ABSTRACT

SCHILTZ, HOLLY KRISTINE. Promoting Visualization Skills through Deconstruction Using Physical Models and a Visualization Activity Intervention. (Under the direction of Maria T. Oliver-Hoyo.)

Visualization skills are important in learning chemistry, as these skills have been shown to correlate to high ability in problem solving. Students' understanding of visual information and their problem-solving processes may only ever be accessed indirectly: verbalization, gestures, drawings, etc. In this research, deconstruction of complex visual concepts was aligned with the promotion of students' verbalization of visualized ideas to teach students to solve complex visual tasks independently. All instructional tools and teaching methods were developed in accordance with the principles of the theoretical framework, the Modeling Theory of Learning: deconstruction of visual representations into model components, comparisons to reality, and recognition of students' their problem-solving strategies.

Three physical model systems were designed to provide students with visual and tangible representations of chemical concepts. The Permanent Reflection Plane Demonstration provided visual indicators that students used to support or invalidate the presence of a reflection plane. The 3-D Coordinate Axis system provided an environment that allowed students to visualize and physically enact symmetry operations in a relevant molecular context. The Proper Rotation Axis system was designed to provide a physical and visual frame of reference to showcase multiple symmetry elements that students must identify in a molecular model.

Focus groups of students taking Inorganic chemistry working with the physical model systems demonstrated difficulty documenting and verbalizing processes and descriptions of visual concepts. Frequently asked student questions were classified, but students also interacted with visual information through gestures and model manipulations. In an effort to characterize how much students used visualization during lecture or recitation, we developed observation rubrics to gather information about students' visualization artifacts and examined the effect instructors' modeled visualization artifacts had on students. No patterns emerged from the passive observation of visualization artifacts in lecture or recitation, but the need to elicit visual information from students was made clear.

Deconstruction proved to be a valuable method for instruction and assessment of visual information. Three strategies for using deconstruction in teaching were distilled from the lessons and observations of the student focus groups: begin with observations of what is given in an image and what it's composed of, identify the relationships between components to find additional operations in different environments about the molecule, and deconstructing steps of challenging questions can reveal mistakes.

An intervention was developed to teach students to use deconstruction and verbalization to analyze complex visualization tasks and employ the principles of the theoretical framework. The activities were scaffolded to introduce increasingly challenging concepts to students, but also support them as they learned visually demanding chemistry concepts. Several themes were observed in the analysis of the visualization activities. Students used deconstruction by documenting which parts of the images were useful for interpretation of the visual. Students identified valid patterns and rules within the images, which signified understanding of arrangement of information presented in the representation. Successful strategy communication was identified when students documented personal strategies that allowed them to complete the activity tasks. Finally, students demonstrated the ability to extend symmetry skills to advanced applications they had not previously seen. This work shows how the use of deconstruction and verbalization may have a great impact on how students master difficult topics and combined, they offer students a powerful strategy to approach visually demanding chemistry problems and to the instructor a unique insight to mentally constructed strategies.

Promoting Visualization Skills through Deconstruction Using Physical Models and a Visualization Activity Intervention

by
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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

Chemistry

Raleigh, North Carolina

2013

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DEDICATION

To my parents, Rod and Karen, for showing such love and pride for everything I've accomplished and to my husband, Vic, for being my home and supporting me in ways I didn't know I needed.

BIOGRAPHY

Holly Kristine Schiltz was born March 20, 1984 to Rod and Karen and grew up in Elkhorn, NE with her sister, Morgan. The Schiltz family was always in the company of an assortment of pets and Holly got her first job at Petco and shadowed veterinarians for each career activity Elkhorn High School offered. Holly always did well in school, graduating 4^{th} in class. Chemistry, physics, and biology were most exciting because they explained so much about the world and the classes just made sense. When faced with the inevitability of making life and death decisions, she was turned away from veterinary medicine. Her success in chemistry and the availability of scholarships for women in chemistry paved the way for her chosen field.

She accepted admission to Iowa State University majoring in Chemistry and minoring in Philosophy. While at ISU, she got involved with the Society of Chemistry Undergraduate Majors (SCUM) where the group performed chemistry demonstrations for schools, boy scouts, and groups visiting the university. During her time at ISU, Holly met Vic Vijayakumar, who would later become her husband. Holly worked in the lab of Dr. Robert Angelici to extract methyl linolenate from FAMEs mixtures, taught several recitations and labs for the chemistry department, and found how much she loved teaching and talking to students about chemistry. With Dr. Angelici's advice, she pursued graduate school at the University of North Carolina at Chapel Hill to study inorganic chemistry and explore the country outside of the Midwest. She graduated with distinction with an ACS certified Bachelor of Science degree in May 2006.

At UNC-Chapel Hill, Holly joined the research group of Dr. Mike Gagné to work on templating dynamic combinatorial libraries with metal ions under the direction of Dr. Mee-Kyung Chung. Unfortunately, the project was not for Holly and she favored her time tutoring high school and undergraduate students in the evenings to her research. Holly won a GAANN scholarship for her second year to enrich her time at UNC with teaching experience, but still sought direction from a former professor at ISU, Dr. Tom Greenbowe. He recommended speaking with Dr. Maria Oliver-Hoyo at North Carolina State University. After speaking with Maria, Holly applied and was accepted to NCSU. She left UNC-Chapel Hill with her Master of Science degree with an emphasis in Inorganic Chemistry in 2008.

Holly joined the Oliver-Hoyo group at NCSU the following fall and conducted the research presented in this dissertation. Holly was lucky to work as a TA for Maria's SCALE-UP general chemistry class and for the inorganic chemistry classes of Dr. Jim Martin and Dr. Walter Weare. During her time in Raleigh, she got engaged and married, bought a house and raised a small flock of chickens, became a godmother, and drove back to Nebraska with Vic and her dogs each Christmas. Under Maria's direction, she learned what it meant to design a research project and evaluate her own work with an objective view. After obtaining her Doctor of Philosophy, Holly will seek teaching opportunities where she can utilize her research knowledge to enhance her teaching methods and make chemistry as enlightening for students as it was for her.

ACKNOWLEDGMENTS

First and foremost, I want to thank Dr. Maria Oliver-Hoyo, my advisor, for everything she has done for me during my time at NC State. She supported my ideas through my own doubt and helped to shape my work into something I am very proud of. I did not know research until watching, listening, and discussing with Maria. I can’t express enough gratitude for advice you’ve offered as a researcher, teacher, and a friend. Maria, you will always be my most valued mentor.

I thank Drs. Bob Beichner, Reza Ghiladi, Jim Martin, and Jerry Whitten for serving on my committee, for their advice during my prelim, and offering advice and guidance when I needed it. My project never would have started if it weren’t for the suggestions of Drs. Ghiladi and Martin. Thank you for giving me access to your students to ask them questions and to teach them about symmetry. I also want to thank Dr. Martin and Dr. Walter Weare for taking me on as a TA. Inorganic has been my favorite class to teach. Jim, I learned so much from discussing the course with you and watching you teach. Discussing the course with you improved my teaching skills and taught me much about inorganic chemistry. Walter, thank you for giving me so much freedom with the intervention.

