:CF2 = C2HF + HF 2.50E14 0.00 86000. !<A
HREF=#70SIM/TSC>70SIM/TSC</A> (EXPT)
CH2:CF2 (+M) = C2HF + HF (+M) 2.50E14 0.00 86000.
LOW /9.00E15 1.00 86000./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

!CHF:CHF[Z] = C2HF + HF 2.50E14 0.00 78000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#70SIM/TSC>70SIM/TSC</A> (CH2:CF2)
CHF:CHF[Z] (+M) = C2HF + HF (+M) 2.50E14 0.00 78000.
LOW / 9.00E15 1.00 78000./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

!CHF:CF2 = C2F2 + HF 2.50E14 0.00 100000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#70SIM/TSC>70SIM/TSC</A> (CH2:CF2)
CHF:CF2 (+M) = C2F2 + HF (+M) 2.50E14 0.00 100000.
LOW / 9.00E15 1.00 100000./
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

!*****
!*** Fluoroethylenes: Decomposition ***
!*****
CH2* + CHF = C2H2 + HF 17.02E19 -2.12 2380. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CH2* + CF2 = C2HF + HF 17.02E19 -2.12 2380. !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CHF + CHF = C2HF + HF 17.02E19 -2.12 2380. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF + CF2 = C2F2 + HF 8.51E19 -2.12 2380. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****

```

```

CH2* + CHF = CH2:CHF          3.10E24 -3.80  2830.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CH2* + CF2 = CH2:CF2          3.10E24 -3.80  2830.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CHF + CHF = CHF:CHF[Z]        3.10E24 -3.80  2830.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF + CF2 = CHF:CF2           3.10E24 -3.80  2830.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CH2* + CHF = CH2:CF + H       1.64E07  1.56  5740.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CH2* + CHF = CHF:CH[Z] + H    1.64E07  1.56  5740.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CH2* + CF2 = CF2:CH + H       3.28E07  1.56  5740.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CHF+CF2)
CHF + CHF = CHF:CF[Z] + H     1.64E07  1.56  5740.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF + CF2 = CF2:CF + H       1.64E07  1.56  5740.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CH2:CF + H = C2H2 + HF        5.98E20 -2.31  1940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF:CH[Z] + H = C2H2 + HF     5.98E20 -2.31  1940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CF2:CH + H = C2HF + HF        5.98E20 -2.31  1940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF:CF[Z] + H = C2HF + HF     5.98E20 -2.31  1940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CF2:CF + H = C2F2 + HF        5.98E20 -2.31  1940.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CH2:CF + H = CH2:CHF          2.40E34 -7.11  5040.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF:CH[Z] + H = CH2:CHF        2.40E34 -7.11  5040.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CF2:CH + H = CH2:CF2          2.40E34 -7.11  5040.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CHF:CF[Z] + H = CHF:CHF[Z]    2.40E34 -7.11  5040.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CHF+CF2)
CF2:CF + H = CHF:CF2          2.40E34 -7.11  5040.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (RRKM)
!*****
CF2:CF2 + M = CF2 + CF2 + M   3.96E50 -9.06  85300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#78SCH/WAG>78SCH/WAG</A> (RRKM)

!*****
!*** Fluoroethylene + H: Association/Stabilization ***
!*****
CH2:CHF + H(+M) = CH2F-CH2 (+M) 4.20E08  1.5  990.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CH2:CHF + H(+M) = CH3-CHF (+M) 4.20E08  1.5  990.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CH2:CF2 + H(+M) = CHF2-CH2 (+M) 4.20E08  1.5  990.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CH2:CF2 + H(+M) = CH3-CF2 (+M) 4.20E08  1.5  990.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CHF:CHF[Z] + H(+M) = CH2F-CHF (+M) 8.40E08  1.5  990.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)

```

```

LOW/6.37E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CHF:CF2 + H(+M)= CHF2-CHF (+M) 4.20E08 1.5 990. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CHF:CF2 + H(+M)= CH2F-CF2 (+M) 4.20E08 1.5 990. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/3.19E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !
CF2:CF2 + H(+M)= CHF2-CF2 (+M) 8.40E08 1.5 990. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
LOW/6.37E27 -2.8 -54./ !
H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/ !

!*****
!*** Fluoroethylene + H: Association with HF-Elimination ***
!*****

!*****
!*** Fluoroethylenes + H: H-Abstraction ***
!*****
CH2:CHF + H = CHF:CH[Z]+ H2 0.33E06 2.53 12241. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
CH2:CHF + H = CH2:CF + H2 0.33E06 2.53 12241. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
CH2:CF2 + H = CF2:CH + H2 0.67E06 2.53 12241. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
CHF:CHF[Z]+ H = CHF:CF[Z]+ H2 0.33E06 2.53 12241. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)
CHF:CF2 + H = CF2:CF + H2 0.33E06 2.53 12241. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H4)

!*****
!*** Fluoroethylenes + F: H-Elimination ***
!*****
C2H4 + F = CH2:CHF + H 4.52E14 0.00 1198. !1999NES/PEY4470
CH2:CHF + F = CH2:CF2 + H 2.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CH2:CHF + F = CHF:CHF[Z]+H 5.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF:CHF[Z] + F = CHF:CF2 + H 4.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF:CF2 + F = CF2:CF2 + H 2.00E12 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!*****
!*** Fluoroethylene + O: Isomerization/decomposition ***
!*****
CH2:CHF + O = CH2F + HCO 5.30E09 1.00 1310. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87CVE>87CVE</A> (FIT)
CHF:CHF[Z]+ O = CH2F + CF:O 7.00E09 1.00 1590. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87CVE>87CVE</A> (FIT)
CH2:CF2 + O = CHF2 + HCO 4.30E09 1.00 1490. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87CVE>87CVE</A> (FIT)
CHF:CF2 + O = CHF2 + CF:O 6.00E09 1.00 1150. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87CVE>87CVE</A> (FIT)
!BAW added these two channels
CHF:CF2 + O = CF2 + CHF:O 0.32E07 2.00 0. ! C2F4+O
CHF:CF2 + O = CHF + CF2:O 0.32E07 2.00 2000. ! C2F4+O
CF2:CF2 + O = CF2 + CF2:O 1.90E09 1.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#87CVE>87CVE</A> (FIT)
!*****
CH2:CHF + O = CH3 + CF:O 5.30E09 1.00 2300. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#74SLA/GUT>74SLA/GUT</A> (FIT)

```

```

!*****
!*** Fluoroethylene + OH: Abstraction of H ***
!*****
CH2:CHF + OH = CHF:CH[Z]+ H2O 2.00E06 2.00 2850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#88TUL>88TUL</A> (C2H4)
CH2:CHF + OH = CH2:CF + H2O 1.00E06 2.00 2850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#88TUL>88TUL</A> (C2H4)
CHF:CHF[Z]+ OH = CHF:CF[Z]+ H2O 2.00E06 2.00 2850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#88TUL>88TUL</A> (C2H4)
CH2:CF2 + OH = CF2:CH + H2O 2.00E06 2.00 2850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#88TUL>88TUL</A> (C2H4)
CHF:CF2 + OH = CF2:CF + H2O 1.00E06 2.00 2850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#88TUL>88TUL</A> (C2H4)
!BAW added
CHF:CF2 +OH = CF2:O + CH2F 2E06 2.00 2850
CHF:CF2 + OH = CHF:O + CHF2 4E06 2.00 2850
!*****
!*** <a name=c2h3>FLUOROVINYLS</a>
!*****
!*****
!*** Fluorovinyl + O2: Addition/decomposition ***
!*****
CH2:CF + O2 = CH2O + CF:O 4.48E26 -4.55 5480. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CHF:CH[Z] + O2 = CHF:O + HCO 4.48E26 -4.55 5480. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CHF:CF[Z] + O2 = CHF:O + CF:O 4.48E26 -4.55 5480. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CF2:CH + O2 = CF2:O + HCO 4.48E26 -4.55 5480. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CF2:CF + O2 = CF2:O + CF:O 4.48E26 -4.55 5480. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
!*****
CH2:CF + O2 = CH2O + CF:O 1.05E38 -8.22 7030. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CHF:CH[Z] + O2 = CHF:O + HCO 1.05E38 -8.22 7030. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CHF:CF[Z] + O2 = CHF:O + CF:O 1.05E38 -8.22 7030. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CF2:CH + O2 = CF2:O + HCO 1.05E38 -8.22 7030. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
CF2:CF + O2 = CF2:O + CF:O 1.05E38 -8.22 7030. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#92WES>92WES</A> (C2H3)
DUP
!*****
!*****
!*** Fluorovinyl + O: Addition/decomposition ***
!*****
CH2:CF + O = CH2CO + F 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (C2H3)
CHF:CH[Z] + O = CHF:CO + H 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (C2H3)
CHF:CF[Z] + O = CHF:CO + F 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (C2H3)

```

```

CF2:CH + O = CF2CO + H 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (C2H3)
CF2:CF + O = CF2CO + F 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (C2H3)

!*****
!*** Fluorovinyl + OH: Addition/decomposition ***
!*****
CH2:CF + OH = CH2CO + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CHF:CH[Z] + OH = CH2CO + HF 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CHF:CF[Z] + OH = CHFCO + HF 2.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CF2:CF + OH = CF2CO + HF 1.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
!*****
CH2:CF + OH = CH3 + CF:O 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CHF:CH[Z] + OH = CH2F + HCO 3.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CHF:CF[Z] + OH = CH2F + CF:O 4.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)
CF2:CF + OH = CHF2 + CF:O 5.00E13 0.00 0. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#86TSA/HAM>86TSA/HAM</A> (C2H3)

!*****
!*** FLUOROETHYNES *****
!*****

!*****
!*** Fluoroethynes + H: Addition/stabilization ***
!*****
C2HF +H (+M)= CH2:CF (+M) 2.80E12 0.00 2410. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#76PAY/STI>76PAY/STI</A> (C2H2)
LOW/1.33E27 -3.5 2410./
H2/2./ CO/2./ CO2/3./ H2O/5./
C2HF +H (+M)= CHF:CH[Z] (+M) 1.40E12 0.00 2410. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#76PAY/STI>76PAY/STI</A> (C2H2)
LOW/0.67E27 -3.5 2410./
H2/2./ CO/2./ CO2/3./ H2O/5./
C2F2 +H (+M)= CHF:CF[Z] (+M) 2.80E12 0.00 2410. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#76PAY/STI>76PAY/STI</A> (C2H2)
LOW/1.33E27 -3.5 2410./
H2/2./ CO/2./ CO2/3./ H2O/5./

!*****
!*** FLUORO-ACETYLENE DESTRUCTION PATHWAYS ***
!*****
!*****
C2HF + O = CF2CO + H 1.00E07 2.00 1900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
C2F2 + O = CF2CO + F 1.00E07 2.00 1900. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
!*****
C2HF + OH = CHF2CO + H 2.18E-4 4.50 -1000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
C2HF + OH = CH2F + CO 2.50E-4 4.00 -2000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
C2HF + OH = HCCO + HF 2.50E-4 4.00 -2000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
C2F2 + OH = CF2CO + H 2.18E-4 4.50 -1000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)
C2F2 + OH = CF2CO + HF 2.50E-4 4.00 -2000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (C2H2)

```

```

!*****
!*** Fluoromethylenes (CHF, CF2): ***
!*****

!*****
!*** Radical combination ***
!*****
CH2F      + CH2  = CH2:CHF  + H    4.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (CH3)
CH2F      + CH2  = C2H4    + F    4.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (CH3)
CHF2      + CH2  = CH2:CF2  + H    4.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (CH3)
CHF2      + CH2  = CH2:CHF  + F    4.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (CH3)
CF3       + CH2  = CH2:CF2  + F    4.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#84WAR>84WAR</A> (CH3)

!*****
!*** Insertion into bonds of methyls ***
!*****
CH2F      + CH2* = CH2:CHF  + H    4.00E12  0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH2)
CH2F      + CH2* = C2H4    + F    2.00E12  0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH2)
CHF2      + CH2* = CH2:CF2  + H    2.00E12  0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH2)
CHF2      + CH2* = CH2:CHF  + F    4.00E12  0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH2)
CF3       + CH2* = CH2:CF2  + F    6.00E12  0.00    0.  !<A HREF=#96BUR/ZAC>96BUR/ZAC</A>
(CH2)
!*****
CH3       + CHF   = CH2:CHF  + H    6.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CH2F      + CHF   = CHF:CHF[Z]+ H    4.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CH2F      + CHF   = CH2:CHF  + F    2.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CHF2      + CHF   = CHF:CF2  + H    2.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CHF2      + CHF   = CHF:CHF[Z]+ F    4.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CF3       + CHF   = CHF:CF2  + F    6.00E12  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
!*****
CH3       + CF2   = CH2:CF2  + H    6.00E12  0.00    3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CH2F      + CF2   = CH2:CF2  + F    2.00E12  0.00    3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CHF2      + CF2   = CF2:CF2  + H    2.00E12  0.00    3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)
CHF2      + CF2   = CHF:CF2  + F    4.00E12  0.00    3500. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH2SING)

!*****
!*** FLUOROKETENE CHEMISTRY ***
!*****
CHFCO + H      = CH2F      + CO      1.13E13  0.00  3428. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (CH2CO)
CHFCO + H      = CFCO      + H2      5.00E13  0.00  8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (CH2CO)
!*****
CHFCO + O      = CHF:O      + CO      1.00E13  0.00  8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF2CO + O      = CF2:O      + CO      1.00E13  0.00  8000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

```



```

CHFCO + OH      = CFCO      + H2O      7.50E12   0.00   2000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (CH2CO)
!*****
CFCO  + H      = CHF      + CO      1.00E14   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (CH2CO)
CFCO  + O      = CF:O     + CO      1.00E14   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#89MIL/BOW>89MIL/BOW</A> (CH2CO)
HCCO  + F      = CHF      + CO      3.00E13   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (H)
CFCO  + F      = CF2      + CO      3.00E13   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (H)

!*****
!*** Fluoromethanes: Reactions with F ***
!*****
CH4   + F      = CH3      + HF      1.33E14   0.50    700.  !NIST CKD
CH3F  + F      = CH2F     + HF      1.35E14   0.00    1200. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#83MAN/SET>83MAN/SET</A> (FIT)
!CH3F + F      = CH2F     + HF      5.58E13   0.00    1000. !Wang
etal, J.ChemTheoryComput., 2005, 1, No2, 201-207
CH2F2 + F      = CHF2     + HF      9.00E13   0.00    1850. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#85CLY/HOD>85CLY/HOD</A> (FIT)
CHF3  + F      = CF3      + HF      4.50E13   0.00    3700. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#85CLY/HOD>85CLY/HOD</A> (FIT)
!CHF3 + F      = CF3      + HF      1.26e13   0.00    2920. !1998LOU/SAW1437-1445, exp, 298-
398K

!*****
!*** CHF:O & CF2:O: Reactions with F ***
!*****
CH3OH + F      = CH3O     + HF      2.62E09   1.44   -205. !<A
HREF=#91GLA/KOS>91GLA/KOS</A> (EXPT)
CH3OH + F      = CH2OH    + HF      4.62E07   1.97   -300. !<A
HREF=#91GLA/KOS>91GLA/KOS</A> (EXPT)
!*****
CH2O  + F      = HCO      + HF      6.00E13   0.00    2000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> <A HREF=#80LEB/FOO>80LEB/FOO</A> (FIT)
CHF:O + F      = CF:O     + HF      2.65E13   0.00    1800. !<A
HREF=#90FRA/ZHA>90FRA/ZHA</A> (EXPT)
!*****
CH3O  + F      = CH2O     + HF      3.00E13   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
HCO   + F      = CO       + HF      1.00E13   0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!*****
!*** Abstraction from fluoroethanes: By F-atom ***
!*****
C2H6  + F      = C2H5     + HF      8.00E12   0.00    300.  !<A
HREF=#60FET/KNO>60FET/KNO</A> (EXPT)
CH3-CH2F + F    = CH2F-CH2 + HF      9.00E13   0.00    800.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH3-CHF2 + F    = CHF2-CH2 + HF      1.00E14   0.00    800.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH3-CF3  + F    = CF3-CH2  + HF      1.00E14   0.00    4000. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
!*****
CH3-CH2F + F    = CH3-CHF  + HF      6.00E13   0.00    200.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH2F-CH2F + F   = CH2F-CHF + HF      1.30E14   0.00    800.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH2F-CHF2 + F   = CHF2-CHF + HF      1.30E14   0.00    800.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH2F-CF3  + F   = CF3-CHF  + HF      6.00E13   0.00    1200. !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
!*****

```

```

CH3-CHF2 + F = CH3-CF2 + HF      3.00E13  0.00   800.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CH2F-CHF2 + F = CH2F-CF2 + HF    3.00E13  0.00  1200.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CHF2-CHF2 + F = CHF2-CF2 + HF    6.00E13  0.00  1200.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
CHF2-CF3 + F = CF3-CF2 + HF     4.00E13  0.00  1400.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (C2H6)
!*****
C2H4 + F = C2H3 + HF      1.00E14  0.00  2000.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (CH4)
CF2:CF2 + F = CF3 + CF2    3.00E13  0.00    0.  !<A
HREF=#80BUT/LAR>80BUT/LAR</A> (EXPT)
C2H2 + F = C2H + HF      1.40E-1  0.00    0.  !1973WIL/ROW301-307

!*****
!*** Fluorovinyl + F: Addition/decomposition ***
!*****
C2H3 + F = C2H2 + HF      2.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CHF:CF[Z] + F = CHF + CF2  1.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)
CF2:CF + F = CF2 + CF2    2.00E13  0.00    0.  !<A
HREF=#96BUR/ZAC>96BUR/ZAC</A> (upper-limit)