I thank the Oliver-Hoyo group members of the past: Deborah Bromfield-Lee and Caroline Christian. Thank you for making me feel so welcome in the group, answering my questions, and taking me seriously so early on. For their assistance with my research, I thank Marc Muñiz, Joan Roque-Peña, and Lavanya Rao. Marc and Joan observed my Friday recitations and collected data for an entire semester. Lavanya helped analyze the complex visualization activities for valid deconstruction statements and assisted with all the nuts and bolts that went into producing a weekly activity. It’s been a pleasure to have your help and be your mentor.

I thank my parents and sister for always helping me keep things in perspective. I love you all so much! Morgan, thank you for being such a wonderful person and so very different from me. You’ve taught me to always consider how other people see the world. Mom and Dad, thank you for always supporting me and showing me that you can do anything. There is always a way and you’ve modeled that for me my whole life. I will always do what I can to deserve your love and pride.

I would never have made it through graduate school without my beloved network friends and family. My lab mates, Marc Muñiz and Sorángel Rodríguez-Velásquez, belong in this section. Marc, you are a genius and your generosity with your knowledge knows no boundaries. Sorángel, I couldn’t have had a sweeter or more fun companion for the hurdles of grad school, conferences, and everyday research. Cynthia Bunders, I love you so much and I’m so glad to have reunited with you at NCSU and fully assimilated you into my animal house. I truly wouldn’t have made it through grad school without you. Thanks to Steve Andrews, Elise Traversa, Jessica Byers, Vishaka Krishnan, Mike Keating, and especially Christi Keating for your friendship. I hope you all know how much you mean to me. I owe my sanity to you! Finally, thanks to my husband, Vic. You are such a good and great man. It’s overwhelming to think how fortunate I am to know you, let alone have you as mine.

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CHAPTER 1.

INTRODUCTION

Visualization is important in chemistry education, as high visual-spatial scores have been found to correlate to better performance on chemistry concepts that require problem solving skills rather than algorithms.[1] The many instructional resources used to explain chemical phenomena generate visual representations that depict different information about a concept. Realizing that these different visual representations (such as graphs, animations, and actual substances and solutions) all describe a different view of the same chemical phenomena and assisting students in becoming well-versed in translating between the different representations used helps to refine students' understanding of chemistry concepts.[2] Even when students have difficulty analyzing visual representations, studies show that visualization skills may be improved. Students with low visual-spatial abilities have gone on to do better in STEM (Science, Technology, Engineering, and Mathematics) courses after spending a semester in a course to improve visualization skills than peers of similar visual-spatial abilities who did not take the course.[3] Even a single repetition of a visualization task results in improvement.[4] In addition, visual-spatial ability has long-term effects on students' career choices and interests and students with high visual-spatial ability are likely to enter STEM professions.[5]

Visually demanding problems in chemistry don't only require visualization skills. Students solve visual tasks with different strategies and may use different combinations of visual and analytical skills on the same kinds of tasks.[6] Fostering problem solving flexibility may help students confidently approach visually complex ideas and problems in chemistry.

Visualization has been shown to enable flexibility when approaching a complex task.[7] In this work, we will discuss a variety of strategies that were used to help students develop their visualization skills and how they were implemented to promote problem-solving skills and to enable students to strategically tackle visually demanding tasks. The goal of this research is to provide a platform for students to accurately communicate their analyses of visual problems. In developing methods to help students recognize their own processes and in analyzing students' interactions with visual representations, we sought to answer three questions:

1. ***To what extent do students document their visual comprehension?***
2. ***What measures are required for students to effectively communicate their problem solving processes?***
3. ***What kind of evidence of visualization deconstruction (if any) do students show after a one-semester intervention tailored to address visualization strategies?***

In an effort to help guide students through difficult visual tasks, such as envisioning symmetry elements in inorganic chemistry, we have developed three physical model systems to provide a context that displays a visual and tangible frame of reference for abstract symmetry elements in molecular models.[8] An activity was designed to accompany each model system to guide students to deconstruct what they observed and to display common problems experienced by students. To understand the model systems' effects on how students learn symmetry and handle conceptual obstacles, we observed and recorded students' questions and interactions with the systems and activities in pilot studies.

Symmetry-based visualization is emphasized in only a portion of Inorganic chemistry courses, but this branch of chemistry incorporates many visually complex topics. In an effort to characterize how much students used visualization during lecture or recitation, we developed observation rubrics to gather information about visualization artifacts students would demonstrate and examined the effect instructors' modeled visualization artifacts had on students.

From what was learned while producing the model systems, outlining their effects on student difficulties in visualizing symmetry elements and operations, and gathering visualization evidence, we developed an intervention to pose difficult visual tasks for students while teaching them to deconstruct the information they were given and communicate their thoughts. The intervention consisted of ten weeks of activities based on complex 2-D images. On the activity worksheets, students were given increasingly difficult tasks and deconstruction questions based on a theoretical framework, the Modeling Theory of Learning.[9] In parallel to teaching students to communicate their visual knowledge and problem-solving processes, evidence of visualization was gathered through students' own documentation. Through exploration of students' documentation, evidence of deconstruction of visualization strategies manifested in four areas: use of deconstruction in direct analysis, pattern determination within the image, communication of a problem-solving strategy, and the extension of symmetry concepts to a new problem. The methods to achieve this evidence provide insight to potentially target students' mental imagery that could lead to misconceptions about chemistry topics.

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CHAPTER 2.

LITERATURE REVIEW

Visualization is an important component in learning chemistry, as chemistry consists of many visually rich topics. Some examples of these topics outlined in a recent review of visualization in chemistry are presented in Table 1.[1] Representations of molecules, reactions, and theories of these topics attempt to bridge how chemistry is taught by instructors and learned by students. Many topics commonly covered in inorganic chemistry courses and the respective textbooks require a level of abstraction that is challenging to demonstrate in an observable, tangible experience. In this work, abstract thought is a general, decontextualized consideration of theoretical concepts derived from observations.[2] Any mental imagery of these abstract concepts is considered a result of visualization: forming mental imagery and actions to think about concepts. Visualization may be characterized or commonly referred to by a number of visualization skills, such as mentally rotating and manipulating figures, recognizing common characteristics between different representations of a figure, and discerning between a figure and its background to name a few examples.[3] In this research, students were encouraged to work with visualization and visual topics. To communicate and

Table 1. Some chemistry topics that benefit from proficiency in visualization.

General	VSEPR and molecular geometry, kinetic molecular theory, stoichiometry represented at the particulate level, crystal structure
Organic	S_N2 reactions, chirality, stereochemistry, molecular representations (such as Newman, Fisher, and Haworth projections, boat and chair conformers, and skeletal formulas)
Inorganic/Physical	Symmetry elements and associated operations
Biochemistry	Biomolecular shapes, enzyme-substrate interactions

model interaction with visual topics to students, it is important to define the intended skills and abstract applications.

The visual topics and representations explored in this research were based in inorganic chemistry due to the level of abstraction and potential benefits of visualization. Symmetry is presented to introduce group theory towards the beginning of numerous inorganic chemistry texts[4, 5, 6] and students' comprehension of the subject as it builds upon symmetry is strongly influenced by their visualization skills. Visual representations are crucial in teaching unobservable abstract concepts such as symmetry and students may use visualization in varying degrees to comprehend what they see. Visual representations appear in many forms, such as textbook images, animation or movies, diagrams, charts, physical objects, and/or vivid descriptions (language that appeals to the senses to elaborate on base definitions) of chemical phenomena. In a review of visual-spatial skills, the authors concluded that advanced visualization skills might be indicative of higher levels of thinking.[7] Students with lower levels of visualization skills may take a model at face value, but providing students with multiple representations, such as models and descriptions, have shown to help them clarify their own misconceptions.[7] Visual representations help to clarify abstract topics. Because visualization is rooted in students' mental imagery, it may only ever be accessed through secondary means such as spatial-visual skills instruments, students' verbal responses, and students' drawings, gestures, or visual representations of their mental images. This work explores how visualization resources and methods were developed to help students both understand visual representations and utilize their own visualization skills to help them communicate their understanding and analysis and enhance their comprehension of the subject matter.

2.1 Visualization in Problem Solving

Emphasis of visualization in chemistry is an important endeavor because it plays a prominent role not only in understanding chemistry concepts, but also with problem solving. The use of visualization as a problem-solving tool benefits students beyond the context of chemistry. In a study where math graduate students solved non-routine problems (problems requiring procedures or strategies instead of algorithms) and were interviewed about their processes afterward, the use of visual imagery allowed for more flexibility in their methods of solving the problems than relying on the recall of known algorithms to reach an answer.[8] Students that relied on memorized formulas found the tasks difficult to complete if the problem variables did not suit the formula they knew. Evidence of underlying visual imagery was determined through drawings, verbal reports, and gestures while working through the problem.[8] In another study, undergraduate students with high spatial ability performed better on tasks requiring problem-solving abilities than students with low spatial ability.[9] Problem solving tasks included crystal structures and stoichiometry instead of problems that used memory or algorithms. Students with high spatial abilities in this study also performed better in the course, overall. This demonstrates that visualization skills and spatial skills have a prominent role in chemistry learning specifically. In another study, spatial ability was related to how much visual information was useful to students at a time.[10] Engineering students with both high and low spatial abilities worked through solving “pictorial creation” problems where they used flat patterns to determine what the final structure would look like (shown in

Figure 1).[10] Participants with high spatial ability were observed to solve the problems by utilizing multiple views (looking across views). Participants with low spatial ability examined one view at a time. Students with low spatial ability were advised to deconstruct visual steps as a problem-solving strategy and as a method to utilize more visual information. This research promoted the use of visual problem-solving processes through documentation of visual analyses. The studies discussed here spoke to the beneficial foundation visualization may have for chemistry. Multiple visual sources and the goal of flexibility in analysis helped to design the visual information students were given in instructional resources throughout this work.

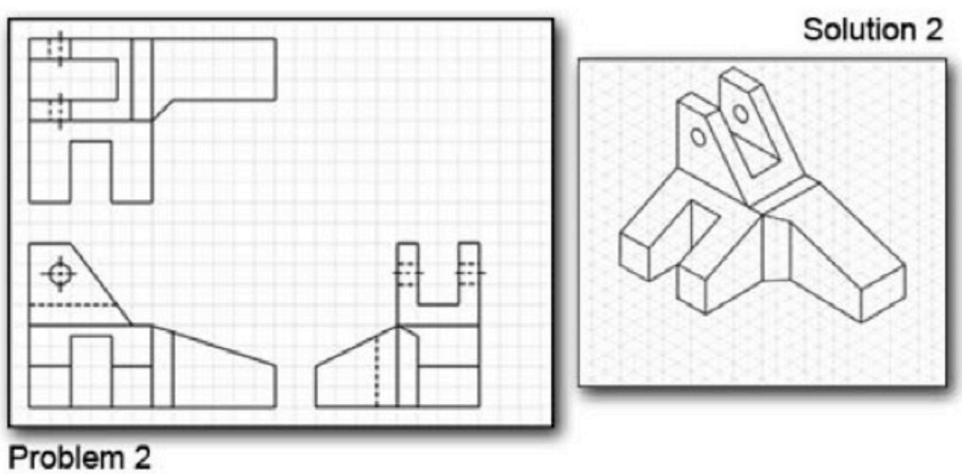

Figure 1. Engineering students with high spatial abilities used the three views (left) at a time to solve the "pictorial creation" problem.[10]

To successfully incorporate information presented in visual representations into students' knowledge of a concept, students must be able to decode, interpret, and evaluate the visual information. Kozma and Russell proposed that problem solving in chemistry might be influenced by a student's representational competence, the ability to see the consistencies of chemical concepts between different representations of the phenomena.[11] They asked students and experts to make connections between videos, graphs, animations, and equations of chemical concepts and found that the experts were more flexible and competent in analyzing, synthesizing, and evaluating the data from the representations they were shown. The different representations each gave information about a specific aspect of the phenomena and experts' ability to incorporate multiple representations into one concept demonstrated a more sophisticated understanding of the chemical concept. In teaching and learning chemistry, communication about attaining representational competence models how to solve problems in chemistry.[11] Modeling interaction with visual representations also sets an example for how to build representational competence. In this research, the cultivation of students' representational competence between verbal and visual representations was crucial in order to gauge the degree of students' conceptual understanding. Based on the connections experts made between representations, Kozma et al. outlined the skills that appear to be the result of representational competence. These skills guided how representational competence was modeled for students in this work.

1. "The ability to identify and analyze features of a particular representation (such as a peak on a coordinate graph) and patterns of features (such as the shape of a line in a graph) and use them as evidence to support claims or to explain, draw inferences, and make predictions about relationships among chemical phenomena or concepts.
2. The ability to transform one representation into another, to map features of one onto those of another, and to explain the relationship (such as mapping a peak on a graph

with the end point of a reaction in a video and a maximum concentration in a molecular-level animation).