!***** delete => addition of C3F7H and C2F5COC3F7 reactions *****
!***** R Hynes' data for FM-200 *****
!
! **** new reactions 14-6-97 R Hynes ****
! start new rxns:
!CF3CO = CF3 + CO          2.2e13    0.00  10000.00
CF3CO (+M) = CF3 + CO (+M) 2.65e14    0.00  12000.00      !Tomas
et al, Zeit.Phys.Chem,214,10,1349,2000
  LOW /2.05E16 0.0 9200.0 /
  TROE/ 1.0 100.0 520.0 /
!***
!*****
CF3CHO + H = CF3CO + H2      4.00e13  0.00   4200.00
CF3CHO + OH = CF3CO + H2O    6.62e11  0.00    0.0
CF3CHO + O = CF3CO + OH      1e12     0.00    0.0
CF3CHO + CH3 = CF3CO + CH4    1e11     0.00   7400.0
CF3CHO + CF3 = CHF3 + CF3CO   1e12     0.00   8400.0
CF3CHO (+M) = CF2CO + HF (+M) 1e13     0.00  30000.0
  LOW /8.75E17 0.0 30000.0 /
  H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
  CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
CF3CHO + F = CF3CO + HF      4e13     0.00   1000.0
CF3CHO (+M) = CF3 + HCO (+M) 4e16     0.00  80000.00
  LOW /3.50E21 0.0 80000.0 /
  H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
  CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
CF3COF+ H = CF3CO + HF      2e13     0.00   3000.00
CF3COF (+M) =CF3+CF:O(+M)    4.3E+16  0.00  90000.00
LOW /3.76E21 0.0 90000.0/
H2O/9.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/

! Novec update, October 4, 2011, addition of reactions for consumption of c2f6,cf3cfo

!CF2:CF2 + F = CF3 + CF2      3.e13     0.0    0.0
!kin db/duplicate
CF3COF + CF3 = CF3CO + CF4    2.e12     0.0   9000.
!est
CF3COF + CF3-CF2 = CF3CO + CF3-CF3 3.e11     0.0  14000.
!est

```

```

CF3-CF3 + CF3 = CF4 + CF3-CF2          3.e12      0.0      11300.
!est
CF3CO + F = CF3 + CF:O                 3.e12      0.0        0.0
!est
CF3CO + F = CF4 + CO                    5.e12      0.0        0.0
!est

! additional reactions, vb, 08/12
CF3 (+ M) = CF2 + F (+ M)               1.0e15      0.0      82370.
!ar=>n2;1800-2200K;Cobos etal.J.PhysChem,A,2010,114,4755-4761
  LOW / 5.0e15  0.0  59660. /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
CH3F /6.00/ CH2F2 /6.00/ CHF3 /6.00/ HF /2.00/
CF3-CF2 = CF2 + CF3                    4.27e15      0.0      56240.
!1991AIN720-725
CF4 + CH3 = CH3F + CF3                  9.64e04      2.41     26130.
!1998BER/MAR179-184
CF3-CF2 + F = CF3 + CF3                 3.16e13      0.0        0.
!Hynes etal,J.PhysChem,1999,103,5967-5977
CF3O + CO = CO2 + CF3                   3.13e10      0.0        0.
!Hynes etal,J.PhysChem,1999,103,5967-5977
CF:O + CF2 = CF3 + CO                   5.4e11      0.0        0.
!x3/Voloshin etal,IEEE TransPlasmaSci,2007,35:1691
CF + CF = C2F2                          5.0e13      0.0        0.
!Hynes etal,J.PhysChem,1999,103,5967-5977
CF2:CF2 + F = CF3-CF2                   3.15e13      0.0       7770.
!x0.5/Hynes etal,J.PhysChem,1999,103,5967-5977
!CF3-CF2 + CF = C3F6                     6.0e11      0.0        0.
!Voloshin etal,IEEE TransPlasmaSci,2007,35:1691

! *** F2 reactions ***
!F + F + M = F2 + M                     1.0e14      0.0        0.
!1971LLO39
F + F + M = F2 + M                       1.0          6339.          !1981BAU/DUX723          9.68e10
F2 + H = F + HF                          2.9e9        1.4         1330.
!1983COH/WES531
F2 + CF3 = CF4 + F                       2.65e12      0.0         2500.
!1986TEI/VED1119
CH3 + F2 = CH3F + F                      4.e12        0.0         1100.
!1981SEE/ROT39-58
CF2 + F2 = CF3 + F                       1.2e12      0.0         3000.
!est
CF:O + F2 = CF2:O + F                    1.e12        0.0          0.
!est
H2 + F2 = HF + F + H                     3.44e12      0.0        19790.
!1975BOK/CHA791-793
F2 + CO = CF:O + F                       4.7e11      0.0        13500.
!1962HER/ARV120
C + F2 = CF + F                          1.7e12      0.0         1500.
!1967MAY/SCH837-844
CF + F2 = CF2 + F                        2.4e12      0.0          0.
!1992PEE/VAN1257-1263, overall rate
C2H4 + F2 = CH2F-CH2 + F                 4.8e10      0.0         4590.
!1967KAP/CHA421-427
CH4 + F2 = CH3 + HF + F                  2.e12        0.0        11230.
!1981SEE/ROT39-58
OH + F2 = HF + F + O                     7.e13        0.0         9000.
!Nosova et al, Comb.Flame,8,163,1964

  CF3CHCH2 + OH      = CF3COCH3      + H          1.0E+12      0.00      4780.      ! hrxn=-
21.3 ref=est class=c.c-o/c.c-h

!! TRIFLUOROPROPENE
  CF3CHCH2 + H      = C2H4      + CF3          5.0E+13      0.00      4780.      ! hrxn=-
5.8 ref=?analog class=c.c-h/c.c-c

```

CF3CHCH2 + H	= CF3CCH2 + H2	4.0E+14	0.00	11850.	!
hrxn=34.3 ref=est class=c-h+h					
CF3CHCH2 + O	= CH3CO + CF3	2.0E+14	0.00	2390.	! hrxn=-
97.4 ref=est					
CF3CHCH2 + OH	= CH3CHO + CF3	1.0E+13	0.00	0.0	! hrxn=-
37.9 ref=est					
CF3CHCH2 + CH3	= C3H6 + CF3	5.0E+12	0.00	11850.	!
hrxn=36.6 ref=est					
!! TRIFLUOROPROPENYL REACTIONS					
CF3CCH + H	= CF3CCH2	6.0E+14	0.00	4780.	! hrxn=-
164.6 ref=calc					
CF3CCH2	= C2H2 + CF3	2.E+13	0.00	37000.	!
hrxn=131.0 ref=					
CF3CCH2 + O2	= CF3CCH + HO2	2.0E+13	0.00	23900.	! hrxn=-
162.1 ref=					
CF3CCH2 + H	= C2H3 + CF3	4.0E+13	0.00	4780.	! hrxn=-
19.3 ref=est					
CF3CCH2 + O	= CH2CO + CF3	5.0E+13	0.00	0.0	! hrxn=-
395.0 ref=analog					
CF3CCH2 + O	= CF3CCH + OH	5.0E+13	0.00	2390.	! hrxn=-
268.1 ref=est					
CF3CCH2 + OH	= CH2CO + CF3 + H	5.0E+13	0.00	9560.	!
hrxn=30? ref=guess					
CF3CCH2 + OH	= CF3CCH + H2O	5.0E+13	0.00	4780.	! hrxn=-
328.4 ref=est					
CF3CCH2 + CH3	= CH3CCH2 + CF3	4.0E+13	0.00	4780.	!
hrxn=11.1 ref=est					
! TRIFLUOROPROPYNE REACTIONS					
CF3CCH + H	= C2H2 + CF3	2.0E+14	0.00	9560.	! hrxn=-
33.6 ref=analog class=c.c-h/c.c-c					
DUPLICATE					
CF3CCH + O	= HCCO + CF3	1.0E+13	0.00	2390.	! hrxn=-
118.2 ref= class=est					
DUPLICATE					
CF3CCH + OH	= CH2CO + CF3	2.0E+14	0.00	4780.	! hrxn=-
126.9 ref=est class=c.c-o/c.c^h/c.c-c					
CF3CCH + CH3	= pC3H4 + CF3	2.0E+14	0.00	9560.	! hrxn=-
2.2 ref=est					
!! TRIFLUOROPROPANONE REACTIONS					
CH3CO + CF3	= CF3COCH3	4.0E+13	0.00	0.0	! hrxn=-
356.6 ref=est					
CF3COCH3 + H	= CH2CO + H2 + CF3	6.0E+14	0.00	23900.	!
hrxn=93.3 ref=est					
CF3COCH3 + OH	= CH2CO + H2O + CF3	5.0E+13	0.00	3585.	!
hrxn=40.8 ref=est					
CF3COCH3 + F	= HF + CH2CO + CF3	1.e13	0.0	10000.	!est
CF3CCH + F	= CF3 + C2HF	5.e13	0.0	11000.	!est
! F,CF3,C2F5-propane reactions					
C3H8 + F	= nC3H7 + HF	3.5e13	0.0	0.	
!1960FET/KNO1064					
C3H8 + F	= iC3H7 + HF	4.1e13	0.0	0.	
!1960FET/KNO1064					
C3H8 + CF3	= nC3H7 + CHF3	5.4e11	0.0	8540.	
!1973ARI/POT1811					
C3H8 + CF3	= iC3H7 + CHF3	1.8e11	0.0	6520.	
!1973ARI/POT1811					
C3H8 + CF3-CF2	= nC3H7 + CHF2-CF3	3.9e11	0.0	7800.	
!1972WHY/CLA689					
C3H8 + CF3-CF2	= iC3H7 + CHF2-CF3	3.3e11	0.0	6100.	
!1972WHY/CLA689					

!F,CF3-ethanol reactions

C2H5OH + F = CH3CH2O + HF 3.8e13 0.0 0.  
!1989KHA/EDE626-632  
C2H5OH + F = CH3CHOH + HF 1.5e13 0.0 0.  
!1989KHA/EDE626-632  
C2H5OH + F = C2H4OH + HF 2.3e13 0.0 0.  
!1989KHA/EDE626-632  
C2H5OH + CF3 = CH3CHOH + CHF3 4.e11 0.0 9700. !est

!F-butane reactions

C4H10 + F = pC4H9 + HF 3.89E13  
0.0 0. !1960FET/KNO1064  
C4H10 + F = sC4H9 + HF 4.68E13  
0.0 0. !1960FET/KNO1064  
iC4H10 + F = iC4H9 + HF  
4.07E13 0.0 0. !1960FET/KNO1064  
iC4H10 + F = tC4H9 + HF  
5.75E13 0.0 0. !1960FET/KNO1064

!\*\*\*\*\*  
!\*\*\* HFO-1234YF REACTIONS \*\*\*  
!\*\*\*\*\*

!\*\*\*\*\*  
!\*\*\* Unimolecular Decomposition of HFO-1234yf \*\*\*  
!\*\*\*\*\*

CH2:CF + CF3 (+ M) <=> CH2CF3 (+ M) 6.812E+14 0.000 0.  
LOW / 2.526E+18 -14.527 9004./  
CH2CF3 (+ M) <=> CF3CCH + HF (+ M) 9.676E+10 0.983 79862.  
LOW / 3.835E+50 -16.425 87927./  
CH2CF3 <=> C2HF + CHF3 6.074E+11 1.184 132824.

!\*\*\*\*\*  
!\*\*\* H-abstraction from HFO-1234yf \*\*\*  
!\*\*\*\*\*

CH2CF3 + H <=> Z-CHCF3 + H2 2.325E+13 0.000 21141.  
CH2CF3 + H <=> E-CHCF3 + H2 2.036E+14 0.000 22192.  
CH2CF3 + CH3 <=> Z-CHCF3 + CH4 5.186E+12 0.000 20934.  
CH2CF3 + CH3 <=> E-CHCF3 + CH4 1.660E+12 0.000 22235.  
CH2CF3 + CF3 <=> Z-CHCF3 + CHF3 1.787E+12 0.000 20965.  
CH2CF3 + CF3 <=> E-CHCF3 + CHF3 8.788E+11 0.000 21186.  
CH2CF3 + O <=> Z-CHCF3 + OH 1.205E+11 0.700 38047.  
!estimated from Tsang J. Phys. Chem. Ref. Data 20 (1991) 221-274  
CH2CF3 + O <=> E-CHCF3 + OH 1.205E+11 0.700 38047.  
!estimated from Tsang J. Phys. Chem. Ref. Data 20 (1991) 221-274  
CH2CF3 + OH <=> Z-CHCF3 + H2O 9.131E+13 0.000 10071.  
CH2CF3 + OH <=> E-CHCF3 + H2O 1.517E+13 0.000 11571.  
CH2CF3 + O2 <=> Z-CHCF3 + HO2 3.580E+13 0.000 60010. !estimated  
as 1/2 rate from 2005HUA/RUS335-341  
CH2CF3 + O2 <=> E-CHCF3 + HO2 3.580E+13 0.000 60010. !estimated  
as 1/2 rate from 2005HUA/RUS335-341

E-CHCF3 <=> Z-CHCF3 6.437E+13 0.000 0.  
!estimated from Benson Thermochemical Kinetics  
Z-CHCF3 <=> C2HF + CF3 1.838E+14 0.344 46611.  
Z-CHCF3 + O (+ M) <=> CHOCF3 (+ M) 2.581E+13 0.000 0.  
LOW / 6.775E+31 -17.096 9613./  
E-CHCF3 + O (+ M) <=> CHOCF3 (+ M) 2.581E+13 0.000 0.  
LOW / 6.955E+31 -17.107 9405./

!\*\*\*\*\*  
!\*\*\* Radical-addition to HFO-1234yf \*\*\*  
!\*\*\*\*\*

CH2CF3 + H <=> CH3CF3 1.137E+14 0.000 4085.

CH3CFCF3 + O (+ M) <=> CH3COFCF3 (+ M)	1.704E+13	0.000	0.
LOW / 1.389E+39 -19.805	12618./		
CH3COFCF3 <=> CH3 + CF3COF	2.456E+12	0.185	207.
CH3COFCF3 <=> CF3 + CH3COF	2.447E+12	0.130	141.
CH2CFCF3 + H <=> CH2CHF3	2.259E+14	0.000	7747.
CH2CHF3 <=> CH2:CHF + CF3	1.059E+14	0.146	33708.
CH2CFCF3 + O (+ M) <=> CH2OCFCF3 (+ M)	3.421E+13	0.000	0.
LOW / 2.922E+01 -10.856	2044./		
CHOCFCF3 + H (+ M) <=> CH2OCFCF3 (+ M)	9.550E+13	0.000	0.
LOW / 8.055E+26 -17.302	8979./		
CF3CF3CO + H (+ M) <=> CHOCFCF3 (+ M)	8.359E+12	0.000	0.
LOW / 2.595E+15 -13.955	4591./		
CO + CF2:CF2 <=> CF3CF3CO	7.866E+11	0.000	0.
CH2CFCF3 + O (+ M) <=> CH2COFCF3 (+ M)	3.000E+13	0.000	0.
LOW / 2.775E+01 -10.964	2056./		
CH2COFCF3 <=> CH2COF + CF3	9.856E+11	0.880	4021.
CH2COFCF3 <=> CF3COF + CH2	8.616E+11	1.132	18465.
CH2CFCF3 + OH (+ M) <=> CH2OHCFCF3 (+ M)	1.640E+13	0.000	0.
LOW / 8.735E+12 -14.202	5054./		
CH2OHCFCF3 <=> CH2OCHF3	5.248E+06	0.992	2041.
CH2OHCFCF3 <=> CHOHCHF3	1.245E+06	1.223	2894.
CH2OCHF3 <=> CH2O + CF3-CHF	4.228E+16	-0.991	6851.
CHOHCHF3 <=> CF3 + CHFCHOH	2.446E+15	0.000	38560.
CH2CFCF3 + OH (+ M) <=> CH2COHF3 (+ M)	1.680E+13	0.000	0.
LOW / 8.760E+12 -14.115	5363./		
CH2COHF3 <=> CH3COFCF3	7.249E+09	0.385	5306.
!*****			
!*** CF3CCH Decomposition ***			
!*****			
CF3CCH + H <=> C2H2 + CF3	5.720E+12	1.740	7700.
DUPLICATE			
CF3CCH + O <=> HCCO + CF3	1.300E+13	0.000	2010.
DUPLICATE			
CF3CCH + OH <=> HCCOH + CF3	6.500E+12	0.000	2000.

## APPENDIX B. GAUSSIAN ARCHIVE FILES

### B.1 Aerosols

HNO<sub>3</sub>

```
1|1|UNPC-MACANDCHEESE-HP|Freq|UB3LYP|6-31++G(d,p)|H1N1O3|MAC AND CHEES
E|22-May-2014|0||#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LY
P/6-31++G(d,p) Freq||HNO3 for solvation||0,1|N,0.0590204919,0.10433621
94,-0.0496494237|O,0.3145918633,0.3715092979,1.3118344054|H,0.59850418
15,-0.4933153803,1.6639553041|O,-0.3107266785,1.0626857522,-0.67533501
81|O,0.2437068217,-1.0452158892,-0.4076052677||Version=IA32W-G09RevB.0
1|State=1-A|HF=-280.9007024|S2=0.|S2-1=0.|S2A=0.|RMSD=9.617e-010|RMSF=
5.116e-006|ZeroPoint=0.0262757|Thermal=0.0298193|
```

MMH

```
1|1|UNPC-MACANDCHEESE-HP|Freq|UB3LYP|6-31++G(d,p)|C1H6N2|MAC AND CHEES
E|22-May-2014|0||#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LY
P/6-31++G(d,p) Freq||MMH for solvation||0,1|C,-0.1219124078,0.09579876
97,0.0459002053|H,-0.5199197843,0.0812358646,1.0665478935|H,0.98238265
49,0.1110451827,0.1085631518|H,-0.4271919434,-0.8313720657,-0.45078612
55|N,-0.681923746,1.2305725056,-0.6801396751|H,-0.4495133016,1.1768832
593,-1.6669415428|N,-0.2460519692,2.5068254178,-0.2196008774|H,-0.8574
51532,2.800839449,0.5369273259|H,0.7127976019,2.4738409465,0.138112921
5||Version=IA32W-G09RevB.01|State=1-A|HF=-151.1945925|S2=0.|S2-1=0.|S2
A=0.|RMSD=2.895e-009|RMSF=1.208e-005|ZeroPoint=0.0815025|Thermal=0.085
7088|
```

HNO<sub>3</sub>-MMH