3. The ability to generate or select an appropriate representation or set of representations to explain or warrant claims about relationships among chemical phenomena or concepts.
4. The ability to explain why a particular representation or set of representations is more appropriate for a particular purpose than alternative representations.
5. The ability to describe how different representations might say the same thing in different ways and how one representation might say something that cannot be said with another."[11]

The research described in this work explored students' analysis of visual representations and worked to help students communicate the conceptually significant facets of those representations. Stieff has conducted research to study the use of visual representations on students' representational competence.[12-13] Stieff et al. used eye fixation data and verbal protocol analysis to investigate if students used multiple representations when answering questions about molecular behavior.[12] They determined that students considered the multiple representations provided, but reported using only the representation they believed to be most relevant.[12] Stieff also studied computer-based visualization tools designed to improve representational competence with supplemental animations.[13] These tools gave students a more sophisticated understanding of the concepts in that students showed more accurate depictions of molecules (space-filling representations rather than ball-and-stick), more dynamic molecular motions, and more accurate particle spacing in different states of matter than students in a traditional, lecture-based classroom.[13] These studies demonstrated that representational competence constitutes incorporating facets of the phenomena into the complete conception of that phenomena and supports the value of focusing attention on the analysis of visual representations.

2.2 Physical, Tangible Models

In the first phase of this research, physical model systems (shown in Figure 2) were developed to allow students to enact symmetry operations and investigate the most challenging portions of their analyses. These models aimed to address students' visual, verbal, and tactile understanding. When developing a visualization resource, providing students with information that reaches multiple senses can reduce the cognitive load (tasks loaded onto the working memory) students require to consider the concept presented in the resource.[7] Physical models provide tangible input to complement what students see while interacting with the models. Using models helps students of high and low spatial ability translate between different molecular representations (Dash-Wedge, Fischer, and Newman)

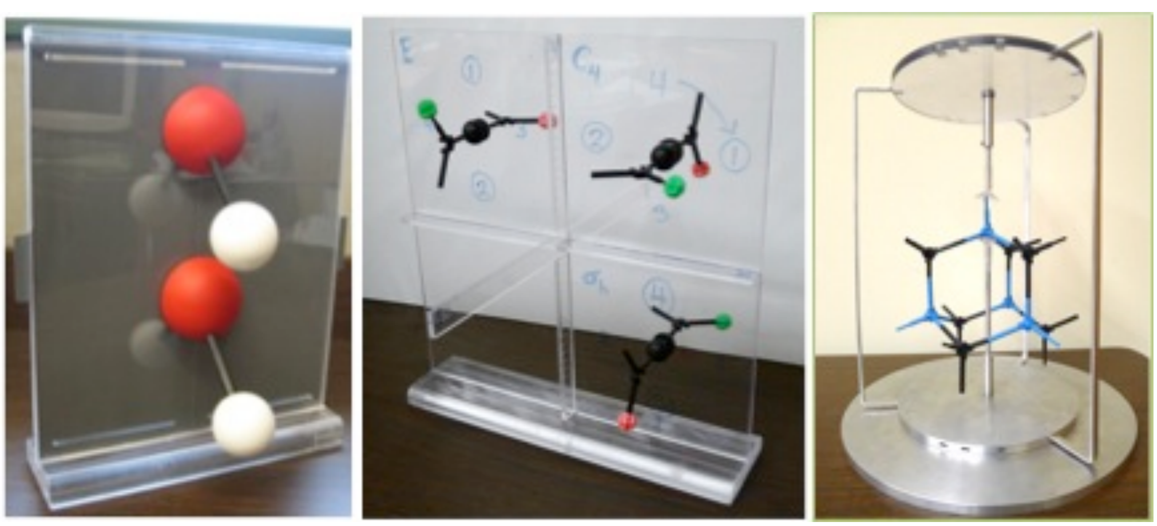

Figure 2. The three physical model systems developed in this research.

with greater accuracy.[14] Though physical models provide another representation of the concepts or procedures they symbolize, perhaps different from students' mental imagery, the models are most beneficial when they make the connection to the concept transparent while additional features remain simple.[15] These points guided the physical model systems developed in this research to provide a clear platform for students to enact symmetry operations and pinpoint what they could not visualize or understand.

Works detailing physical model resources for topics related to symmetry and group theory have previously been published.[16-21] Some activities use tangible examples in which students may explore occurrences of symmetry.[16-18] One comprehensive activity required students to determine all the rotation axes and reflection planes of a tennis ball.[16] Another activity demonstrated how symmetry was removed by adding more treads to tires.[17] The symmetry of role-playing dice gave students practice with high symmetry point groups and differentiated between elements and operations.[18] These activities provide students with specific tactile examples to practice symmetry, but do not allow student to address their own specific obstacles. The physical models developed in this research guide students with specific examples, but are designed to allow students to incorporate their own molecular models and address examples from their own coursework.

Other resources allow students to interact with models and emphasize specific symmetry elements and operations.[19-21] Mirrors have been used with pattern blocks to identify and explain reflection symmetry elements.[19] Poster board models representing specific point groups have allowed students to enact the operations on a specialized system that displays all the operations for that group.[20] Tinkertoys were used to explore C_2 rotation axes perpendicular to the principle rotation axis with a modified modeling kit to also demonstrate and reaffirm locations of reflection planes.[21] The variety of tangible resources developed to assist students in visualizing symmetry concepts encountered in chemistry attests to the range of difficulties students have in the subject. Physical models are a valuable visual resource because they allow students to actively interact with the material and provide students with representations external to their working memory and concrete experiences to support their understanding of symmetry. The models developed in this research address symmetry visually and physically as the aforementioned resources do, but they also focus on students' communication of their analyses of symmetry within these examples. The model systems promote translation between verbal and visual representations through students' documented problem-solving processes.

2.3 Visualization Interventions

Though this research explored students' interaction with visual problems, it was important to consider the motivation and methods of research seeking to improve students' visualization to understand the extent and means by which students could improve their visualization skills. Different strategies have been investigated to determine whether or not students may improve their general visualization or improve their visualization in inorganic concepts.[22-27] In one study, a group of students given more time and access to working with molecular modeling computer programs performed better on a posttest compared to students who were not exposed to the additional training.[22] This points to the fact that development of these skills requires time and practice. In another study, an on-going symmetry activity required general chemistry students to search their everyday surroundings for symmetry elements and keep a journal of their observations in order to give them insight to these visualization skills for use in future organic and inorganic chemistry courses, where symmetry would be revisited.[23] Though students' verbalization skills may be targeted through these journals, this research structured students' documented visual observations with procedural deconstruction to frame their visualization as a problem-solving strategy. Another project that provided on-going symmetry exposure targeted high school students and related symmetry to everyday objects, models, animations, crystals, and x-ray crystallography.[24] The students retained knowledge three weeks after the unit conclusion, but students reported that they found symmetry confusing and difficult to understand.[24] In the research presented in this dissertation, students were similarly encouraged to make connections to real world examples, but were also required to acknowledge and communicate deconstructed aspects of the connections to support understanding. In another study, computer simulations, ball-and-stick physical models, and 2-D perspective drawings were given to students to aid in their understanding of stereochemical concepts.[25] All students given help performed better than the group without additional resources, but the computer simulation showed the most improvement perhaps because it guided students through the transformation of manipulating a mental image.[25] Additionally, as demonstrated in research into mental rotation skills, repeated exposure to a specific kind of visualization task results in improved performance.[26] Repeated exposure does not guarantee that students will be able to critically analyze new visualization problems. This research sought to improve the quality of students' interaction with visual representations. Instead of improving students' visualization directly, we promoted the analysis of visual problems as a strategy where students would employ visual and verbal knowledge.

Website and computer simulation resources can produce very detailed examples of symmetry operations and interactions with specific molecules. For these to be effective conceptual representations, students must understand the spatial implications of the computer representations, such as interpreting shading and depth cues. Though 3-D computer simulations are powerful instruments to give students practice in visualization, computer monitors are still 2-D and the skill of transforming 2-D to 3-D remains untapped if the simulation is the sole resource. To address this problem, an exercise in producing 2-D images from a collection of wooden cubes allowed students to methodically practice 2-D to 3-D transformations.[27] This exercise supplemented an assignment in exploring molecular structure of literature molecules and substances to teach students the translation of 2-D images to a 3-D knowledge of the structures.[27] The physical model systems also address 2-D to 3-D translation, but the whole of this research promotes translation between verbal and visual (2-D and 3-D) understanding to ensure that students comprehend what they translated. The studies discussed here showed that building visualization skills requires time and practice and may not necessarily result in improved chemistry knowledge. With the development of physical model systems, we sought to supplement visual information about symmetry elements and operations with tangible information by way of physical (3-D) model systems. To address how effective the physical and visual information would be in students' symmetry comprehension, verbal comprehension was built through structured deconstruction of the visual problems students encountered.

2.4 Deconstruction

In this research, deconstruction refers to a procedural breakdown and examination of the components of a concept or representation involved in the formation of mental constructs. The Modeling Theory of Learning, the theoretical framework used in this research, outlines several principles to create successful thought-revealing activities for students.[28] The first principle declares the need to construct a model of the problem that must be solved, but in order to construct this model, the problem must be deconstructed into its simplest parts and the relationships, operations, and patterns inherent in the problem must be examined and understood.[28] The procedural deconstruction of the tasks and students' analyses was emulated in this work to effectively elicit students' problem-solving processes.

The concept of deconstruction has been documented to have many advantages in learning and instruction. Deconstruction has been used to help students build a more practical sense of reality by breaking down the meanings of classroom instructional models and asking students to discuss the similarities and differences between the models and what they represent and subsequently, how the models can be improved.[29] Eichinger claims that this helps to account for any shortcomings of the models and encourages "student ownership of concepts." Deconstruction has been successfully incorporated into the planning, instruction, and assessment of middle school science classes to improve students' progress in learning the material.[30] During Katsh-Singer's instruction, students were asked deconstructive questions about components, relationships, meanings, and consequences of the topics presented in class. In this scenario, the author claimed that deconstructive questions provided both remediation and challenge for the students because they included both simple clarification questions and deeper cognitive questions. Deconstruction was described as a safety net for students because they were able to provide more responses to deconstructed scenarios of a topic than with a direct, singular presentation of a topic.[30] In this research, analysis of visual representations was encouraged through deconstruction to make the visual problems approachable.

Deconstruction also supports critical problem solving. The thought process ("nature of thought") necessary to progress in science may be interpreted as deconstruction. Humans understand science from many partial points of view and analyze knowledge through "a process of redefinition of the meanings and reorganization of conceptual structures".[31] The ability to deconstruct and understand that only specific aspects of a concept are represented in scientific models is indicative of higher levels of thought.[32] As students progress toward an expert level of thought, they understand that a model adds a particular facet of a concept and that this concept is more comprehensive than any single model can display. Connecting multiple representations of chemical concepts (videos, graphs, animations, and equations) helps students build an inclusive and accurate understanding of the concept from the partial representations.[11, 33] Promoting familiarity with multiple representations of a concept fosters a refined understanding of the interrelations of the deconstructed parts of the concept. Rather than a specific problem-solving method, these points emphasize the strengths of deconstruction as a thought process regarding scientific concepts. Previous to this work, structured deconstruction had not been applied to help students analyze visual representations.

General deconstruction is prevalent in many symmetry-related instructional tools to date. In an activity exploring the symmetry elements and operations of the D_{4h} point group, students use a grid of the sixteen possible orientations of a labeled square to break down the possibilities of different operations on the square.[34] Tuvi-Arad and Bonder used online visualization tools to teach high school teachers about symmetry elements and continuous symmetry, which involves investigating how far a structure is from being perfectly symmetrical by deconstruction of the parts of the structure that make it different.[35] These activities show how students may successfully approach complex visual topics by first examining deconstructed portions of a task. In this work, deconstruction was addressed through a structural framework and elevated beyond a breakdown of parts to an introspective examination of the relationships and patterns inherent in the tasks.

2.5 Scaffolding

Late in this research, scaffolding was employed to promote student interaction with advanced visual content. Scaffolding has been used with students of a variety of levels. It refers to the process in which instructors provide decreasing amounts of guidance to help students accomplish higher cognitive goals that would be difficult to attain alone.[36] An article outlining scaffolding methods to assist young children with problem solving suggests the following advantages of using scaffolding: maintaining the subject's interest, simplifying the task to ensure manageability, keeping the subject on track, calling attention to discrepancies between the subject's work and correct work/assumptions, controlling and managing frustration, and demonstrating a final solution.[37] A study using scaffolding to teach density and buoyancy also outlined several principles to guide their scaffolding methods: affective supports, articulation, focusing, modeling, problematizing, and promoting shared understandings.[38] Articulation allows instructors insight to students' thoughts to see if they're on track to understanding or solving the task. Focusing steers students' attention to the relevant aspects of the problem, while modeling allows the instructor to raise students' attention to a more difficult task or portion of the task and demonstrate how students solve similar tasks. Problematizing calls attention to discrepancies and conflicts that students must overcome and encourages students to challenge themselves and reflect further. Articulation, focus, and problematization echo the principles outlined by the Modeling Theory of Learning within documentation, model construction, and self-assessment. The similarities suggest that scaffolding would favorably introduce thought-eliciting tasks that would help students complete higher-level problems.

Another interpretation of scaffolding is to give students supports that enable them to deal with more complex content and advanced abilities than they would otherwise be able to handle (rather than a scheduled decrease of guidance).[39] This view of scaffolding was taken into consideration while scaffolding the visual components of the intervention. In an in-depth analysis of scaffolding, Reiser determined two mechanisms of scaffolding from previously discussed guidelines: structuring and problematizing. Structuring consists of the decomposition of a complex problem into more manageable parts, removing unnecessary options, and monitoring student progress. Problematizing still calls attention to discrepancies and conflict, but also encourages expression of ideas and making decisions. Within the complex visualization activities in this research, students were given complex problems and room to discern between unnecessary options. At the college level, scaffolding has been used to immerse students in NMR and IR spectroscopy activities that are initially beyond their skill and knowledge capabilities.[40] Here, Livengood introduced material that was too complex for students to handle on their own and made it approachable by breaking the concepts up and offering supports of organic chemistry relationships that students had already covered. This example demonstrates how scaffolding may be utilized through the planned dispersal of supports rather than gradual removal. Livengood's work interpreted scaffolding as a dispersal of supports from organic chemistry to help students Scaffolding offers an effective way to challenge students while not alienating them from tasks that seem above their ability. In solving visual tasks within the intervention presented in this work, scaffolding made the images of advanced content approachable and allowed students to work through their mental images independently.