```
1\1\GINC-TRANSMOGRIFIER\Freq\RB3LYP\6-31++G(d,p)\C1H7N3O3\CDNEEDHA\05-
Mar-2014\0\|#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-3
1++G(d,p) Freq\\HNO3 1MMH solvation\\0,1|N,-0.2680699807,-0.0835999072
,0.1552901882|O,-0.3547957646,-0.4590701505,1.3319430481|O,0.739226314
2,-0.0647657827,-0.5214158394|O,-1.4023531,0.3504265147,-0.4392846499\
H,-2.2267278205,0.2032235389,0.26864468|H,-3.485870932,-0.9100634152,1
.4316699131|N,-3.3441088808,0.0744053149,1.2053936147|N,-3.0072189446,
0.6950201441,2.49024072|H,-2.0458447879,0.3977007356,2.6727596785|H,-2
.9448314281,1.6968288186,2.3007829771|C,-4.6214632892,0.6157506924,0.7
125479046|H,-4.4759391443,1.6569952617,0.4095845292|H,-4.9285883313,0.
0419871257,-0.1651376002|H,-5.3991492041,0.5699087328,1.4829458297\\Ve
rsion=AM64L-G09RevB.01\State=1-A|HF=-432.117832\RMSD=6.092e-09\RMSF=1.
686e-05\ZeroPoint=0.109004\Thermal=0.1177302\
```

HNO<sub>3</sub>-2MMH

```
1\1\GINC-TRANSMOGRIFIER\Freq\RB3LYP\6-31++G(d,p)\C2H13N5O3\CDNEEDHA\06
-Mar-2014\0\|#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31++G(d,p) Freq\\HNO3 2MMH solvation\\0,1|N,-0.2834385928,0.1562587726
,0.2783439613|O,-0.7033209244,-0.868151552,0.9005821156|O,0.8567408213
,0.2370356913,-0.1628326249|O,-1.1081788207,1.1478982242,0.122323984|H
,-2.3889938332,0.7356411202,0.7590754045|H,-2.9655253521,-0.6736104963
,1.3938566187|N,-3.2666293573,0.296828233,1.2689079323|N,-3.4972310635
,0.8362697981,2.59937194|H,-2.6447628357,0.5913982915,3.1468222198|H,-
3.5050850098,1.8510936859,2.491129283|C,-4.4866746735,0.354822877,0.4
336819777|H,-4.744492875,1.4015694946,0.2619929194|H,-4.2730729962,-0.
1257066115,-0.5232031074|H,-5.304899414,-0.1474014915,0.9513213787|H,-
0.5790273162,-0.5509501148,3.0314833994|N,-0.9495237124,-0.0762301037,
```

3.8590893028\N,-1.0494831891,-0.9752861714,4.9759484856\H,-1.908405190  
7,-1.5093902558,4.8845495031\H,-0.2654289902,-1.6296313219,4.995262681  
7\C,-0.0712819333,1.047524098,4.1988833839\H,0.0193731532,1.6970693722  
,3.3223310539\H,-0.5132606111,1.6097697859,5.0255085545\H,0.9380979385  
,0.7275769489,4.4981231716\\Version=AM64L-G09RevB.01\State=1-A\HF=-583  
.3254109\RMSD=5.433e-09\RMSF=1.961e-06\ZeroPoint=0.1940085\Thermal=0.2  
085044\

#### 2HNO<sub>3</sub>-MMH

1\1\GINC-TRANSMOGRIFIER\Freq\RB3LYP\6-31++G(d,p)\C1H8N4O6\CDNEEDHA\11-  
Mar-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-3  
1++G(d,p) Freq\HNO3 MMH solvation\0,1\N,-0.9339671656,-0.669449332,  
0.6722119253\O,-0.7722109791,0.4878576993,1.0773671601\O,-0.0895489691  
, -1.401708844,0.2125489667\O,-2.1932385231,-1.1824729593,0.7455948941\  
H,-2.8133347178,-0.4281277014,1.1199398692\H,-4.6270730368,0.300694026  
3,2.0789523446\N,-3.8047974013,0.7181765189,1.6395272989\N,-3.11108078  
86,1.4031986457,2.6999214092\H,-2.1304528395,1.4692577711,2.4192532819  
\H,-3.480676002,2.3499018178,2.8178898034\C,-4.1969760037,1.5940372927  
,0.5226072553\H,-3.2986545188,1.9746551121,0.0299742012\H,-4.768462270  
3,1.0008050485,-0.1961913044\H,-4.814608969,2.4390778917,0.8568293057\  
H,-3.3354642286,0.5555490172,4.0929530325\O,-3.466249488,0.0427671007,  
4.9808012045\N,-4.7477363074,-0.4262965489,4.9860882711\O,-5.431715054  
3,-0.20859787,3.9801640718\O,-5.0889173333,-1.0130374591,5.9850450453\  
\Version=AM64L-G09RevB.01\State=1-A\HF=-713.044376\RMSD=4.523e-09\RMSF  
=4.515e-06\ZeroPoint=0.138621\Thermal=0.1516934\

#### HNO<sub>3</sub>-3MMH

1\1\GINC-TRANSMOGRIFIER\Freq\RB3LYP\6-31++G(d,p)\C3H19N7O3\CDNEEDHA\09-  
Mar-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-  
31++G(d,p) Freq\HNO3 3MMH solvation\0,1\N,-0.3258350856,2.3799734174  
,0.8438702889\O,-1.0162311383,3.3810572595,1.1559538561\O,0.7642686428  
,2.1253328197,1.3775285796\O,-0.8009429938,1.5684304965,-0.0481454162\  
H,-3.5311456357,0.5633615642,0.3307348475\N,-3.4362602044,1.5957975468  
,0.5962723397\N,-3.3933525591,1.6527809119,2.0469093185\H,-2.688661869  
1,0.9488757081,2.3250096744\H,-2.963318361,2.5555124596,2.2620539115\C  
, -4.5417080206,2.4082457647,0.0487621646\H,-4.5607469947,2.2802162676,  
-1.0356989411\H,-4.3688854857,3.4584352554,0.2912675204\H,-5.479130802  
8,2.0721104683,0.4932774354\H,-0.3049378853,0.2857339204,3.0788336007\  
N,-1.0608514025,-0.31435177,2.7413047189\N,-0.6376374262,-0.9866027115  
,1.5347996103\H,-0.4349101614,-0.2430046685,0.859486034\H,0.2433480995  
, -1.4828920239,1.7017883186\C,-1.4093511701,-1.2909319693,3.7701403852  
\H,-1.6853173774,-0.7562665883,4.6840037191\H,-2.2678798355,-1.8797135  
848,3.4340750468\H,-0.5873806343,-1.9869628436,4.0079579288\H,-2.50567  
04793,1.8729173986,0.1936556636\N,-3.1784171576,-1.067708115,-0.180292  
6705\H,-2.4706632515,-1.4162833171,0.4806601283\C,-4.2924628942,-2.008  
9452277,-0.2939161308\H,-4.7264357035,-2.1613075009,0.6990454976\H,-5.  
0523224204,-1.592454992,-0.9602814595\H,-3.9837317988,-2.9873615674,-0  
.693487478\N,-2.5765499235,-0.8544185836,-1.4755856272\H,-1.9062614423  
, -0.0921163949,-1.3789854143\H,-2.041365218,-1.6817629669,-1.751352972  
2\\Version=AM64L-G09RevB.01\State=1-A\HF=-734.5455048\RMSD=4.195e-09\R  
MSF=3.154e-06\ZeroPoint=0.279593\Thermal=0.2990513\

#### 3HNO<sub>3</sub>-MMH

1\1\GINC-TRANSMOGRIFIER\Freq\RB3LYP\6-31++G(d,p)\C1H9N5O9\CDNEEDHA\18-  
Mar-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-3  
1++G(d,p) Freq\3HNO3 MMH solvation\0,1\N,-0.7279614718,-0.3069891179  
,0.6541191146\O,-0.8150994135,0.7403085059,1.3066690703\O,0.2821264634  
, -0.8187329124,0.2347638116\O,-1.8902023034,-0.9610689827,0.371450626\  
H,-2.6659923475,-0.3853763014,0.7568693757\H,-4.7209064266,-0.05838344



7,1.4736691271\N,-3.8976337642,0.5224507806,1.3012994902\N,-3.47869379  
 28,1.0422774948,2.5802267854\H,-2.4831337744,1.2628807163,2.4985007424  
 \H,-3.989203972,1.8980101032,2.8149765884\C,-4.2161204279,1.5734956472  
 ,0.3186899913\H,-3.3079926944,2.1341913335,0.0835471714\H,-4.579179105  
 ,1.0906163299,-0.5920420272\H,-4.9869345281,2.2639469028,0.6867763259\  
 H,-3.7897293353,0.0427400775,3.6834739824\O,-4.1441245008,-0.728343905  
 5,4.3375511364\N,-5.1880643793,-0.2144386315,5.0170093749\O,-5.2667719  
 854,0.9966848031,5.1390802192\O,-5.9849374912,-1.0416707278,5.46275727  
 86\O,-6.2989102859,-1.1773499873,2.3414331784\N,-6.5075232418,-2.39271  
 18778,2.3661001964\O,-6.7049198278,-3.1252083014,1.4286845736\O,-6.526  
 9949293,-2.9962178384,3.5955852569\H,-6.2970771559,-2.2909698283,4.262  
 9529498\\Version=AM64L-G09RevB.01\State=1-A\HF=-993.9570096\RMSD=8.732  
 e-10\RMSF=2.717e-06\ZeroPoint=0.1656742\Thermal=0.1837552\

4HNO<sub>3</sub>-MMH

1\1\GINC-TRANSMOGRIFIER\Freq\UB3LYP\6-31++G(d,p)\C1H10N6O12\CDNEEDHA\0  
 9-Jun-2014\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6  
 -31++G(d,p) Freq\MMH 4HNO3 Internal Coord Fix\0,1\N,0.1539900153,-0.  
 3290308506,-0.1396830351\O,0.042890085,0.1129799069,1.012229836\O,1.17  
 45382861,-0.5278844633,-0.7445125196\O,-1.0032442804,-0.6235302199,-0.  
 808577906\H,-1.7709268622,-0.4622093095,-0.1526167466\H,-3.0640552742,  
 -1.041170761,1.5533159862\N,-3.0266032041,-0.2056610964,0.9561878277\N  
 ,-2.5870670497,0.8733811076,1.8306580759\H,-1.5661235571,0.7751003692,  
 1.9335201721\H,-2.7847989443,1.7957357994,1.3964238396\C,-4.3839176115  
 ,0.0573623501,0.4263950103\H,-4.3554216634,0.9258979469,-0.2355137924\  
 H,-4.6673517705,-0.8221152142,-0.1545744488\H,-5.1183758996,0.21262311  
 96,1.2228765995\H,-3.0858358922,0.8682344946,2.757159463\O,-4.26235157  
 71,0.5477798657,3.9174485494\N,-4.4783138924,0.9487519654,5.1062072993  
 \O,-4.3619956776,2.177221039,5.3863913791\O,-4.8098985031,0.1325375557  
 ,5.9832592295\O,-5.568674159,-2.1823572748,3.5626977944\N,-4.366950919  
 9,-2.2926880928,3.6826609808\O,-3.5521325941,-2.5493966967,2.800070375  
 7\O,-3.8214116123,-2.1342479717,4.9264733085\H,-4.406998273,-1.4656636  
 156,5.3937825412\O,-5.1001875437,4.2484951864,2.7757640321\N,-4.076480  
 9707,3.6973383151,2.4432505015\O,-3.6862658178,3.4830322106,1.28923659  
 26\O,-3.2237136724,3.2477969066,3.4060611969\H,-3.7820542199,2.9503033  
 229,4.2410974578\\Version=AM64L-G09RevB.01\State=1-A\HF=-1274.8712077\  
 S2=0.\S2-1=0.\S2A=0.\RMSD=4.962e-09\RMSF=2.031e-06\ZeroPoint=0.1950019  
 \Thermal=0.2176978\

**B.2 HFO-1234yf sub-mechanism**

HFO-1234yf

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.048741	E(Thermal)=	0.055094
E(SCF)=	-512.679319	DE(MP2)=	-1.454875
DE(CBS)=	-0.158522	DE(MP34)=	-0.028908
DE(CCSO)=	-0.029130	DE(Int)=	0.043226
DE(Empirical)=	-0.074330		
CBS-QB3 (0 K)=	-514.333115	CBS-QB3 Energy=	-514.326762
CBS-QB3 Enthalpy=	-514.325818	CBS-QB3 Free Energy=	-514.364002

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4\CDNEEDHA\07-Jan-2015\0\#p o  
 pt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom=di  
 hedral\HFO-1234yf Thermochemistry\0,1\C,0,0.0159857282,0.2257166945,  
 -0.052817652\H,0,0.0351620643,0.694999025,0.9190604724\H,0,0.941739645  
 9,0.0887469599,-0.5950769649\C,0,-1.1291755106,-0.1757496054,-0.570842  
 0959\C,0,-2.4846362987,-0.0465797785,0.074488493\F,0,-1.2204018387,-0.

7659879334,-1.7745857821\F,0,-3.3162054627,0.6877524446,-0.6878546685\F,0,-3.0574609278,-1.2528303583,0.2440431887\F,0,-2.3942440262,0.5439328021,1.2790728904\\Version=ES64L-G09RevD.01\State=1-A\HF/CbsB3=-512.6793185\E2(CBS)/CbsB3=-1.6133966\CBS-Int/CbsB3=0.0432262\OIii/CbsB3=12.8375676\MP2/CbsB4=-513.6756023\MP4(SDQ)/CbsB4=-513.7045106\MP4(SDQ)/6-31+G(d')=-513.6885291\QCISD(T)/6-31+G(d')=-513.7176586\CBSQB3=-514.3331153\

E-CHCFCF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.035223	E(Thermal)=	0.041683
E(SCF)=	-512.027472	DE(MP2)=	-1.403858
DE(CBS)=	-0.154643	DE(MP34)=	-0.031896
DE(CCSL)=	-0.034913	DE(Int)=	0.041192
DE(Empirical)=	-0.073150		
CBS-QB3(0 K)=	-513.649516	CBS-QB3 Energy=	-513.643055
CBS-QB3 Enthalpy=	-513.642111	CBS-QB3 Free Energy=	-513.681123

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H1F4(2)\CDNEEDHA\06-Jan-2015\0\#\p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom =dihedral\\Abstraction Species 2 Thermochemistry\\0,2\C,0,0.2196038721,0.3766027593,0.0979278563\H,0,-0.0915864317,0.4610354209,1.1227177588\C,0,1.1338583322,-0.1351924366,-0.6751785945\C,0,1.1800773692,0.0113085512,-2.17679272\F,0,2.1756609442,-0.8754691671,-0.2233852063\F,0,2.3208471714,0.6096896679,-2.5653258659\F,0,1.132918813,-1.1916627786,-2.7776337336\F,0,0.1489523926,0.743688224,-2.6212921136\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-512.0274717\E2(CBS)/CbsB3=-1.5585005\CBS-Int/CbsB3=0.041192\OIii/CbsB3=12.3080378\MP2/CbsB4=-512.9772995\MP4(SDQ)/CbsB4=-513.0091951\MP4(SDQ)/6-31+G(d')=-513.0015213\QCISD(T)/6-31+G(d')=-513.0364338\CBSQB3=-513.6495155

Z-CHCFCF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.035328	E(Thermal)=	0.041753
E(SCF)=	-512.028580	DE(MP2)=	-1.403650
DE(CBS)=	-0.154563	DE(MP34)=	-0.031867
DE(CCSL)=	-0.034999	DE(Int)=	0.041152
DE(Empirical)=	-0.073087		
CBS-QB3(0 K)=	-513.650266	CBS-QB3 Energy=	-513.643841
CBS-QB3 Enthalpy=	-513.642897	CBS-QB3 Free Energy=	-513.681833

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H1F4(2)\CDNEEDHA\06-Jan-2015\0\#\p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom =dihedral\\Abstraction Species 3 Thermochemistry\\0,2\C,0,0.0132794591,0.2515944788,0.0469352849\C,0,0.0951226535,-0.1581923346,1.2806839429\C,0,1.3260264337,-0.0452441855,2.1548085715\F,0,-0.9216093833,-0.7426785662,1.9424492815\F,0,1.0724161206,0.6869441095,3.2531103035\F,0,1.7407805103,-1.2568354655,2.5631094204\F,0,2.3342018169,0.5390835731,1.4852764334\H,0,0.611252877,0.7253286277,-0.7084358707\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-512.0285796\E2(CBS)/CbsB3=-1.5582129\CBS-Int/CbsB3=0.0411524\OIii/CbsB3=12.293326\MP2/CbsB4=-512.9778968\MP4(SDQ)/CbsB4=-513.009764\MP4(SDQ)/6-31+G(d')=-513.0020714\QCISD(T)/6-31+G(d')=-513.0370708\CBSQB3=-513.650266\

CH<sub>3</sub>CFCF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.058333	E(Thermal)=	0.065587
E(SCF)=	-513.248104	DE(MP2)=	-1.447633
DE(CBS)=	-0.159982	DE(MP34)=	-0.035984
DE(CCSL)=	-0.027035	DE(Int)=	0.043108
DE(Empirical)=	-0.075027		

CBS-QB3 (0 K)= -514.892326 CBS-QB3 Energy= -514.885072  
CBS-QB3 Enthalpy= -514.884128 CBS-QB3 Free Energy= -514.925176  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\06-Jan-2015\0\#\n  
p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom  
=dihedral\Species 4 H-addition Thermochemistry\0,2\C,0,-0.0523896903  
,0.0165226465,-0.0281035411\H,0,-0.4811754528,0.4955411933,0.851967918  
1\H,0,0.9162345602,-0.4214213881,0.2538840666\C,0,-0.974236808,-1.0139  
484592,-0.5530363096\C,0,-1.785937317,-1.9173236987,0.3134064513\F,0,-  
0.6317347202,-1.5842967925,-1.7230014518\F,0,-2.7769256341,-2.51037601  
85,-0.3712529471\F,0,-1.0425540607,-2.9116713361,0.8708703573\F,0,-2.3  
282221902,-1.2169388011,1.3317867525\H,0,0.1372443511,0.7760557348,-0.  
7907435242\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-513.2481042\E  
2(CBS)/CbsB3=-1.6076156\CBS-Int/CbsB3=0.0431075\OIii/CbsB3=12.9392892\  
MP2/CbsB4=-514.238415\MP4(SDQ)/CbsB4=-514.2743995\MP4(SDQ)/6-31+G(d')=  
-514.2504811\QCISD(T)/6-31+G(d')=-514.2775164\CBSQB3=-514.8923262\

CH<sub>3</sub>COFCF<sub>3</sub>

Temperature= 298.150000 Pressure= 1.000000  
E(ZPE)= 0.062446 E(Thermal)= 0.070230  
E(SCF)= -588.143657 DE(MP2)= -1.659747  
DE(CBS)= -0.182865 DE(MP34)= -0.042304  
DE(CCSO)= -0.034279 DE(Int)= 0.049622  
DE(Empirical)= -0.085384  
CBS-QB3 (0 K)= -590.036167 CBS-QB3 Energy= -590.028384  
CBS-QB3 Enthalpy= -590.027440 CBS-QB3 Free Energy= -590.069196  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\24-Oct-2014\0\  
\#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save geom=dih  
edral\O-addition to Species 4 to convert to products of TSb11 or TSb1  
2\0,2\C,0,0.0262037696,-0.0316176668,0.0160086835\H,0,-0.1225146124,0  
.0619209491,1.0892869968\H,0,1.0489317529,-0.3332436329,-0.2099606756\  
C,0,-0.9116176862,-1.1215429334,-0.5625435383\C,0,-0.6404287525,-2.512  
6431753,0.1076265554\F,0,-0.5882489324,-1.2968415716,-1.9101861656\F,0  
,-1.4449012795,-3.4498569624,-0.4004212139\F,0,0.6304685669,-2.8888177  
501,-0.0926554752\F,0,-0.8521678267,-2.4360506419,1.4293738734\H,0,-0.  
2004331798,0.9095985087,-0.4816780885\O,0,-2.1571436629,-0.7514367151,  
-0.3707313589\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.143657  
2\E2(CBS)/CbsB3=-1.8426118\CBS-Int/CbsB3=0.049622\OIii/CbsB3=14.729746  
6\MP2/CbsB4=-589.2788206\MP4(SDQ)/CbsB4=-589.3211246\MP4(SDQ)/6-31+G(d  
')=-589.2973065\QCISD(T)/6-31+G(d')=-589.331585\CBSQB3=-590.0361674\

CH<sub>2</sub>CHFCF<sub>3</sub>

Temperature= 298.150000 Pressure= 1.000000  
E(ZPE)= 0.057218 E(Thermal)= 0.064519  
E(SCF)= -513.244826 DE(MP2)= -1.444924  
DE(CBS)= -0.159072 DE(MP34)= -0.036647  
DE(CCSO)= -0.026565 DE(Int)= 0.043023  
DE(Empirical)= -0.074973  
CBS-QB3 (0 K)= -514.886765 CBS-QB3 Energy= -514.879464  
CBS-QB3 Enthalpy= -514.878520 CBS-QB3 Free Energy= -514.919247  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\06-Jan-2015\0\#\n  
p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom  
=dihedral\Species 5 H-addition Thermochemistry\0,2\C,0,-0.0336016228  
,0.1717342953,0.0157788624\H,0,0.0364741234,1.0027394267,0.7040400779\  
H,0,0.7598400234,-0.5599287049,-0.0360646092\C,0,-1.2867803828,-0.0204  
662571,-0.7453314647\C,0,-2.3561610486,-0.8076441745,0.0318855543\F,0,  
-1.856650814,1.211178027,-1.0607091999\F,0,-3.4839802582,-0.9375103227  
,-0.6848827237\F,0,-1.8939199029,-2.0468326635,0.3026161397\F,0,-2.670  
7602737,-0.2163226609,1.1948241277\H,0,-1.1192295917,-0.5688055476,-1.  
6783890936\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-513.2448255\E

2 (CBS) /CbsB3=-1.6039962\CBS-Int/CbsB3=0.0430232\OIii/CbsB3=12.9276534\  
MP2/CbsB4=-514.2325066\MP4 (SDQ) /CbsB4=-514.2691533\MP4 (SDQ) /6-31+G (d')  
=-514.2451476\QCISD (T) /6-31+G (d')=-514.2717123\CBSQB3=-514.8867649\

CH<sub>2</sub>OCFCF<sub>3</sub>

Temperature= 298.150000 Pressure= 1.000000  
E (ZPE)= 0.049464 E (Thermal)= 0.057476  
E (SCF)= -587.497098 DE (MP2)= -1.618889  
DE (CBS)= -0.180416 DE (MP34)= -0.042897  
DE (CCSD)= -0.032632 DE (Int)= 0.048242  
DE (Empirical)= -0.082756  
CBS-QB3 (0 K)= -589.356981 CBS-QB3 Energy= -589.348969  
CBS-QB3 Enthalpy= -589.348025 CBS-QB3 Free Energy= -589.392362  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4O1 (3)\CDNEEDHA\07-Jan-2015\0\  
\#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge  
om=dihedral\Species 6 O-addition Thermochemistry\0,3\C,0,0.002231998  
4,0.0433519027,0.0041685416\H,0,-0.1569462065,0.5282286948,0.994406902  
4\C,0,1.4465152438,0.0689877367,-0.3610686514\C,0,2.3738275707,-1.0957  
977956,-0.2878616387\F,0,2.0574319068,1.2565466535,-0.3278943662\F,0,3  
.4033137528,-0.9723871735,-1.1389701133\F,0,2.9046244127,-1.2522992338  
,0.9528250769\F,0,1.7070226689,-2.2319946115,-0.5793251674\H,0,-0.3530  
52294,-0.9895716406,0.1338244255\O,0,-0.8052555642,0.7479043696,-0.854  
5437036\Version=ES64L-G09RevD.01\State=3-A\HF/CbsB3=-587.4970977\E2 (C  
BS) /CbsB3=-1.7993043\CBS-Int/CbsB3=0.0482425\OIii/CbsB3=14.2528112\MP2  
/CbsB4=-588.5950794\MP4 (SDQ) /CbsB4=-588.637976\MP4 (SDQ) /6-31+G (d')=-58  
8.6225739\QCISD (T) /6-31+G (d')=-588.6552061\CBSQB3=-589.3569806\

CH<sub>2</sub>COFCF<sub>3</sub>

Temperature= 298.150000 Pressure= 1.000000  
E (ZPE)= 0.047790 E (Thermal)= 0.055827  
E (SCF)= -587.507206 DE (MP2)= -1.620349  
DE (CBS)= -0.179864 DE (MP34)= -0.042024  
DE (CCSD)= -0.034045 DE (Int)= 0.048148  
DE (Empirical)= -0.082703  
CBS-QB3 (0 K)= -589.370252 CBS-QB3 Energy= -589.362216  
CBS-QB3 Enthalpy= -589.361271 CBS-QB3 Free Energy= -589.403857  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4O1 (3)\CDNEEDHA\15-Sep-2014\0\  
\#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save geom=dih  
edral\Species 7 O-addition Thermochemistry\0,3\C,0,-0.0469444916,0.0  
171742968,0.0716766145\H,0,-0.216367047,0.0839485166,1.1364730928\H,0,  
0.9373439871,-0.0870229767,-0.3574408472\C,0,-1.2578125067,-0.09501332  
67,-0.8098517905\C,0,-1.7134439825,-1.6240003051,-0.9289824237\F,0,-2.  
3391237155,0.5287305237,-0.1802254017\F,0,-2.7986434522,-1.735945,-1.6  
952304277\F,0,-0.7272553436,-2.350275175,-1.4631508047\F,0,-1.99408172  
11,-2.1058399116,0.2853949085\O,0,-1.0204505921,0.3497074912,-2.023129  
7476\Version=ES64L-G09RevD.01\State=3-A\HF/CbsB3=-587.507206\E2 (CBS) /  
CbsB3=-1.8002126\CBS-Int/CbsB3=0.048148\OIii/CbsB3=14.2403102\MP2/CbsB  
4=-588.6068216\MP4 (SDQ) /CbsB4=-588.6488455\MP4 (SDQ) /6-31+G (d')=-588.63  
29425\QCISD (T) /6-31+G (d')=-588.6669875\CBSQB3=-589.3702521\

CHOCFCF<sub>3</sub>

Temperature= 298.150000 Pressure= 1.000000  
E (ZPE)= 0.040377 E (Thermal)= 0.047834  
E (SCF)= -586.959725 DE (MP2)= -1.629608  
DE (CBS)= -0.179486 DE (MP34)= -0.035661  
DE (CCSD)= -0.040406 DE (Int)= 0.047733  
DE (Empirical)= -0.083908  
CBS-QB3 (0 K)= -588.840684 CBS-QB3 Energy= -588.833227  
CBS-QB3 Enthalpy= -588.832283 CBS-QB3 Free Energy= -588.874778

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H1F4O1(2)\CDNEEDHA\07-Jan-2015\0\
\#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge
om=dihedral\Species 8 O addition decomposition species\0,2\C,0,-0.05
95752286,-0.0852885308,0.0231783246\H,0,0.078879156,0.0018732232,1.116
2985799\C,0,1.137009256,0.0926114822,-0.7418623251\C,0,1.2347022289,0.
0162206392,-2.2497779924\F,0,0.3826402272,0.8730032442,-2.8311237789\F
,0,0.9415879572,-1.2193434768,-2.6888800002\F,0,2.4780284941,0.3188916
431,-2.6488990092\F,0,2.2744853083,0.3187128638,-0.1028421168\O,0,-1.1
436939567,-0.316681088,-0.4959416819\Version=ES64L-G09RevD.01\State=2
-A\HF/CbsB3=-586.9597251\E2(CBS)/CbsB3=-1.809094\CBS-Int/CbsB3=0.04773
27\OIii/CbsB3=14.1941591\MP2/CbsB4=-588.0683485\MP4(SDQ)/CbsB4=-588.10
40094\MP4(SDQ)/6-31+G(d')=-588.0958805\QCISD(T)/6-31+G(d')=-588.136286
4\CBSQB3=-588.8406844\

```

CH<sub>2</sub>COF

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                    0.034967 E(Thermal)=                0.039021
E(SCF)=                    -251.261656 DE(MP2)=                -0.756271
DE(CBS)=                   -0.080576 DE(MP34)=                -0.024993
DE(CCSD)=                  -0.020202 DE(Int)=                 0.023109
DE(Empirical)=             -0.038311
CBS-QB3 (0 K)=             -252.123933 CBS-QB3 Energy=          -252.119880
CBS-QB3 Enthalpy=         -252.118935 CBS-QB3 Free Energy=      -252.150753

```

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C2H2F1O1(2)\CDNEEDHA\07-Jan-2015\0\
\#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge
om=dihedral\Species 9 O addition decomposition product\0,2\C,0,-0.08
18951293,0.,-0.025649556\C,0,0.0016848342,0.,1.4068715323\H,0,0.958651
2927,0.,1.9086278817\H,0,-0.9196031453,0.,1.9711973345\O,0,-1.06940793
59,0.,-0.7015551894\F,0,1.1534819669,0.,-0.611254005\Version=ES64L-G0
9RevD.01\State=2-A\HF/CbsB3=-251.2616559\E2(CBS)/CbsB3=-0.8368467\CBS
-Int/CbsB3=0.0231086\OIii/CbsB3=6.4780225\MP2/CbsB4=-251.7982983\MP4(S
DQ)/CbsB4=-251.8232912\MP4(SDQ)/6-31+G(d')=-251.8074231\QCISD(T)/6-31+
G(d')=-251.8276254\CBSQB3=-252.123933\

```

CF<sub>3</sub>CCH

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                    0.032828 E(Thermal)=                0.038263
E(SCF)=                    -412.573942 DE(MP2)=                -1.193666
DE(CBS)=                   -0.127878 DE(MP34)=                -0.018141
DE(CCSD)=                  -0.027418 DE(Int)=                 0.035992
DE(Empirical)=             -0.059134
CBS-QB3 (0 K)=             -413.931359 CBS-QB3 Energy=          -413.925924
CBS-QB3 Enthalpy=         -413.924980 CBS-QB3 Free Energy=      -413.959413

```

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H1F3\CDNEEDHA\07-Jan-2015\0\#p o
pt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom=di
hedral\Species 10 4-center concerted reaction product Restricted Open
Shell Basis Set to Eliminate Spin Contamination\0,1\C,0,0.0000000557
,0.0000000019,-0.0306988745\H,0,0.0000000557,0.0000000019,1.032927294\
C,0,0.0000000557,0.0000000019,-1.2278394262\C,0,0.0000000557,0.0000000
019,-2.6882233779\F,0,1.2536107449,0.0437770378,-3.1772901322\F,0,-0.5
888932638,-1.1075472193,-3.1772901322\F,0,-0.6647173141,1.0637701874,-
3.1772901322\Version=ES64L-G09RevD.01\State=1-A1\HF/CbsB3=-412.573942
4\E2(CBS)/CbsB3=-1.3215437\CBS-Int/CbsB3=0.0359922\OIii/CbsB3=10.21309
57\MP2/CbsB4=-413.3999463\MP4(SDQ)/CbsB4=-413.4180877\MP4(SDQ)/6-31+G(
d')=-413.4110205\QCISD(T)/6-31+G(d')=-413.4384389\CBSQB3=-413.9313592\