2.6 Verbalization with Respect to Visualization

The motivation of the research presented here was to understand students' visualization processes and challenges. Verbalization is a crucial bridge to communicating visualization. Even though mental imagery may be evidenced through secondary means like drawings, gestures, or instruments designed to measure visualization skills, verbalizing one's intentions, thoughts, and interpretations of concepts is most common for both instructors and students. Using verbalization to express mental imagery may not adequately relay the extent of students' visual understanding if they are unaccustomed to describing visual ideas and representations. Habraken recommends teaching to the pictorial language of chemistry because of the prevalence of visuospatial thinking outside of school and within chemistry due to modern technology.[41] Instead of decreasing logical-mathematical and verbal teaching, it has a place in translating visual thinking into speech and writing to build upon students' representational competence. In a study exploring the role of visualization in solving math problems, evidence of graduate students' visualization, such as drawing, verbal reports, and gestures indicated the type of thinking that was taking place.[8] Visual imagery was used to either make sense of a problem, solve it, or both and though it required more time than using a formula, it let the graduate students be more flexible with their problem-solving methods.[8] These conclusions were based on a verbal discussion of the students' problem-solving processes. Any mental imagery and reasons for such images were relayed through verbalization. When working with complex tasks, encouraging students to articulate their thoughts helps them make sense of the problems and manage their progress on completing the task.[42] This ties verbalization in as a major element of scaffolding and relates to the Modeling Theory of Learning through documentation. Through verbalization, students may clarify visual information through, communicate their progress, consider verbal guidance from the instructor, and finally relay their visual understanding of visualization tasks.

2.7 Understanding Visualization through Brain Function

Studies of visualization in learning science rarely venture into discussions of brain function, but it is important to illustrate the emphasis of secondary means to access visual thought processes. Visualization is difficult to categorize and is intertwined with other skills used to understand, process, and relay information.[43-50] Evidence of different kinds of visualization and the interconnectivity between multiple senses attest to the complicated facets of mental imagery. Rock and Victor established a discrepancy paradigm when they conducted intersensory conflict studies in the 1960s between sight and touch.[43] Students' visual perception was so powerful that they favored sight and altered the memory of what they touched to match what they saw. The researchers concluded that vision dominates when a subject's vision is manipulated to conflict with what a subject sense through touch.[43] Later work replicating the same intersensory conflicts discounted that vision always dominated, but concluded that both vision and touch have roles in affect, spatial cognition, and guidance.[44] Despite which sensory input dominates, the results of these studies indicate that clear physical information is important for students to understand the spatial representation of objects with the best accuracy.

Figure 3. Subjects responded to numbers in either a number line (left) or clock (right) with the hand that was closest to where the number would appear if the line or clock were in front of the subject.[46]

Though physical and visual input affect one another, physical representations offer important information that is inaccessible while relying on vision alone. Haptic feedback in a sensitive simulated feedback device inspired more interest and engagement in scientific topics because the immersive environment allowed students to connect with the topic based on concrete experiences.[45] Furthermore, mental imagery may manifest in how people respond physically.[46] The connection between visualization and physical response was studied by having participants physically point out a number on an ascending list (number line) or on a clock. Visual-spatial thinking manifested in which hand a subject used to respond to a number based on its location in the image in their minds. Based on the visualized number line or clock, subjects chose a number with the hand that would be closest to the side of an actual number line or clock that contained that number (see Figure 3).[46] Based on the evidence that touch and sight are so influential on each other, providing physical resources to visual topics will only add to students' mental imagery and enhance their understanding. The physical model systems developed in this research provided a physical platform for students to explore and determine visualization problems in their analysis of symmetry problems.

Figure 4. When the right eye is covered, the researcher was able to communicate with the "right" brain, which could communicate through left hand gestures.[47]

Evidence of students' visualization may be accessed through verbalization, but the two require separate brain processes. Split-brain studies, a now defunct treatment for epilepsy, demonstrated the disconnect between brain halves and each hemisphere's ability to understand visual and verbal information. In one case study of split-brain patients, a right-handed patient's left eye was covered and he could point and describe visual cues given to him. When the same patient's right eye was covered, only his left hand could point to visual cues. When the researcher verbally questioned the patient about his choice, the patient would verbally deny any knowledge of his left hand's motion.[47] Figure 4 illustrates the brain hemisphere responsible for left eye and hand activity. The portion of the brain responsible for verbal communication was cut off from what the patient's right hemisphere experienced. This demonstrates that verbalization is not coincident with visualization and some transfer must occur in the brain to understand visual information received verbally or to communicate mental imagery. The translation between visual and verbal understanding was a key point in this research when students found documentation to be so challenging.

Translation is not only required between visualization and verbalization. Chemistry utilizes a variety of visualization skills. Targeting different visualization skills lends insight to the variety of visualization that occurs in the brain. One study investigated the impact of physical and verbal interference on working memory.[48] Students were trained with visual (representative images and spatial relations) or verbal (vivid description) memory strategies and given a list of directions to recall. While recalling the directions, they were asked to perform concurrent interference tasks: verbalizing "Ba-Be-Bi-Bo-Bu" or tapping the corners of a square on the table. Verbalization hindered recall more than tapping for both visual and verbal training strategies and visual training strategies helped students with both high and low spatial ability retain more information than the verbal, vivid description strategies.[48] A self-report measure of mental imagery, the Object-Spatial Imagery Questionnaire, was developed and validated to predict an individual's preference for either spatial visualization or object visualization, a term representing appearance and detailed imagery.[49] The separation of visualization skills is supported by research of a brain-damaged patient's visualization skills.[50] Damage to the parietal cortex results in impairment of spatial skills such as mental rotation and maze learning, while damage to the temporal cortex results in impairment of tasks that require visual discrimination between objects. These visual skills were shown to be distinct from one another because damage to one lobe did not affect the visual skills associated with the undamaged lobe.[50] By separating thinking abilities through targeted tasks (or damage to specific brain areas), different visualization skills and verbalization are shown to be distinct and to operate independently. Visual tasks in everyday life and in chemistry courses require the combination of skills that are physically based in multiple locations in the brain. This research utilized deconstruction to teach students to pool their thinking skills and senses in order to ease the translation of representations that speak to a particular skill.

In this work, student improvement in visualization skills was targeted through multiple, varying representations of chemical concepts to provide students space to work on communicating the translation of these representations: physical representations, visual examples with additional visual frames of reference, and meaningful descriptions of the parts, relations, and patterns within complex images. To help students analyze and comprehend the representations, they were taught to deconstruct the concepts and verbalize the deconstruction process to unify the mental imagery and verbal understanding of their own visualization strategies.