```

CH<sub>2</sub>OHCFCF<sub>3</sub>

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                    0.063714 E(Thermal)=                0.071995

```

E(SCF)= -588.122164 DE(MP2)= -1.679276  
 DE(CBS)= -0.183642 DE(MP34)= -0.036452  
 DE(CCSO)= -0.031891 DE(Int)= 0.049753  
 DE(Empirical)= -0.085604  
 CBS-QB3 (0 K)= -590.025561 CBS-QB3 Energy= -590.017280  
 CBS-QB3 Enthalpy= -590.016336 CBS-QB3 Free Energy= -590.060669  
 1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\07-Jan-2015\0\  
 \#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge  
 om=dihedral\Species 11 OH-addition Thermochemistry\0,2\C,0,0.0433445  
 179,0.0245167734,0.0231631944\H,0,0.0934834173,-0.0035113899,1.1176890  
 999\C,0,1.4205394258,0.023762282,-0.5381492737\C,0,2.1032980307,-1.183  
 7276697,-1.0894304905\F,0,2.2658572502,0.956059655,-0.0829387634\F,0,3  
 .1731384596,-0.8586253777,-1.8303087376\F,0,2.5361156079,-2.0241559274  
 ,-0.1133846528\F,0,1.2460433156,-1.8879267815,-1.8597141367\H,0,-0.475  
 0705432,-0.8800270377,-0.3147517388\O,0,-0.6769403973,1.21129706,-0.28  
 7698697\H,0,-0.7387249581,1.27788976,-1.2468551106\Version=ES64L-G09R  
 evD.01\State=2-A\HF/CbsB3=-588.1221635\E2(CBS)/CbsB3=-1.8629184\CBS-Int/  
 CbsB3=0.0497535\Oiii/CbsB3=14.764879\MP2/CbsB4=-589.2740345\MP4(SDQ)  
 /CbsB4=-589.3104864\MP4(SDQ)/6-31+G(d')=-589.2784563\QCISD(T)/6-31+G(d  
 ')=-589.3103474\CBSQB3=-590.0255609\

CH<sub>2</sub>COHF<sub>2</sub>

Temperature= 298.150000 Pressure= 1.000000  
 E(ZPE)= 0.061477 E(Thermal)= 0.069700  
 E(SCF)= -588.139928 DE(MP2)= -1.679755  
 DE(CBS)= -0.182802 DE(MP34)= -0.035497  
 DE(CCSO)= -0.031949 DE(Int)= 0.049691  
 DE(Empirical)= -0.085563  
 CBS-QB3 (0 K)= -590.044327 CBS-QB3 Energy= -590.036104  
 CBS-QB3 Enthalpy= -590.035160 CBS-QB3 Free Energy= -590.077668  
 1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\07-Jan-2015\0\  
 \#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge  
 om=dihedral\Species 12 OH-addition Thermochemistry\0,2\C,0,0.0416764  
 619,-0.0513052374,-0.0147400801\H,0,0.1606167743,-0.4539823093,0.98013  
 01376\H,0,0.7861104824,0.5959869162,-0.4531577367\C,0,-1.222161132,-0.  
 2810560215,-0.7454774587\C,0,-1.6628222184,-1.7671484545,-0.7496670317  
 \F,0,-2.2800400383,0.3775020159,-0.0776015172\F,0,-2.7922921994,-1.910  
 9249073,-1.478356672\F,0,-0.7190233423,-2.5419309422,-1.3070780393\F,0  
 ,-1.9010108833,-2.2210797728,0.4874419243\O,0,-1.1188641842,0.19784944  
 12,-2.0288780398\H,0,-1.9451089731,0.0121127656,-2.4940726448\Version  
 =ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.1399284\E2(CBS)/CbsB3=-1.862  
 5574\CBS-Int/CbsB3=0.0496911\Oiii/CbsB3=14.7572491\MP2/CbsB4=-589.2931  
 772\MP4(SDQ)/CbsB4=-589.3286747\MP4(SDQ)/6-31+G(d')=-589.2973378\QCISD  
 (T)/6-31+G(d')=-589.3292869\CBSQB3=-590.044327\

CH<sub>2</sub>OCHF<sub>2</sub>

Temperature= 298.150000 Pressure= 1.000000  
 E(ZPE)= 0.062371 E(Thermal)= 0.070240  
 E(SCF)= -588.131100 DE(MP2)= -1.654970  
 DE(CBS)= -0.182528 DE(MP34)= -0.043706  
 DE(CCSO)= -0.032338 DE(Int)= 0.049649  
 DE(Empirical)= -0.085403  
 CBS-QB3 (0 K)= -590.018025 CBS-QB3 Energy= -590.010157  
 CBS-QB3 Enthalpy= -590.009212 CBS-QB3 Free Energy= -590.051885  
 1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\07-Jan-2015\0\  
 \#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge  
 om=dihedral\Species 13 OH-addition H-transfer Thermochemistry\0,2\C,  
 0,0.0648177465,-0.0335602934,0.0702653091\H,0,0.2406857873,-0.26420843  
 5,1.1359356794\C,0,1.4022985017,0.1123458799,-0.6575763468\C,0,2.16343

35425,-1.2048037225,-0.763518309\F,0,2.1990534998,1.0087222986,0.03667  
 87338\F,0,3.36373781,-1.0445934475,-1.3339031172\F,0,2.3492524413,-1.7  
 72800215,0.4436453024\F,0,1.4525377543,-2.0734602117,-1.5193128908\H,0  
 ,-0.4973697924,-0.904494822,-0.3149680939\O,0,-0.7386806343,1.06152332  
 85,-0.0275990441\H,0,1.2445748148,0.5001881705,-1.6670676529\Version=  
 ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.1310998\E2(CBS)/CbsB3=-1.8374  
 984\CBS-Int/CbsB3=0.049649\OIii/CbsB3=14.7340661\MP2/CbsB4=-589.261544  
 5\MP4(SDQ)/CbsB4=-589.3052504\MP4(SDQ)/6-31+G(d')=-589.2819259\QCISD(T  
 )/6-31+G(d')=-589.3142638\CBSQB3=-590.0180251\

CHOHCHFCF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.063292	E(Thermal)=	0.071514
E(SCF)=	-588.127531	DE(MP2)=	-1.683173
DE(CBS)=	-0.183632	DE(MP34)=	-0.035862
DE(CCSD)=	-0.032432	DE(Int)=	0.049797
DE(Empirical)=	-0.085588		
CBS-QB3 (0 K)=	-590.035128	CBS-QB3 Energy=	-590.026906
CBS-QB3 Enthalpy=	-590.025962	CBS-QB3 Free Energy=	-590.069244

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\07-Jan-2015\0\  
 \#p opt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar ge  
 om=dihedral\Species 14 OH-addition H-transfer Thermochemistry\0,2\C,  
 0,0.0021541868,0.0116318967,0.0044209032\H,0,-0.0495844077,0.164854280  
 4,1.0714696441\C,0,1.2713953965,-0.0101722079,-0.7280188828\C,0,2.3780  
 041471,-0.7290616136,0.0434962118\F,0,1.7579102404,1.2971646005,-1.010  
 9714142\F,0,3.5581580651,-0.6201644765,-0.5835962567\F,0,2.5232933826,  
 -0.2379250989,1.2875295959\F,0,2.0869890447,-2.0419661585,0.1493202606  
 \O,0,-1.1763823003,0.2066810561,-0.6347274037\H,0,1.1726149295,-0.5087  
 155448,-1.6990493608\H,0,-1.05517818,0.1483630243,-1.5899281365\Versi  
 on=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.1275312\E2(CBS)/CbsB3=-1.8  
 668056\CBS-Int/CbsB3=0.0497973\OIii/CbsB3=14.7592099\MP2/CbsB4=-589.28  
 29262\MP4(SDQ)/CbsB4=-589.3187878\MP4(SDQ)/6-31+G(d')=-589.2868216\QCI  
 SD(T)/6-31+G(d')=-589.3192535\CBSQB3=-590.0351283\

CF<sub>3</sub>CFCO

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.030283	E(Thermal)=	0.037479
E(SCF)=	-586.363573	DE(MP2)=	-1.662256
DE(CBS)=	-0.178230	DE(MP34)=	-0.018351
DE(CCSD)=	-0.034416	DE(Int)=	0.048640
DE(Empirical)=	-0.081545		
CBS-QB3 (0 K)=	-588.259447	CBS-QB3 Energy=	-588.252251
CBS-QB3 Enthalpy=	-588.251307	CBS-QB3 Free Energy=	-588.292077

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3F4O1\CDNEEDHA\07-Jan-2015\0\#p o  
 pt=(calcall,tight) freq=hinderedrotor cbs-qb3 guess=save polar geom=di  
 hedra\Species 16 Thermochemistry\0,1\C,0,0.0317446686,-0.092347469,  
 0.0426516213\C,0,-0.0000890721,0.1338165987,1.3459904201\C,0,1.2897963  
 934,-0.0124192239,-0.7451091785\O,0,-0.0231789998,0.3323361096,2.48524  
 65988\F,0,1.588286768,-1.1792395102,-1.3454809788\F,0,-1.1009146833,-0  
 .4096822737,-0.6281814016\F,0,2.3107483603,0.3124779717,0.0781109647\F  
 ,0,1.2220642723,0.9150579391,-1.7178430149\Version=ES64L-G09RevD.01\S  
 tate=1-A\HF/CbsB3=-586.3635731\E2(CBS)/CbsB3=-1.8404859\CBS-Int/CbsB3=  
 0.0486404\OIii/CbsB3=14.0837019\MP2/CbsB4=-587.5031195\MP4(SDQ)/CbsB4=  
 -587.5214702\MP4(SDQ)/6-31+G(d')=-587.5214702\QCISD(T)/6-31+G(d')=-587  
 .5558864\CBSQB3=-588.2594467\

a<sub>1</sub>-CF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.055838	E(Thermal)=	0.067093

E (SCF) = -848.880414 DE (MP2) = -2.330012  
DE (CBS) = -0.259728 DE (MP34) = -0.043738  
DE (CCSD) = -0.052173 DE (Int) = 0.068158  
DE (Empirical) = -0.121106  
CBS-QB3 (0 K) = -851.563174 CBS-QB3 Energy = -851.551919  
CBS-QB3 Enthalpy = -851.550974 CBS-QB3 Free Energy = -851.605141  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C4H2F7(2)\CDNEEDHA\09-Oct-2014\0\#\n  
p opt=(calcall,qst3,noeigentest) freq cbs-qb3 guess=save geom=dihedral  
\\al TS for CF3 abstraction from HFO-1234yf\0,2\C,0,-0.0316112288,-0.  
3725198784,-0.1550265048\H,0,-0.0772984075,-0.9649785405,0.7449899456\  
H,0,1.2528094882,-0.1715547038,-0.6910084843\C,0,-1.0210730211,0.18166  
4983,-0.8136652211\C,0,-2.4860057313,0.1097531035,-0.4442035809\F,0,-0.  
.8395825785,0.9045759807,-1.9348106236\F,0,-2.9901724703,1.3386479663,  
-0.2383027758\F,0,-3.2016884448,-0.4627473958,-1.4275200095\F,0,-2.663  
3493605,-0.6093876864,0.6765605682\C,0,2.436670148,-0.0214438403,-1.14  
63672501\F,0,2.4821282577,-0.4250332398,-2.4136931984\F,0,3.2632740675  
,-0.7629688881,-0.4058298738\F,0,2.786766496,1.2601892014,-1.065059425  
3\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-848.8804136\E2 (CBS)  
/CbsB3=-2.58974\CBS-Int/CbsB3=0.0681581\OIii/CbsB3=20.554233\MP2/CbsB4=-8  
50.4512228\MP4 (SDQ) /CbsB4=-850.4949609\MP4 (SDQ) /6-31+G(d')=-850.476202  
7\QCISD(T) /6-31+G(d')=-850.5283755\CBSQB3=-851.5631743\

a<sub>1</sub>-CH<sub>3</sub>

Temperature = 298.150000 Pressure = 1.000000  
E (ZPE) = 0.076355 E (Thermal) = 0.085930  
E (SCF) = -552.204945 DE (MP2) = -1.615943  
DE (CBS) = -0.176619 DE (MP34) = -0.052296  
DE (CCSD) = -0.041016 DE (Int) = 0.049025  
DE (Empirical) = -0.085142  
CBS-QB3 (0 K) = -554.050580 CBS-QB3 Energy = -554.041006  
CBS-QB3 Enthalpy = -554.040062 CBS-QB3 Free Energy = -554.088710  
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C4H5F4(2)\CDNEEDHA\26-Oct-2014\0\#\n  
p opt=(calcall,tight,ts,noeigentest) freq cbs-qb3 guess=save geom=dihedral  
\\al TS for CH3 abstraction from HFO-1234yf\0,2\C,0,-0.0000424456  
,-0.0086619791,-0.0002578733\H,0,0.0000250141,-0.0223432268,1.07833024  
8\H,0,1.2582960882,-0.0046570407,-0.6412287331\C,0,-1.0513087518,0.004  
2137621,-0.7837202687\C,0,-2.4963181665,0.0028225888,-0.3465186715\F,0  
,-0.9620063545,0.0209783331,-2.1324257629\F,0,-3.1423543122,1.09477993  
76,-0.7975740167\F,0,-3.1485284347,-1.0737199742,-0.8249172372\F,0,-2.  
5961637577,-0.0138014722,0.9942818328\C,0,2.3735870891,-0.0007739861,-  
1.2492457524\H,0,3.1298580583,0.055567148,-0.4690090779\H,0,2.34582743  
43,0.8788826531,-1.8882471348\H,0,2.3971515538,-0.9342278173,-1.806993  
7884\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-552.2049448\E2 (CBS)  
/CbsB3=-1.7925627\CBS-Int/CbsB3=0.0490255\OIii/CbsB3=14.360631\MP2/Cbs  
B4=-553.3293977\MP4 (SDQ) /CbsB4=-553.3816939\MP4 (SDQ) /6-31+G(d')=-553.3  
381788\QCISD(T) /6-31+G(d')=-553.3791944\CBSQB3=-554.0505801\

a<sub>1</sub>-H

Temperature = 298.150000 Pressure = 1.000000  
E (ZPE) = 0.046608 E (Thermal) = 0.054219  
E (SCF) = -513.136290 DE (MP2) = -1.445795  
DE (CBS) = -0.159683 DE (MP34) = -0.038391  
DE (CCSD) = -0.037459 DE (Int) = 0.043117  
DE (Empirical) = -0.076240  
CBS-QB3 (0 K) = -514.804133 CBS-QB3 Energy = -514.796522  
CBS-QB3 Enthalpy = -514.795577 CBS-QB3 Free Energy = -514.836906  
1\1\GINC-BL1\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\29-Sep-2014\0\#\n  
p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save  
geom=dihedral\\al TS for H abstraction from HFO-1234yf\0,2\C,0,-0.01



97996049,0.0020825397,0.05057728\H,0,0.1515386621,0.0018725317,1.11364  
 18643\H,0,1.2733665084,0.005155302,-0.7742347846\C,0,-1.1316097957,0.0  
 000515222,-0.6405299955\C,0,-2.5275079853,-0.0033354314,-0.0569091634\  
 F,0,-1.1708662074,0.0006979646,-1.9856059459\F,0,-3.2188587421,1.07951  
 77007,-0.4541699041\F,0,-3.2138774856,-1.0890892094,-0.454954976\F,0,-  
 2.4870235337,-0.0037167804,1.2863791258\H,0,1.9857417517,0.0067628631,  
 -1.2002563623\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-513.136290  
 1\E2(CBS)/CbsB3=-1.6054778\CBS-Int/CbsB3=0.0431169\OIii/CbsB3=12.80284  
 26\MP2/CbsB4=-514.122518\MP4(SDQ)/CbsB4=-514.1609094\MP4(SDQ)/6-31+G(d  
 ')=-514.1362806\QCISD(T)/6-31+G(d')=-514.1737397\CBSQB3=-514.8041334\

a<sub>1</sub>-OH

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.052878	E(Thermal)=	0.062040
E(SCF)=	-588.044993	DE(MP2)=	-1.676530
DE(CBS)=	-0.185304	DE(MP34)=	-0.041452
DE(CCSB)=	-0.041568	DE(Int)=	0.050046
DE(Empirical)=	-0.086607		
CBS-QB3 (0 K)=	-589.973530	CBS-QB3 Energy=	-589.964368
CBS-QB3 Enthalpy=	-589.963424	CBS-QB3 Free Energy=	-590.009871

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\04-Nov-2014\0\  
 \#p opt=(calcall,tight,ts,noeigentest) freq cbs-qb3 guess=save geom=di  
 hedra1\TS for OH abstraction from HFO-1234yf\0,2\C,0,0.0086069535  
 ,0.0323050944,0.0280682462\H,0,-0.0151528484,-0.0112520983,1.106409156  
 4\H,0,1.197529313,0.098446715,-0.4897623076\C,0,-1.014412788,0.0310050  
 066,-0.7937368094\C,0,-2.471400523,-0.0082250154,-0.3989738448\F,0,-0.  
 8691673589,0.0653398351,-2.1344813298\F,0,-3.1235308002,1.0742492335,-  
 0.8565887728\F,0,-3.0788326557,-1.0928503937,-0.9108912383\F,0,-2.6029  
 637693,-0.0446312065,0.9371110514\H,0,1.6991230442,-0.1472643964,-2.05  
 6811002\O,0,2.1274448575,0.0029712474,-1.1985493473\\Version=ES64L-G09  
 RevD.01\State=2-A\HF/CbsB3=-588.0449934\E2(CBS)/CbsB3=-1.8618343\CBS-I  
 nt/CbsB3=0.0500456\OIii/CbsB3=14.6352676\MP2/CbsB4=-589.195751\MP4(SDQ  
 )/CbsB4=-589.2372026\MP4(SDQ)/6-31+G(d')=-589.1974566\QCISD(T)/6-31+G(  
 d')=-589.239025\CBSQB3=-589.9735305\

a<sub>2</sub>-CF<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.055878	E(Thermal)=	0.067061
E(SCF)=	-848.878908	DE(MP2)=	-2.330836
DE(CBS)=	-0.259524	DE(MP34)=	-0.043908
DE(CCSB)=	-0.052472	DE(Int)=	0.068154
DE(Empirical)=	-0.121139		
CBS-QB3 (0 K)=	-851.562754	CBS-QB3 Energy=	-851.551571
CBS-QB3 Enthalpy=	-851.550627	CBS-QB3 Free Energy=	-851.604118

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C4H2F7(2)\CDNEEDHA\10-Oct-2014\0\  
 #p opt=(calcall,qst3,noeigentest) freq cbs-qb3 guess=save geom=dihedra1  
 \TSa2 for abstraction of H by CH3\0,2\C,0,-0.0059982077,-0.000554876  
 ,-0.0214311085\H,0,-0.0568620243,-0.0002400963,1.3922348012\H,0,1.0123  
 878336,-0.0014680709,-0.3838370165\C,0,-1.1124498837,0.0002272235,-0.7  
 280507356\C,0,-2.5241588491,0.0015062479,-0.1940675954\F,0,-1.11812312  
 66,-0.000029179,-2.0791356843\F,0,-3.1956686513,1.0860676122,-0.616839  
 5128\F,0,-3.197484243,-1.0820863128,-0.6164351905\F,0,-2.535737914,0.0  
 017673681,1.1507734619\C,0,0.0894030897,-0.0001124654,2.6547946147\F,0  
 ,-0.4666949236,1.0904823201,3.1751238113\F,0,-0.4685425432,-1.08955396  
 24,3.1755632159\F,0,1.4013942527,-0.0011717603,2.9060736314\\Version=E  
 S64L-G09RevD.01\State=2-A\HF/CbsB3=-848.8789079\E2(CBS)/CbsB3=-2.59036  
 \CBS-Int/CbsB3=0.0681544\OIii/CbsB3=20.5552238\MP2/CbsB4=-850.4506628\  
 MP4(SDQ)/CbsB4=-850.4945705\MP4(SDQ)/6-31+G(d')=-850.4757818\QCISD(T)/  
 6-31+G(d')=-850.5282534\CBSQB3=-851.5627541\

a<sub>2</sub>-CH<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076443	E(Thermal)=	0.085918
E(SCF)=	-552.202932	DE(MP2)=	-1.616254
DE(CBS)=	-0.176581	DE(MP34)=	-0.052505
DE(CCSB)=	-0.041333	DE(Int)=	0.049033
DE(Empirical)=	-0.085214		
CBS-QB3 (0 K)=	-554.049345	CBS-QB3 Energy=	-554.039869
CBS-QB3 Enthalpy=	-554.038925	CBS-QB3 Free Energy=	-554.086500

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C4H5F4(2)\CDNEEDHA\06-Oct-2014\0\#\#  
p opt=(calcall,qst3,noeigentest) freq cbs-qb3 guess=save geom=dihedral  
\TSa2 for abstraction of H by CH3\0,2\C,0,0.0197485541,0.0880984593,  
-0.0235022586\H,0,0.0511373484,0.0494521076,1.3989489752\H,0,1.0113662  
211,0.167760289,-0.4469587802\C,0,-1.1024509138,0.0314632149,-0.702119  
863\C,0,-2.5014446047,-0.0793159095,-0.1528243018\F,0,-1.1439235159,0.  
0679015177,-2.0589855983\F,0,-3.2549695918,0.9684695507,-0.5378097396\  
F,0,-3.1090466599,-1.1940620875,-0.6022472587\F,0,-2.5080451304,-0.119  
7656889,1.1904996691\C,0,0.1891164754,0.0231041119,2.6548663226\H,0,1.  
2605136257,0.0869635246,2.8338394451\H,0,-0.2451682212,-0.9231635267,2  
.9686636381\H,0,-0.3614888267,0.8870459189,3.0195012006\Version=ES64L  
-G09RevD.01\State=2-A\HF/CbsB3=-552.2029322\E2(CBS)/CbsB3=-1.7928353\C  
BS-Int/CbsB3=0.049033\Oiii/CbsB3=14.3642938\MP2/CbsB4=-553.3279217\MP4  
(SDQ)/CbsB4=-553.3804266\MP4(SDQ)/6-31+G(d')=-553.3369479\QCISD(T)/6-3  
1+G(d')=-553.3782813\CBSQB3=-554.0493446\

a<sub>2</sub>-H

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.046707	E(Thermal)=	0.054253
E(SCF)=	-513.134114	DE(MP2)=	-1.445856
DE(CBS)=	-0.159672	DE(MP34)=	-0.038593
DE(CCSB)=	-0.037663	DE(Int)=	0.043131
DE(Empirical)=	-0.076331		
CBS-QB3 (0 K)=	-514.802389	CBS-QB3 Energy=	-514.794844
CBS-QB3 Enthalpy=	-514.793900	CBS-QB3 Free Energy=	-514.835105

1\1\GINC-BL1\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\17-Sep-2014\0\#\#  
p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save  
geom=dihedral\TS a2 for H abstraction by H from HFO-1234yf to form s  
pecies 2\0,2\C,0,-0.0179358442,-0.000000241,0.0796332357\H,0,-0.0112  
242029,-0.000004927,1.6175015202\H,0,1.0037622107,0.0000008892,-0.2668  
80248\C,0,-1.1458825201,0.0000023121,-0.5871510481\C,0,-2.5445784908,0  
.0000007672,-0.0203658432\F,0,-1.1892048794,0.0000066367,-1.9414713085  
\F,0,-3.2251558956,1.084371417,-0.4355836939\F,0,-3.2251562957,-1.0843  
669847,-0.4355905813\F,0,-2.537003401,-0.0000035064,1.3200295816\H,0,0  
.0763820918,-0.0000075637,2.4396371114\Version=ES64L-G09RevD.01\State  
=2-A\HF/CbsB3=-513.134114\E2(CBS)/CbsB3=-1.605528\CBS-Int/CbsB3=0.0431  
315\Oiii/CbsB3=12.811737\MP2/CbsB4=-514.1207409\MP4(SDQ)/CbsB4=-514.15  
93336\MP4(SDQ)/6-31+G(d')=-514.1346102\QCISD(T)/6-31+G(d')=-514.172272  
8\CBSQB3=-514.8023892\

a<sub>2</sub>-OH

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.053646	E(Thermal)=	0.062446
E(SCF)=	-588.041747	DE(MP2)=	-1.677061
DE(CBS)=	-0.185207	DE(MP34)=	-0.041550
DE(CCSB)=	-0.041999	DE(Int)=	0.050049
DE(Empirical)=	-0.086673		
CBS-QB3 (0 K)=	-589.970542	CBS-QB3 Energy=	-589.961742
CBS-QB3 Enthalpy=	-589.960797	CBS-QB3 Free Energy=	-590.005697

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\05-Dec-2014\0\
\#p opt=(calcall,ts,noeigentest) freq cbs-qb3 guess=save geom=dihedral
\TSa2 for abstraction of H by OH\0,2\C,0,0.0357663234,-0.0267167491,
0.0647424128\H,0,0.0573042073,-0.1414133776,1.3640382979\H,0,1.0411576
603,0.0005039177,-0.3332492826\C,0,-1.0782383292,0.0143204515,-0.63201
1206\C,0,-2.4913280115,0.0284999684,-0.1051473471\F,0,-1.0799838066,0.
0495824501,-1.9813639897\F,0,-3.1504475861,1.1153639106,-0.5418290053\
F,0,-3.1733130162,-1.052071904,-0.5169347315\F,0,-2.5156506712,0.04488
89329,1.2424558929\H,0,-0.6943064911,0.6377350045,2.6167936295\O,0,0.1
271211648,0.1361766327,2.4964771098\Version=ES64L-G09RevD.01\State=2-
A\HF/CbsB3=-588.0417465\E2(CBS)/CbsB3=-1.8622678\CBS-Int/CbsB3=0.05004
89\OIii/CbsB3=14.6370031\MP2/CbsB4=-589.1934925\MP4(SDQ)/CbsB4=-589.23
50429\MP4(SDQ)/6-31+G(d')=-589.1956186\QCISD(T)/6-31+G(d')=-589.237617
4\CBSQB3=-589.970542\

```

a<sub>11</sub>

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                      0.031847 E(Thermal)=                0.039403
E(SCF)=                      -511.942055 DE(MP2)=                -1.413937
DE(CBS)=                     -0.156477 DE(MP34)=                -0.029338
DE(CCSD)=                    -0.037797 DE(Int)=                0.041565
DE(Empirical)=              -0.072051
CBS-QB3 (0 K)=               -513.578243 CBS-QB3 Energy=                -513.570687
CBS-QB3 Enthalpy=           -513.569743 CBS-QB3 Free Energy=        -513.612655
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H1F4(2)\CDNEEDHA\15-Oct-2014\0\#
p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save
geom=dihedral\TSa11 beta scission of Species 3 to produce CF3 and HC
CF\0,2\C,0,-0.0434037387,0.0000078733,-0.12294514\C,0,-0.4192258373,-
0.0000039255,1.0278993387\C,0,1.5238944531,-0.0000000353,2.3665583315\
F,0,-1.2108525057,-0.0000177506,2.0446578988\F,0,1.5140053317,1.090871
3032,3.1247812126\F,0,1.5140216554,-1.090883556,3.1247639015\F,0,2.579
4209324,0.0000142223,1.5647159098\H,0,0.5134505427,0.0000190851,-1.027
9103117\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-511.9420549\E2(C
BS)/CbsB3=-1.5704134\CBS-Int/CbsB3=0.0415646\OIii/CbsB3=12.105101\MP2/
CbsB4=-512.8986737\MP4(SDQ)/CbsB4=-512.9280122\MP4(SDQ)/6-31+G(d')=-51
2.9207842\QCISD(T)/6-31+G(d')=-512.9585809\CBSQB3=-513.5782431\

```

b<sub>1</sub>

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                      0.049635 E(Thermal)=                0.057111
E(SCF)=                      -513.173888 DE(MP2)=                -1.447798
DE(CBS)=                     -0.158963 DE(MP34)=                -0.032582
DE(CCSD)=                    -0.034191 DE(Int)=                0.042884
DE(Empirical)=              -0.075660
CBS-QB3 (0 K)=               -514.830563 CBS-QB3 Energy=                -514.823088
CBS-QB3 Enthalpy=           -514.822143 CBS-QB3 Free Energy=        -514.863191
1\1\GINC-BL1\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\17-Sep-2014\0\#
p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save
geom=dihedral\Transition state b1 for H addition to yf to make Speci
es 4\0,2\C,0,0.0170622752,-0.2053356864,0.0099147521\H,0,-0.163250875
1,0.0702426449,1.0375633794\H,0,0.9391249782,0.0978289506,-0.466444935
9\C,0,-0.8280068742,-1.011828399,-0.6199555334\C,0,-2.1222008409,-1.54
54294475,-0.0649721893\F,0,-0.6322928843,-1.4212401304,-1.882247682\F,
0,-3.1721952061,-1.1214495479,-0.7926842657\F,0,-2.1385119045,-2.89116
32024,-0.0841559514\F,0,-2.3059083228,-1.1440924925,1.2045435014\H,0,-
0.6467870918,1.8563572527,-0.4792894273\Version=ES64L-G09RevD.01\Stat
e=2-A\HF/CbsB3=-513.1738875\E2(CBS)/CbsB3=-1.6067613\CBS-Int/CbsB3=0.0
428839\OIii/CbsB3=12.8211752\MP2/CbsB4=-514.1607142\MP4(SDQ)/CbsB4=-51
4.193296\MP4(SDQ)/6-31+G(d')=-514.1762309\QCISD(T)/6-31+G(d')=-514.210

```

4222\CBSQB3=-514.8305628\

b<sub>2</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.050255	E(Thermal)=	0.057169
E(SCF)=	-513.166053	DE(MP2)=	-1.445392
DE(CBS)=	-0.158937	DE(MP34)=	-0.034276
DE(CCSD)=	-0.036078	DE(Int)=	0.042655
DE(Empirical)=	-0.076206		
CBS-QB3 (0 K)=	-514.824033	CBS-QB3 Energy=	-514.817119
CBS-QB3 Enthalpy=	-514.816175	CBS-QB3 Free Energy=	-514.855794

1\1\GINC-BL1\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\29-Sep-2014\0\#\n#  
p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save  
geom=dihedral\\b2 TS for H addition to HFO-1234yf\\0,2\C,0,-0.0418806  
482,-0.0190978773,-0.0527350125\H,0,-0.0322941688,-0.0321096798,1.0267  
228238\H,0,0.8904392623,-0.0785627595,-0.5970281455\C,0,-1.1942294683,  
0.1584223333,-0.7068103883\C,0,-2.5659356833,0.0194259938,-0.072997536  
2\F,0,-1.2646148545,0.0963356788,-2.0476686984\F,0,-3.4658606568,0.849  
9071859,-0.6153708901\F,0,-3.0266897124,-1.2361024155,-0.2446457273\F,  
0,-2.5052899949,0.2594211093,1.2481934251\H,0,-1.2707457646,2.12081259  
21,-0.6256275502\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-513.166  
0532\E2(CBS)/CbsB3=-1.6043294\CBS-Int/CbsB3=0.0426548\OIii/CbsB3=12.79  
71639\MP2/CbsB4=-514.1505262\MP4(SDQ)/CbsB4=-514.1848022\MP4(SDQ)/6-31  
+G(d')=-514.1661717\QCISD(T)/6-31+G(d')=-514.2022497\CBSQB3=-514.82403  
32\

b<sub>111</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.058830	E(Thermal)=	0.067150
E(SCF)=	-588.098913	DE(MP2)=	-1.678758
DE(CBS)=	-0.183528	DE(MP34)=	-0.038468
DE(CCSD)=	-0.038332	DE(Int)=	0.049598
DE(Empirical)=	-0.085830		
CBS-QB3 (0 K)=	-590.015401	CBS-QB3 Energy=	-590.007081
CBS-QB3 Enthalpy=	-590.006137	CBS-QB3 Free Energy=	-590.049233

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\26-Oct-2014\0\  
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=sa  
ve geom=dihedral\\TSb11 from Oaddition to Species 4 product to form OC  
HCF3 and CH3\\0,2\C,0,0.0879711455,0.3258101163,0.0968312714\H,0,0.012  
9058227,0.1653032805,1.164153344\H,0,1.0676613637,0.2723026186,-0.3600  
569025\C,0,-0.735155154,-1.5116177421,-0.6450453948\C,0,0.3332687632,-  
2.4857041252,-0.08107129\F,0,-0.4550317931,-1.270567997,-1.9642891623\  
F,0,0.0538718192,-3.7247441257,-0.5136037771\F,0,1.5768501262,-2.17985  
8422,-0.4777338788\F,0,0.3004668939,-2.4863754176,1.2558695693\H,0,-0.  
6427678761,0.979239233,-0.3606352718\O,0,-1.8559002325,-1.4569986122,-  
0.2168587088\\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.098913\  
E2(CBS)/CbsB3=-1.8622864\CBS-Int/CbsB3=0.049598\OIii/CbsB3=14.6211637\  
MP2/CbsB4=-589.2517441\MP4(SDQ)/CbsB4=-589.2902123\MP4(SDQ)/6-31+G(d')  
=-589.2661651\QCISD(T)/6-31+G(d')=-589.3044968\CBSQB3=-590.0154014\

b<sub>112</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.060740	E(Thermal)=	0.068838
E(SCF)=	-588.102507	DE(MP2)=	-1.676135
DE(CBS)=	-0.184963	DE(MP34)=	-0.039727
DE(CCSD)=	-0.041132	DE(Int)=	0.049444
DE(Empirical)=	-0.086097		
CBS-QB3 (0 K)=	-590.020376	CBS-QB3 Energy=	-590.012278
CBS-QB3 Enthalpy=	-590.011334	CBS-QB3 Free Energy=	-590.054340

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\26-Oct-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save
geom=dihedral\TSb12 from Oaddition to Species 4 product to form OC
HCH3 and CF3\0,2\C,0,-0.1111061528,0.1689054326,-0.0468223705\H,0,-0.
1682695676,0.2046355809,1.0396091976\H,0,0.9048563969,0.3553173912,-0.
3885938059\C,0,-0.6281808328,-1.1694341782,-0.5422287882\C,0,0.7994863
83,-2.4141446312,0.1287389084\F,0,-0.323633387,-1.3184598538,-1.891753
2812\F,0,0.533447874,-3.6189615205,-0.317678097\F,0,1.9623524352,-1.98
07722627,-0.3334026657\F,0,0.7738040006,-2.368115526,1.4483214491\H,0,
-0.7681294592,0.935701322,-0.4646470547\O,0,-1.6117833899,-1.740232103
3,-0.1028890589\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.1025
065\E2(CBS)/CbsB3=-1.8610981\CBS-Int/CbsB3=0.0494441\OIii/CbsB3=14.632
3699\MP2/CbsB4=-589.2523473\MP4(SDQ)/CbsB4=-589.2920744\MP4(SDQ)/6-31+
G(d')=-589.268183\QCISD(T)/6-31+G(d')=-589.309315\CBSQB3=-590.0203765\
b21
Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                    0.055389 E(Thermal)=                0.062955
E(SCF)=                    -513.184433 DE(MP2)=                -1.436862
DE(CBS)=                   -0.160192 DE(MP34)=                -0.039099
DE(CCSD)=                  -0.035301 DE(Int)=                0.042678
DE(Empirical)=             -0.076484
CBS-QB3 (0 K)=              -514.834302 CBS-QB3 Energy=            -514.826737
CBS-QB3 Enthalpy=          -514.825793 CBS-QB3 Free Energy=      -514.869004
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4(2)\CDNEEDHA\10-Oct-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save
geom=dihedral\TSb21 for beta scission of Species 5\0,2\C,0,-0.00681
45412,0.020560338,0.0254936134\H,0,0.0198408411,0.0848323489,1.1050326
822\H,0,0.9031131693,-0.2001825738,-0.5148474704\C,0,-1.1727300009,0.1
059785011,-0.6430687478\C,0,-1.8051149933,-2.0817072047,-0.9371561488\
F,0,-2.3039399032,0.4739520797,-0.0007247923\F,0,-3.0001723037,-2.1167
600369,-1.5234318109\F,0,-0.895902824,-2.6602050023,-1.7228566805\F,0,
-1.8517002964,-2.6975602679,0.2381179731\H,0,-1.2572017823,0.209250125
,-1.7186393992\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-513.18443
27\E2(CBS)/CbsB3=-1.5970537\CBS-Int/CbsB3=0.0426778\OIii/CbsB3=12.8234
431\MP2/CbsB4=-514.1633341\MP4(SDQ)/CbsB4=-514.2024326\MP4(SDQ)/6-31+G
(d')=-514.1780905\QCISD(T)/6-31+G(d')=-514.2133915\CBSQB3=-514.8343024
C21
Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                    0.046835 E(Thermal)=                0.054831
E(SCF)=                    -587.480027 DE(MP2)=                -1.628400
DE(CBS)=                   -0.182292 DE(MP34)=                -0.041634
DE(CCSD)=                  -0.040400 DE(Int)=                0.047836
DE(Empirical)=             -0.082830
CBS-QB3 (0 K)=              -589.360911 CBS-QB3 Energy=            -589.352916
CBS-QB3 Enthalpy=          -589.351972 CBS-QB3 Free Energy=      -589.394968
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4O1(3)\CDNEEDHA\15-Oct-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save
geom=dihedral\TSc21 beta scission of Species 7 to form Species 9 a
nd CF3\0,3\C,0,0.0353055905,-0.0129353509,0.0468373852\H,0,0.04093246
31,0.1328225734,1.1168440938\H,0,0.9492754273,-0.1157356586,-0.5186646
78\C,0,-1.2334798309,-0.0473120353,-0.6738091473\C,0,-1.6695750223,-1.
9399445078,-0.8478583802\F,0,-2.2963913139,0.270524696,0.1621609394\F,
0,-2.8572390083,-2.0806362214,-1.3964358117\F,0,-0.7296565264,-2.50263
22322,-1.5877834788\F,0,-1.6539376315,-2.4378381466,0.3795993604\O,0,-
1.3144871154,0.283468602,-1.8716942069\Version=ES64L-G09RevD.01\State
=3-A\HF/CbsB3=-587.480027\E2(CBS)/CbsB3=-1.8106923\CBS-Int/CbsB3=0.047
8363\OIii/CbsB3=14.0602561\MP2/CbsB4=-588.5867124\MP4(SDQ)/CbsB4=-588.
628346\MP4(SDQ)/6-31+G(d')=-588.6124375\QCISD(T)/6-31+G(d')=-588.65283

```

73\CBSQB3=-589.3609108\

C<sub>22</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.044952	E(Thermal)=	0.053545
E(SCF)=	-587.460903	DE(MP2)=	-1.636947
DE(CBS)=	-0.179504	DE(MP34)=	-0.037013
DE(CCSO)=	-0.037759	DE(Int)=	0.048002
DE(Empirical)=	-0.083046		
CBS-QB3 (0 K)=	-589.342217	CBS-QB3 Energy=	-589.333624
CBS-QB3 Enthalpy=	-589.332680	CBS-QB3 Free Energy=	-589.376877

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4O1(3)\CDNEEDHA\15-Oct-2014\0\  
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save  
geom=dihedral\TSc22 beta scission of Species 7 to form CF3CFO and  
CH2\0,3\C,0,0.2143229449,0.0410014161,0.1170178771\H,0,-0.0058728841,  
0.0028509735,1.1741555339\H,0,1.0296432917,-0.3171319369,-0.493497483\  
C,0,-1.6475702897,-0.1667662321,-0.9667670544\C,0,-1.7500540405,-1.712  
793384,-0.8853147445\F,0,-2.4299584814,0.3786697251,0.0070125347\F,0,-  
2.9248994599,-2.0880416433,-1.4158351782\F,0,-0.7665839107,-2.27927717  
06,-1.5895935674\F,0,-1.698684472,-2.1677341361,0.3728076851\O,0,-1.36  
37956343,0.4260045598,-1.9671127601\Version=ES64L-G09RevD.01\State=3-  
A\HF/CbsB3=-587.4609029\E2(CBS)/CbsB3=-1.8164507\CBS-Int/CbsB3=0.04800  
15\Oiii/CbsB3=14.1233587\MP2/CbsB4=-588.5771781\MP4(SDQ)/CbsB4=-588.61  
41915\MP4(SDQ)/6-31+G(d')=-588.5983504\QCISD(T)/6-31+G(d')=-588.636109  
1\CBSQB3=-589.3422175\

d<sub>11</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.058953	E(Thermal)=	0.066369
E(SCF)=	-588.043394	DE(MP2)=	-1.686398
DE(CBS)=	-0.185739	DE(MP34)=	-0.039591
DE(CCSO)=	-0.037455	DE(Int)=	0.050230
DE(Empirical)=	-0.085415		
CBS-QB3 (0 K)=	-589.968810	CBS-QB3 Energy=	-589.961394
CBS-QB3 Enthalpy=	-589.960450	CBS-QB3 Free Energy=	-590.002190

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\11-Dec-2014\0\  
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=save  
geom=dihedral\TS d11 for H-transfer of OH hydrogen to CF\0,2\C,0,  
-0.0588263739,-0.1138999071,0.0304732842\H,0,-0.0959286662,-0.18553814  
76,1.1194880035\C,0,1.3284256427,0.0774047754,-0.4926468667\C,0,1.8038  
513999,-0.7148738398,-1.6935860666\F,0,2.3156690971,0.2294000129,0.420  
4318111\F,0,2.9163155579,-0.1876580853,-2.2207828812\F,0,2.0780081057,  
-1.9906665301,-1.3480225508\F,0,0.8508137007,-0.7403714193,-2.63948955  
15\H,0,-0.6440074306,-0.9045079813,-0.4419886591\O,0,-0.413200638,1.20  
18082735,-0.4650483141\H,0,0.7879890823,1.2494447055,-0.877280386\Ver  
sion=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.0433945\E2(CBS)/CbsB3=-1  
.8721376\CBS-Int/CbsB3=0.0502303\Oiii/CbsB3=14.6638933\MP2/CbsB4=-589.  
2023549\MP4(SDQ)/CbsB4=-589.2419458\MP4(SDQ)/6-31+G(d')=-589.2118964\Q  
CISD(T)/6-31+G(d')=-589.2493514\CBSQB3=-589.9688104\

d<sub>12</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.058627	E(Thermal)=	0.066616
E(SCF)=	-588.027291	DE(MP2)=	-1.696279
DE(CBS)=	-0.185298	DE(MP34)=	-0.034384
DE(CCSO)=	-0.035293	DE(Int)=	0.050262
DE(Empirical)=	-0.085660		
CBS-QB3 (0 K)=	-589.955316	CBS-QB3 Energy=	-589.947327
CBS-QB3 Enthalpy=	-589.946383	CBS-QB3 Free Energy=	-589.989194