2.8 Conclusion

The work discussed in this dissertation provided a platform of deconstruction for students to accurately communicate their analyses of visual problems. The literature presented here documents some existing methods devised to help students relate to abstract topics, specifically symmetry within inorganic chemistry. Visualization skills are important to promote in chemistry, as they are indicative of higher levels of conceptual understanding and contribute to problem solving abilities.[9, 11] Advanced visualization skills correlate to resourceful, flexible problem solving while lower-level visualization may hinder students from understanding and completing tasks that require problem-solving skills.[8, 10] Instead of aiming to improve visualization skills, this research sought methods to help students work with visual problems using whatever skills (visual and logical) were available to them and to help students communicate how they interacted with these problems. This research differs from other visualization interventions by placing emphasis on the analysis of visual representations rather than visual methods used in analysis. Deconstruction and scaffolding offer plausible strategies to make visualization more approachable for students that have difficulty with visual tasks or understanding the visual information associated with chemistry concepts. A specific, procedural form of deconstruction was used throughout this work as a method that could be applied to any problem, but that has not been explicitly used within visualization. Scaffolding enabled students to handle advanced chemistry content.

Visualization is closely related to touch and verbalization. Touch combined with sight may give students information about spatial relationships that cannot be taught with 2-D images. Verbalization is key to translating and relating visual information. This literature review has included documented efforts to understand and enhance visualization skills. This dissertation used effective methods reported in the literature (such as scaffolding) in aims to improve students' visualization skills. New resources were developed to enhance visualization skills through physical models and verbal communication. This project aimed to help students manage the complex visual information associated with inorganic chemistry and help make sophisticated visualization more attainable for students through platforms where students could verbalize their interactions with deconstructive and structured environments.

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CHAPTER 3.

THEORETICAL FRAMEWORK

Lesh et al. developed a framework for creating thought-revealing activities to promote and document how students develop a method to solve problems in a way that allows students to recognize their own problem solving processes.[1] The foundation of the thought-revealing activities came from the need to keep students thinking productively during interviews. In a preliminary study, Lesh et al. determined the most effective interviewers were those that interfered the least with students as they verbalized their problem solving.[1] However, even if the interviewer asked the right questions and pulled out procedural information from the students as they worked, examining hours of video and audiotape offered external observations about descriptions and replies rather than deliberate explanations from the students. Their activities evolved into decision-making tools with steps for the students to complete along the way. This involved students being required to document their answers and reasons for each step. The outcome of this deliberate documentation was an abundance of students' thoughts about solving the steps instead of only the outcome decision for the problem. Without documented progress, the process may be lost since students value and remember the outcome above all else. As the students in the study worked through the activities, the authors shifted their focus to the developing knowledge rather than how much the students knew in the end. They found their processes to be more valuable than the outcomes and sought to determine the mechanisms students use to "develop a construct from situated to decontextualized knowledge." From their work, they developed six principles that include Model Construction, Reality, Self-Assessment, Construct Documentation, Construct Shareability and Reusability, and Effective Prototype principles.[1] The first three principles specify how the activities should guide students to think about the problem they'll need to solve. The last three principles provide guidelines for how the thought processes are consciously documented. These guidelines directed the physical model instructional materials and intervention activities developed in this project in order to

Table 2. The six original framework principles as outlined by Lesh, et al.

Principle	**Task Characteristics Pertaining to the Principle**
Model Construction	The task puts students in a situation where they recognize the need to generate a model for interpreting the given information, possible processes, and goals in a complex, problem-solving situation. A model is a system with the following components: • *Elements* • *Relationships* (among elements) • *Operations* (describing how elements interact) • *Patterns or Rules* (apply to relationships and operations)
Reality	Some aspect(s) of the task will be meaningful to students in order to encourage them to "make sense of the situation based on extensions of their own personal knowledge and experiences."
Self-Assessment	The task implies appropriate criteria for assessing the validity of creative solutions. Students are able to judge whether they've solved the task and when they need to improve or refine their responses for a given purpose.
Construct Documentation	Questions are posed in a way that students will clearly reveal how they are thinking about the situation by leaving an "audit trail" of responses outlining the given information, possible processes, and goals that they took into account.
Construct Shareability and Reusability	Tasks challenge students to go beyond personally solving a singular problem to developing general ways of thinking. Focus is placed on the process to make it easier to gauge the mastery of a concept rather than the answer produced.
Effective Prototype	After the task is completed, the solution provides a useful prototype, or metaphor, for interpreting future situations. It cues students to think back on the process when they encounter similar situations.

gain valuable insight to students' processes of visualization before the processes are forgotten in favor of the final outcome of problems posed to the students. These principles are described in Table 2.

The research by Lesh et al. is founded on constructivism. As students learn, the knowledge they take away comes from actively constructing it.[2] Students take in a version of a concept every time it is presented to them and arrange it, along with any other information about that concept, into something compatible with existing knowledge. Lesh et al. define these active assemblies of fitting new information into a larger picture as mental constructs. Mental constructs are "models or conceptual systems embedded in a variety of representational systems." Staver gives guidelines for how knowledge may be constructed and explains that knowledge may come from individuals, communities, and any social interactions.[3] The construction of learning and descriptive language must be useful, practical and adaptive, and learning and language give coherency to individual experiences and the collective knowledge of the community.[3] Every time a student experiences a concept (whether in courses or in everyday life), the experiences will contribute to what the student knows about the concept. Mental constructs are not only shaped by what the student experiences in the classroom, but by how peers (the community) regard the topic. When forming mental constructs, they are working to build and shape their understanding of a concept. Lesh et al. emphasize that mental constructs are things of value that students produce rather than a superficial afterthought that may not lead to permanent understanding. They describe the production of a mental construct as consisting of assembly, sorting, differentiating, reorganizing, and refining a system and going beyond these to encompass all representations of a concept in the student's mind. Abstract concepts are challenging to relate to students and instructors cannot be certain that the constructs students build will represent the important characteristics of the concepts presented in class.

The activities based on this framework specifically guide students to develop their own model systems, mental constructs of the situation and factors surrounding the problem to be solved. Lesh et al. argue that a modeling system is needed when students need to make predictions based on underlying patterns or regularities, when constructions or explanations are specifically asked for, when decisions must be justified or explained, and/or when students must analyze or assess alternative conclusions, explanations, or interpretations from others. Upon reading the activity, students may not immediately know that they must construct a model to solve it, but they will understand that a plan is needed to sort out the information step by step. We propose that when students are required to work through activities to examine abstract visualizations (where it is not possible for them to know what they are supposed to see), they will construct explicit conceptual steps and documentation that support their own mental processes. In order to modify the framework originally developed to address middle school math to college inorganic visualization, the principles were translated into questions in order for students to navigate through the deconstruction of visualization tasks. This framework offers a method to shape activities bringing forth descriptions of what students are visualizing and providing insight into the process to benefit both students and instructors.