```

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\15-Dec-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=sa
ve geom=dihedral\TSd12 for Htransfer from CH2OH to CF\0,2\C,0,-0.046
011792,0.0417021353,0.1302727854\H,0,0.1036963307,0.5543270226,1.37058
46535\C,0,1.2215334788,0.012631151,0.8836604549\C,0,1.9566545986,-1.24
2594375,1.2403200758\F,0,2.0642566536,1.0373417467,0.5253933116\F,0,2.
8945553205,-1.0304342886,2.1747472852\F,0,1.0757447777,-2.1525053317,1
.7140454041\F,0,2.575142687,-1.8113070725,0.1736215389\H,0,-0.71442063
48,-0.8003115096,0.2500872705\O,0,-0.1636864214,0.7122731059,-1.053852
8547\H,0,0.6330577231,1.2437595261,-1.1824593582\Version=ES64L-G09Rev
D.01\State=2-A\HF/CbsB3=-588.0272908\E2(CBS)/CbsB3=-1.8815768\CBS-Int/
CbsB3=0.0502617\OIii/CbsB3=14.7017062\MP2/CbsB4=-589.1948925\MP4(SDQ)/
CbsB4=-589.2292765\MP4(SDQ)/6-31+G(d')=-589.1954933\QCISD(T)/6-31+G(d'
)=-589.2307865\CBSQB3=-589.9553158\

```

d<sub>21</sub>

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                      0.057742 E(Thermal)=                0.065056
E(SCF)=                      -588.061895 DE(MP2)=                -1.692631
DE(CBS)=                     -0.185720 DE(MP34)=                -0.036743
DE(CCSO)=                    -0.036573 DE(Int)=                0.050309
DE(Empirical)=              -0.085549
CBS-QB3 (0 K)=              -589.991060 CBS-QB3 Energy=          -589.983745
CBS-QB3 Enthalpy=          -589.982801 CBS-QB3 Free Energy=      -590.023661
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\11-Dec-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=sa
ve geom=dihedral\TS d21 for H-transfer of OH Hydrogen to CH3\0,2\C,0
,-0.0627464118,-0.1051257869,-0.0506011905\H,0,-0.1879015957,-0.170525
2194,1.0236481096\H,0,0.9342031585,-0.1499338992,-0.4755324097\C,0,-1.
0744006983,0.6635301609,-0.8409796972\C,0,-1.9912752187,1.6488019402,-
0.1045119292\F,0,-0.5446956614,1.3362716773,-1.9191827892\F,0,-3.01515
51645,2.0306860975,-0.8758398433\F,0,-2.4900422859,1.0748089975,1.0069
142211\F,0,-1.3077374271,2.7442116497,0.2690360803\O,0,-1.7361001922,-
0.5012750164,-1.2237943949\H,0,-0.8077737626,-1.1022095513,-0.61418174
39\Version=ES64L-G09RevD.01\State=2-A\HF/CbsB3=-588.0618952\E2(CBS)/C
bsB3=-1.8783516\CBS-Int/CbsB3=0.0503091\OIii/CbsB3=14.6852496\MP2/CbsB
4=-589.2275967\MP4(SDQ)/CbsB4=-589.2643395\MP4(SDQ)/6-31+G(d')=-589.23
37885\QCISD(T)/6-31+G(d')=-589.2703613\CBSQB3=-589.9910602\

```

d<sub>111</sub>

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                      0.059757 E(Thermal)=                0.068006
E(SCF)=                      -588.081035 DE(MP2)=                -1.662250
DE(CBS)=                     -0.183713 DE(MP34)=                -0.044193
DE(CCSO)=                    -0.040675 DE(Int)=                0.049343
DE(Empirical)=              -0.086904
CBS-QB3 (0 K)=              -589.989670 CBS-QB3 Energy=          -589.981421
CBS-QB3 Enthalpy=          -589.980477 CBS-QB3 Free Energy=      -590.024559
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\15-Dec-2014\0\
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=sa
ve geom=dihedral\TSd111 for beta-scission from species 13\0,2\C,0,-0
.1350376675,-0.0277123846,0.0286937793\H,0,-0.0022455185,0.0392092065,
1.1240601486\C,0,1.9787877925,0.0319229037,-0.2439836303\C,0,2.5060037
12,-1.3050182361,0.2117400858\F,0,2.3910771155,1.0385588642,0.52805001
42\F,0,3.8532053827,-1.3348308126,0.1786676048\F,0,2.1250215185,-1.593
4936344,1.4669612856\F,0,2.0500428097,-2.2712872012,-0.6057837711\H,0,
-0.2111940543,-1.0541823981,-0.3769141256\O,0,-0.518027079,0.944472128
,-0.6298605842\H,0,2.0197695592,0.2431777001,-1.3070777196\Version=ES
64L-G09RevD.01\State=2-A\HF/CbsB3=-588.0810347\E2(CBS)/CbsB3=-1.845962

```

9\CBS-Int/CbsB3=0.0493426\OIii/CbsB3=14.6867404\MP2/CbsB4=-589.2177336  
\MP4 (SDQ) /CbsB4=-589.2619261\MP4 (SDQ) /6-31+G(d')=-589.2372275\QCISD(T)  
/6-31+G(d')=-589.2779023\CBSQB3=-589.9896697\

d<sub>121</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.060558	E(Thermal)=	0.069261
E(SCF)=	-588.063342	DE(MP2)=	-1.672432
DE(CBS)=	-0.184286	DE(MP34)=	-0.038344
DE(CCSO)=	-0.039646	DE(Int)=	0.049424
DE(Empirical)=	-0.086853		
CBS-QB3 (0 K)=	-589.974919	CBS-QB3 Energy=	-589.966216
CBS-QB3 Enthalpy=	-589.965272	CBS-QB3 Free Energy=	-590.010907

1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H3F4O1(2)\CDNEEDHA\15-Dec-2014\0\  
\#p opt=(calcall,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=sa  
ve geom=dihedral\TSd121 for beta-scission of species 14\0,2\C,0,0.03  
32020072,0.2390107515,0.0345780458\H,0,-0.045184502,0.2493771765,1.113  
8133175\C,0,1.2218391528,0.4068026181,-0.5861706434\C,0,1.6609062958,-  
1.8449603668,-1.2968643218\F,0,2.3096124909,0.708016252,0.156537342\F,  
0,2.8064936515,-2.0306454014,-1.953073711\F,0,1.5407136524,-2.74662813  
88,-0.3266961982\F,0,0.6318224936,-1.9902498141,-2.1636943918\O,0,-1.1  
313887418,-0.0476939877,-0.5888295783\H,0,1.3442995746,0.6137573655,-1  
.641868368\H,0,-0.9698432518,-0.2421357802,-1.5207287951\Version=ES64  
L-G09RevD.01\State=2-A\HF/CbsB3=-588.0633416\E2(CBS)/CbsB3=-1.8567181\  
CBS-Int/CbsB3=0.0494242\OIii/CbsB3=14.6457653\MP2/CbsB4=-589.2081726\MP  
P4(SDQ)/CbsB4=-589.2465164\MP4(SDQ)/6-31+G(d')=-589.2147059\QCISD(T)/6  
-31+G(d')=-589.2543515\CBSQB3=-589.9749193\

u<sub>2</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.038815	E(Thermal)=	0.046720
E(SCF)=	-512.418156	DE(MP2)=	-1.499951
DE(CBS)=	-0.161480	DE(MP34)=	-0.018689
DE(CCSO)=	-0.035860	DE(Int)=	0.044754
DE(Empirical)=	-0.073083		
CBS-QB3 (0 K)=	-514.123650	CBS-QB3 Energy=	-514.115744
CBS-QB3 Enthalpy=	-514.114800	CBS-QB3 Free Energy=	-514.156612

1\1\GINC-BL1\Mixed\CBS-QB3\CBS-QB3\C3H2F4\CDNEEDHA\28-Aug-2014\0\#p o  
pt=(calcall,tight,qst3,noeigentest) freq=hinderedrotor cbs-qb3 guess=s  
ave geom=dihedral\TS CBS-QB3 u2 HFO-1234yf -> HCCF + CHF3 QST3\0,1\C  
,0,0.0631310678,0.0019015103,-0.0577111779\H,0,-0.2966163454,-0.000241  
3688,1.3702448904\H,0,0.8737155367,0.0025210786,-0.7527615138\C,0,-1.0  
783013317,0.0018411776,0.4335956519\C,0,-1.3610104164,-0.0015474541,2.  
5790363478\F,0,-2.3896405734,0.002976899,0.2747748808\F,0,-2.078104911  
7,1.0865656624,2.8820794223\F,0,-2.0795527647,-1.0897096866,2.87845154  
99\F,0,-0.2494618482,-0.0035972142,3.3649253972\Version=ES64L-G09RevD  
.01\State=1-A\HF/CbsB3=-512.4181555\E2(CBS)/CbsB3=-1.661431\CBS-Int/Cb  
sB3=0.0447545\OIii/CbsB3=12.6222438\MP2/CbsB4=-513.4555099\MP4(SDQ)/Cb  
sB4=-513.4741991\MP4(SDQ)/6-31+G(d')=-513.4523536\QCISD(T)/6-31+G(d')=  
-513.4882138\CBSQB3=-514.1236495\

u<sub>3</sub>

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.040339	E(Thermal)=	0.047157
E(SCF)=	-512.519436	DE(MP2)=	-1.482198
DE(CBS)=	-0.159803	DE(MP34)=	-0.023236
DE(CCSO)=	-0.032828	DE(Int)=	0.044094
DE(Empirical)=	-0.073648		
CBS-QB3 (0 K)=	-514.206716	CBS-QB3 Energy=	-514.199898



```

CBS-QB3 Enthalpy=          -514.198954 CBS-QB3 Free Energy=          -514.238147
1\1\GINC-BL0\Mixed\CBS-QB3\CBS-QB3\C3H2F4\CDNEEDHA\27-Aug-2014\0\#\#p o
pt=(calcall,tight,qst3,noeigentest) freq cbs-qb3 guess=save geom=dihed
ral\TS u3 HFO-1234yf -> HF + CF3CCH CBSQB3 QST3\0,1\C,0,-0.014058563
,0.0009133021,-0.0044651942\H,0,0.0159590415,-0.0003984176,1.067886064
8\H,0,0.8088450704,0.0044328292,-1.1321203082\C,0,-0.8144302994,0.0001
552592,-0.9690656927\C,0,-2.0690928035,-0.0019601734,-1.7654542951\F,0
,0.4379662309,0.0049969611,-2.2874068122\F,0,-2.1823304202,1.082555806
3,-2.5371114464\F,0,-2.1769131002,-1.0850499939,-2.5398858123\F,0,-3.0
936869567,-0.0056445689,-0.8880317687\Version=ES64L-G09RevD.01\State=
1-A\HF/CbsB3=-512.5194363\E2(CBS)/CbsB3=-1.6420007\CBS-Int/CbsB3=0.044
0941\OIII/CbsB3=12.7199259\MP2/CbsB4=-513.5431075\MP4(SDQ)/CbsB4=-513.
566344\MP4(SDQ)/6-31+G(d')=-513.5423407\QCISD(T)/6-31+G(d')=-513.57516
83\CBSQB3=-514.2067162\

```

### B.3 PMMA/TMA

PMMA

```

1\1\GINC-MRBUN\Freq\UB3LYP\6-31++G(d,p)\C6H12O2\CDNEEDHA\06-May-2014\0
\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31++G(d,p)
Freq\PMMA IR Spectrum Calc ++\0,1\C,-0.2994681172,-0.0540098949,-0.1
450307776\H,-0.3125417273,-0.2009177489,0.940613657\H,0.725793187,-0.2
208968971,-0.4933609916\H,-0.9459800535,-0.8075045744,-0.6023452027\C,
-0.7459631422,1.3780277407,-0.5208873584\C,0.1913579314,2.409784002,0.
1269834033\H,1.2133963039,2.2546486396,-0.2347759342\H,-0.1121559345,3
.4313491618,-0.1180547456\H,0.1912008617,2.3177780698,1.2166056094\C,-
0.7339952392,1.5423084944,-2.0584576107\H,-1.3874117111,0.8126663531,-
2.5437556666\H,-1.0596187258,2.5463719601,-2.352077626\H,0.2849896544,
1.3974028684,-2.4339791317\C,-2.1721282386,1.607888724,-0.0048765993\O
,-2.5087460812,2.4648190058,0.7881686968\O,-3.0519743039,0.7277340675,
-0.5409200536\C,-4.4204345634,0.8650318519,-0.115119566\H,-4.805049623
2,1.8533915145,-0.3783249462\H,-4.9685118595,0.0852629161,-0.643678446
9\H,-4.4997144996,0.7274486901,0.9660203037\Version=AM64L-G09RevB.01\
State=1-A\HF=-386.3609887\S2=0.\S2-1=0.\S2A=0.\RMSD=4.233e-09\RMSF=2.0
76e-06\ZeroPoint=0.1741855\Thermal=0.1842297\

```

PMMA-TMA Coordinated

```

1\1\GINC-MRBUN\Freq\UB3LYP\6-311++G(d,p)\C9H21Al1O2\CDNEEDHA\23-May-20
14\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-311++G(
d,p) Freq\PMMA TMA optimization 6311+.log start\0,1\C,0.0010567469
,0.0071319857,0.0120252354\H,0.0126795383,0.0249283623,1.1024604217\H,
1.0341648977,0.0062483674,-0.344520778\H,-0.4658142683,-0.9263987527,-
0.3139493518\C,-0.7342593009,1.2347766404,-0.5694493802\C,-0.072612307
5,2.5364712473,-0.055793278\H,0.9636848126,2.5718671788,-0.4012611329\
H,-0.5851922855,3.4217198633,-0.4417563462\H,-0.0734797055,2.581086031
8,1.0346622415\C,-0.7036568178,1.1958473585,-2.1044155113\H,-1.1754360
651,0.2900718746,-2.4907799295\H,-1.2219637745,2.0511347172,-2.5401557
585\H,0.3347494609,1.2118180657,-2.4444100538\C,-2.1828274667,1.231237
5698,-0.0883850314\O,-3.150272183,1.3329424335,-0.8318735926\O,-2.2989
426337,1.1256622345,1.2257981231\C,-3.6302497911,1.1361556419,1.801667
4098\H,-4.2133662668,0.3046061005,1.4082312917\H,-3.4738501754,1.02657
2915,2.871482463\H,-4.1273870293,2.0783224773,1.5759078643\Al,-4.98494
75708,1.4633466675,-1.7094189164\C,-5.7612516456,3.0160513247,-0.72893
21883\C,-5.69303288,-0.3470163376,-1.2738311644\C,-4.4758864027,1.7935
14164,-3.5998657954\H,-5.0785205966,3.8743813737,-0.6860544654\H,-6.66
33265833,3.3727422815,-1.2430385383\H,-6.0673965151,2.7887026805,0.299

```

7667381\H,-6.6353726085,-0.525896042,-1.8079338084\H,-5.011721078,-1.1507447759,-1.5799642854\H,-5.9143225735,-0.4949561342,-0.20916386\H,-3.8816355,0.9782321589,-4.0298803981\H,-5.3665133041,1.8959507593,-4.2334770903\H,-3.8992629757,2.7180859404,-3.7271149189\Version=AM64L-G09 RevB.01\State=1-A\HF=-748.7209109\S2=0.\S2-1=0.\S2A=0.\RMSD=1.920e-09\RMSF=3.439e-06\ZeroPoint=0.2809798\Thermal=0.3007393\

Product A

1\1\GINC-N3I1-5\Freq\UB3LYP\6-311++G(d,p)\C9H21A11O2\ROOT\11-Jun-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-311++G(d,p) Freq\PMMA-TMA 4-center product\0,1\C,-0.1542127798,0.0675937417,-0.1005480096\C,0.354676591,-0.0882993777,1.3463087516\H,1.4407841,0.0429148982,1.3684964785\H,-0.0919027514,0.659030065,2.0039392675\H,0.140752936,-1.0796300952,1.7550476858\C,0.4729144353,-1.0325105225,-0.9782879393\H,0.2578767175,-2.037312464,-0.6050379958\H,0.1226549393,-0.9628082297,-2.0103666624\H,1.5605042393,-0.9171115416,-0.9864729383\C,0.2924276413,1.4405072539,-0.6412200023\H,-0.0462931595,1.5851313118,-1.6683699484\H,-0.106608181,2.2521679521,-0.0318466221\H,1.3847677858,1.5036354081,-0.6274149332\C,-1.7248898357,-0.0205187656,-0.1549908944\O,-2.1712269801,1.0665355731,0.6664852109\O,-2.1399605571,0.1827189479,-1.476215802\Al,-3.2814959258,-0.0871227268,-2.7293189394\C,-4.8252939967,-1.2693682735,-2.4531891394\H,-5.4931459015,-0.8867292564,-1.6729189897\H,-5.420488937,-1.3826969298,-3.3646177793\H,-4.5161937319,-2.2705200986,-2.133175953\C,-2.9015083962,0.8331142417,-4.4132956904\H,-2.491504058,0.1343384144,-5.152856558\H,-3.8074682979,1.2573861738,-4.8594140806\H,-2.172837132,1.638197347,-4.2880512144\C,-3.554987101,1.3479816543,0.7080278318\H,-3.9572966451,1.5833692351,-0.2853871388\H,-4.1422518007,0.5322871579,1.1466492642\H,-3.6663655398,2.2314599033,1.3378518454\C,-2.2884440425,-1.3473826256,0.3774858244\H,-1.9037393916,-2.1884540894,-0.2004560198\H,-2.0290612277,-1.4932274605,1.4265811391\H,-3.3762529455,-1.3599963327,0.2899134625\Version=EM64L-G09RevA.02\State=1-A\HF=-748.7248568\S2=0.\S2-1=0.\S2A=0.\RMSD=4.586e-10\RMSF=3.506e-06\ZeroPoint=0.2842693\Thermal=0.3027782\

Product B

1\1\GINC-MRBUN\Freq\UB3LYP\6-311++G(d,p)\C7H15A11O2\CDNEEDHA\07-May-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-311++G(d,p) Freq\PMMA-TMA 6-center product\0,1\C,-0.1035234533,-0.134960196,-0.1197769169\C,-0.2168987972,-0.0827925898,1.4208310559\H,0.7802229437,0.031727563,1.853958971\H,-0.8343881659,0.7578247309,1.7411355058\H,-0.6531363676,-1.0034406865,1.8180034982\C,0.75012167,-1.3343791627,-0.5568605369\H,0.3243212381,-2.2762785868,-0.2054659297\H,0.8306971505,-1.3916018366,-1.6441472556\H,1.7568211633,-1.2359372555,-0.1419963842\C,0.508805288,1.1850592556,-0.6409717955\H,0.5960089542,1.1788831705,-1.7309258147\H,-0.0989776176,2.042646447,-0.3482766793\H,1.511427325,1.3092022373,-0.2234746538\C,-1.5081195819,-0.2470233958,-0.6830563344\O,-2.3935355692,0.6465137677,-0.4453465997\O,-1.8873414574,-1.2215839928,-1.4156870048\Al,-3.6499749244,-0.3822723742,-1.520063971\C,-4.984068641,-1.3137946833,-0.4302618926\H,-5.8225088317,-0.6559218151,-0.1743937343\H,-5.4099573016,-2.1709952387,-0.9641387626\H,-4.5679069671,-1.6901550015,0.5096506856\C,-3.9847590769,0.4317374816,-3.2694960906\H,-4.3437620728,-0.3083482717,-3.9937808559\H,-4.7544194517,1.2096681425,-3.2087156648\H,-3.0882222053,0.8942778519,-3.694408836\Version=AM64L-G09RevB.01\State=1-A\HF=-668.9352877\S2=0.\S2-1=0.\S2A=0.\RMSD=4.867e-09\RMSF=2.599e-07\ZeroPoint=0.2071992\Thermal=0.2216925\

Product C

1\1\GINC-BL1\Freq\UB3LYP\6-31++G(d,p)\C13H27A11O4\CDNEEDHA\25-Aug-2014\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31++G(d,p)

) Freq\2 Pendant Group unconnected PMMA Product\0,1\C,-0.053337682,0.4959631274,0.1087633709\C,-0.7526300312,1.2660805058,1.2474178172\H,-0.0343871874,1.9327259426,1.7371010085\H,-1.5833184379,1.8634682917,0.8646932344\H,-1.1488565732,0.5803269631,2.0041100146\C,1.0924478888,-0.3659724908,0.6653222429\H,0.7237105121,-1.0985382186,1.3905383483\H,1.6059352251,-0.9109959349,-0.1309204741\H,1.8222652237,0.2749527869,1.1721194639\C,0.4980778814,1.4995976705,-0.9353898448\H,0.9916733248,0.980713786,-1.7640267255\H,-0.3039563182,2.1208644103,-1.3443379724\H,1.2351843359,2.1550923193,-0.458603833\C,-1.083605273,-0.3667396702,-0.6150261742\O,-2.2431651984,0.0496480808,-0.87926552\O,-0.79080311,-1.5600685039,-1.0259512112\A1,-2.5382423699,-1.8269848426,-1.8166534378\C,-2.7654662973,-1.2064599452,-3.6803233947\H,-3.2484772337,-1.9580222117,-4.3182225749\H,-3.381672509,-0.2993513181,-3.7176668044\H,-1.8043856267,-0.9568392882,-4.1506907933\C,-3.9261222792,-2.5687712517,-0.6192528994\H,-4.5929845553,-1.7802502079,-0.2493151899\H,-4.552063186,-3.3165465129,-1.1239548521\H,-3.4897699033,-3.0587384355,0.2621857678\C,0.2637480069,-4.9172738869,-2.3524081948\C,0.8203321354,-6.263026212,-2.8499466838\H,1.8859270146,-6.3183477971,-2.604619578\H,0.3183946702,-7.1113450793,-2.3765856267\H,0.7159973051,-6.3701616471,-3.9335949613\C,1.0112405926,-3.7475861359,-3.0354813371\H,0.8965521424,-3.7838300315,-4.1244686264\H,0.6488729756,-2.7841361153,-2.6722588131\H,2.0792561237,-3.8265483667,-2.8073492772\C,0.4234082988,-4.8117873483,-0.8151727273\H,0.0570432871,-3.8509494664,-0.4480610807\H,-0.1122076284,-5.6192452658,-0.3037110529\H,1.4849321025,-4.8998045232,-0.5612050579\C,-1.2245921131,-4.7606645395,-2.6609117138\O,-1.8843565725,-3.7524306387,-2.4209967846\O,-1.7914917883,-5.8292528621,-3.2195201258\C,-3.2058738124,-5.7451871642,-3.5192124931\H,-3.7728812329,-5.5640815328,-2.604379342\H,-3.3903286275,-4.9383823859,-4.2308543449\H,-3.4604669449,-6.7114766782,-3.9517047589\Version=ES64L-G09RevD.01\State=1-A\HF=-1055.1920503\S2=0.\S2-1=0.\S2A=0.\RMSD=3.231e-09\RMSF=1.759e-06\ZeroPoint=0.838035\Thermal=0.4099797\

## APPENDIX C. RELEVANT PRIME DATA

### C.1 QoIs

Table B.1: Experimental shock-tube ignition-delay QoIs.

<i>Equiv ratio <math>\phi</math></i>	<i>P(atm)</i>	<i>T(K)</i>	<i><math>\tau</math> (ms)</i>	<i>Uncertainty Bounds of <math>\tau</math></i>		<i>PRIME ID</i>	<i>Ref.</i>
0.17	0.32	2007	0.0426	0.0201	0.0903	a00000451*	[126]
		1768	0.0756	0.0365	0.1565	a00000452*	
		1580	0.1341	0.0637	0.2825	a00000453*	
0.50	0.34	2224	0.0662	0.0460	0.0951	a00000448*	[126]
		1969	0.1063	0.0750	0.1507	a00000449*	
		1767	0.1709	0.1184	0.2466	a00000450*	
1.50	0.33	2090	0.0461	0.0276	0.0768	a00000445*	[126]
		1838	0.0829	0.0511	0.1346	a00000446*	
		1640	0.1493	0.0912	0.2444	a00000447*	
0.39	2.18	1412	0.1392	0.0840	0.2306	a00000382*	[127]
		1318	0.2096	0.1280	0.3433	a00000383*	
		1237	0.3157	0.1916	0.5201	a00000384*	
0.75	2.10	1311	0.2494	0.1131	0.5500	a00000385	[127]
		1266	0.3113	0.1423	0.6808	a00000386*	
		1223	0.3885	0.1740	0.8676	a00000387*	
1.00	2.04	1299	0.3125	0.1338	0.7296	a00000454*	[127]
		1257	0.3659	0.1626	0.8234	a00000455*	
		1218	0.4284	0.1916	0.9579	a00000456*	
1.00	1.94	1454	0.0273	0.0192	0.0390	a00000370*	[128]
		1269	0.0616	0.0438	0.0866	a00000371*	
		1126	0.1386	0.0988	0.1946	a00000372*	
1.00	0.71	1352	0.0498	0.0308	0.0806	a00000373	[129]
		1180	0.0992	0.0621	0.1585	a00000374	
		1047	0.1977	0.1234	0.3168	a00000375	
1.00	1.45	1161	0.2021	0.0880	0.4637	a00000460*	[130]
		1027	0.4783	0.2087	1.0961	a00000461*	
		921	1.1324	0.4753	2.6977	a00000462*	
1.00	2.35	1023	0.2167	0.0997	0.4711	a00000463*	[130]
		974	0.4857	0.2323	1.0156	a00000464	
		930	1.0888	0.5212	2.2747	a00000465	
0.50	1.05	999	1.0014	0.7424	1.3508	a00000388	[131]
		972	1.4996	1.1135	2.0195	a00000389	

Table B.1 Continued

		947	2.2456	1.6521	3.0525	a00000390	
0.50	3.99	1015	0.7533	0.4799	1.1826	a00000391	
		995	1.4457	0.9244	2.2609	a00000392*	[131]
		976	2.7743	1.7571	4.3804	a00000393*	
0.50	15.86	1093	0.8912	0.7036	1.1288	a00000394	
		1067	1.5758	1.2490	1.9882	a00000395	[131]
		1042	2.7864	2.1811	3.5596	a00000396	
1.00	1.01	1411	0.1112	0.0760	0.1628	a00000415*	
		1197	0.2988	0.2062	0.4329	a00000416	[131]
		1039	0.8025	0.5445	1.1829	a00000417	
1.00	3.96	1103	0.1333	0.0563	0.3153	a00000418	
		1052	0.3919	0.1708	0.8992	a00000419	[131]
		1005	1.1528	0.4936	2.6926	a00000420	
1.00	16.39	1174	0.0505	0.0359	0.0711	a00000421	
		1115	0.2506	0.1786	0.3517	a00000422	[131]
		1063	1.2436	0.8793	1.7590	a00000423*	
0.10	3.69	1221	0.0739	0.0204	0.2675	a00000439*	
		1108	0.3037	0.0866	1.0650	a00000440	[132]
		1014	1.2486	0.3554	4.3863	a00000441*	
0.10	1.01	1372	0.0410	0.0300	0.0560	a00000427	
		1162	0.1455	0.1085	0.1950	a00000428	[132]
		1007	0.5158	0.3859	0.6894	a00000429	
0.10	4.17	1074	0.1147	0.0471	0.2792	a00000430	
		1022	0.4968	0.2112	1.1687	a00000431*	[132]
		975	2.1530	0.9012	5.1438	a00000432*	
0.10	17.78	1113	0.3755	0.1473	0.9572	a00000433*	
		1055	1.0493	0.4138	2.6609	a00000434	[132]
		1003	2.9324	1.1114	7.7368	a00000435	
0.10	0.94	1608	0.0810	0.0279	0.2350	a00000436	
		1299	0.2626	0.0930	0.7416	a00000437*	[132]
		1090	0.8520	0.3000	2.4195	a00000438	
0.10	16.31	1192	0.1241	0.0579	0.2660	a00000442	
		1136	0.5109	0.2456	1.0629	a00000443*	[132]
		1084	2.1028	1.0091	4.3820	a00000444*	
0.50	0.99	1534	0.0811	0.0509	0.1292	a00000397	
		1262	0.2668	0.1709	0.4167	a00000398	[132]
		1072	0.8779	0.5654	1.3630	a00000399	
0.50	4.08	1183	0.0939	0.0417	0.2116	a00000400	
		1118	0.3172	0.1446	0.6960	a00000401*	[132]

Table B.1 Continued

		1059	1.0718	0.4861	2.3631	a00000402*	
		1192	0.1853	0.1101	0.3117	a00000403	
0.50	15.57	1144	0.5729	0.3427	0.9576	a00000404	[132]
		1101	1.7710	1.0402	3.0153	a00000405	
		1623	0.0849	0.0280	0.2577	a00000406*	
3.99	1.06	1308	0.2522	0.0883	0.7208	a00000407	[132]
		1096	0.7491	0.2651	2.1165	a00000408	
		1297	0.0565	0.0136	0.2351	a00000409	
3.99	3.98	1164	0.1954	0.0483	0.7897	a00000410	[132]
		1057	0.6756	0.1623	2.8127	a00000411*	
		1143	0.1697	0.0979	0.2941	a00000412	
3.99	14.87	1069	0.7237	0.4231	1.2381	a00000413	[132]
		1004	3.0870	1.7975	5.3016	a00000414	
		1009	0.2344	0.1048	0.5244	a00000457	
0.42	3.28	972	0.8252	0.3762	1.8102	a00000458*	[133]
		938	2.9051	1.2947	6.5184	a00000459*	
		1062	0.3217	0.1535	0.6742	a00000376	
1.00	3.56	1012	1.0194	0.4931	2.1072	a00000377*	[133]
		966	3.2307	1.5479	6.7428	a00000378*	
		1296	0.2278	0.1284	0.4041	a00000466	
1.00	1.00	1184	0.3902	0.2287	0.6657	a00000467	[134]
		1089	0.6685	0.3927	1.1379	a00000468	
		1564	0.1707	0.1630	0.1787	a00000472	
1.03	1.00	1411	0.3018	0.2893	0.3149	a00000473	[134]
		1286	0.5337	0.5118	0.5566	a00000474*	
		1386	0.1634	0.1407	0.1898	a00000469*	
1.47	1.00	1280	0.2403	0.2089	0.2763	a00000470*	[134]
		1190	0.3532	0.3071	0.4062	a00000471*	
		1270	0.0263	0.0230	0.0300	a00000361	
1.00	33.00	1242	0.0592	0.0519	0.0676	a00000362	[135]
		1215	0.1337	0.1168	0.1529	a00000363	
		1714	0.0235	0.0176	0.0315	a00000364	
1.00	64.00	1578	0.0423	0.0320	0.0558	a00000365	[135]
		1461	0.0760	0.0569	0.1013	a00000366	
		1327	0.1031	0.0866	0.1226	a00000367	
1.00	64.00	1311	0.1438	0.1220	0.1695	a00000368*	[135]
		1295	0.2007	0.1695	0.2376	a00000369*	
		1566	0.0668	0.0283	0.1576	a00000424	
0.25	1.32	1365	0.1137	0.0502	0.2575	a00000425	[136]

Table B.1 Continued

		1210	0.1933	0.0856	0.4366	a00000426*	
		1045	0.5000	0.3152	0.7931	a00000379	
2.00	5.00	1016	1.3800	0.8768	2.1720	a00000380	[137]
		990	3.8100	2.3867	6.0823	a00000381	

\*Indicates target was not included in final, reduced dataset

Table B.2: Experimental flame-speed QOIs.

<i>Equiv ratio <math>\phi</math></i>	<i>P</i> ( <i>atm</i> )	<i>Flame speed</i> ( <i>ms</i> )	<i>PrIMe ID</i>	<i>Ref.</i>
0.6	1	81.88	a00000476	
0.85	10	45.3	a00000483	
0.85	15	26.9	a00000482	
0.85	20	18.35	a00000481	
1.5	20	80.9	a00000479	[138]
1.65	1	280.21	a00000477	
2	20	64.05	a00000480	
4	1	165.29	a00000478	
2.5	15	28.7	a00000484	
2.5	25	27.7	a00000485	[139]