3.1 Framework Translation

Using the six principles of the thought-revealing activities and the rationale that lead to these principles' development, we shaped and revised specific questions that could be applied to visual tasks. The translated principles are shown in Table 3. Within the task characteristics, possible questions and commands to work into the activities are shown in italics. These translations apply the framework to the activities that accompany the physical model systems. To use the original framework as Lesh et al. did, a committee of instructors would have spent time developing visualization scenarios that would evoke all six principles. Because one of the general goals of this research was to encourage students to use visualization as a tool for learning chemistry, the principles were utilized directly through individual questions applied to visual tasks. The activities incorporated an assembly of tasks composed of questions that each aligned with one of the six principles rather than one task that evoked all of them.

3.2 Framework Modification

The first generation of questions referred to varying problems surrounding different symmetry elements with open-ended questions to emphasize each guiding principle. The questions encouraged students to expand on their visual mental constructs as well as to apply content knowledge of symmetry and point groups. From the pilot studies, we found that students were unable even to verbalize each of the requested questions as they struggled with the documentation that each principle required. Complying with symmetry rules, students needed to reach a correct verbal answer about a visual representation, but the mental processes to get to that point may be entirely visual and difficult for students to translate

Table 3. Questions developed to elicit the goals of the six principles within the framework.

Principle	**Task Characteristics Pertaining to the Principle**
Model Components	• Elements: *What are the simplest parts of the image/problem/object/situation?* • Relationships: *How are the elements related to each other? (Surroundings, positions, numbers)* • Operations: *How do the elements interact? (Movement, intersections, changes)* • Patterns/Rules: *What patterns and rules do the operations and relationships adhere to (that you observe or infer)?*
Reality	• Students are able to use their real-life sense-making abilities. • Students' transfer their spatial skills to the chemistry context. They should see that the logical skills they have may be used in chemistry as it's as real a context as everyday life. *Have you experienced the same operations or patterns before? How did you handle the situation at that time?*
Self-Assessment	• Students identify the end goal and assess their ideas. They should be able to tell when the question will be answered and the problem solved. *Voice your frustrations, uncertainties, and where you get stuck.*
Construct Documentation	• Write down thoughts/answers to questions right away rather than moving on to the next question. • Verbally ID the start and end point of the visualized process. *Describe the "motion", changes, or paths to get from start to end: rotation, reflection, paper folding.*
Combined Shareability and Reusability	• Tie to reality so students know they're using a strategy—require them to transfer the knowledge. • Students should be able to explain what they did/are doing. *Describe some other ways you could manipulate the image/problem either using the motion required or something knew.* *Imagine you must use the relationships, operations, and patterns on an assortment of fruits. What obstacles do you encounter? Do your patterns and rules change?*
Effective Prototype	• The activity should require students to reflect on the entirety of process. Students should remember how they approached and what helped them to succeed. • Sharing a prototype may be the same as identifying their process as a tool—combine! *Focus on the overall process and help the instructor/a classmate understand. How did you begin? What do you need to consider in order to move on from the beginning?*

verbally. Brain research shows that visual skills induce activity in a different part of the brain than verbal skills.[4] Therefore, visualization may be instantaneous and independent from verbalization for students. The additional task of examining their mental images before verbalization and documentation may have made the tasks more difficult. Students were unprepared to analyze, adapt, or justify their visual ideas like they did with more concrete tasks. To help the framework principles be more applicable and relatable to the subject matter, the questions needed more structure and transparency.

The principles were analyzed within a visual context, simplified to questions that students could address individually, and the questions that evoke each principle were edited to be more explicit and direct. To emphasize deconstruction of a visual task, the Model Construction principle was kept in its entirety and the activity questions for both the Physical Model Systems and the Complex Visualization Activity Intervention focused on identifying model components. This involved identifying elements, relationships, operations, and patterns/rules as described in Table 3. The Reality principle was used in a comparative capacity. If visual tasks based in a chemistry context resembled an image or task a student had previously experienced, the Reality principle could help them to transfer existing skills early on. Questions that were exclusive to the Self-Assessment and Construct Documentation principles were omitted. These principles represented elements that were expressed in the other fields and became repetitive when developed into activity questions. Students would fulfill the Construct Documentation principle each time they wrote down their answers and the Self-Assessment principle would be apparent when students could or could not answer the direct questions, but would also fit into the final constructed principle.

The final principle, Share and Reuse the Strategy, evolved from the combination of the Self-Assessment, Construct Shareability and Reusability, and Effective Prototype principles. All of these principles employ a reflection aspect that would help students acknowledge the visualization process they'd established to better prepare them for a similar task in the future. This new principle requires students to acknowledge the process of coming to a conclusion about the task. Self-Assessment is represented when students reflect upon and evaluate their own steps. The Effective Prototype principle was, in effect, a more formal and defined version of the Construct Shareability and Reusability. Recounting the plan to solve the problem and naming it an official strategy are one in the same to students who are more interested in understanding the actual topic rather than how they understand. The principle uses 'strategy' in place of 'tool' or 'prototype'. For this work, the end recognition of a students' own visual problem-solving strategy was more important than prompting the students to differentiate between sharing the process they used and acknowledging that process as an official tool. Together, the three remaining principles highlight the most impactful characteristics of the original framework. Streamlining three principles into one helped to focus students' reflection into a point that could potentially help them on future visualization tasks. The modified framework summarized in Table 4 guided the design of the activity worksheets and discussion with students.

This research focused on the analytical merits of the framework rather than the reporting merits. Though students documented their answers, the purpose of this documentation was to help them outline the deconstruction of their own mental images. The questions on the activities were ultimately simplified to those that proved crucial to help students understand their own processes. The physical models and visual activity intervention aim to teach students to deconstruct complex visualization problems and more direct and transparent framework principles helped align the framework with the goals of this research.

Table 4. Modified framework principles.

Principle	**Description and Questions Imparting the Principle**
Model Construction/Components	• Deconstruct the visual into the outlined components. *Dissect and identify the parts of the visual problem. Answer the following questions to help organize all the parts that have been deconstructed.* o Elements: *What are the simplest parts of the image/problem/object/situation? (Atoms, bonds, edges, faces)* o Relationships: *How are the elements related to each other? (Surroundings, positions, numbers)* o Operations: *How do the elements interact? (Movement, intersections, changes)* o Patterns/Rules: *What patterns and rules do the operations and relationships adhere to (that you observe or infer)?*
Compare Tasks to Reality	• Prompt students to transfer relevant visual skills early. *Connect the visual to reality. Have you ever seen anything like this visual or its parts before? Does it resemble or remind you of anything?*
Share and Reuse the Strategy	• Find the start and end points and describe the process to prompt reflection. *After reading the summary question, what strategy would you use to answer it? If you cannot answer the question, describe the steps you took to make sense of the visuals given.*

3.3 Activity Design

Providing students with physical models and complex visuals are both alternative ways to represent abstract visual concepts. This framework was used to design activities twice within this research: first for the physical model systems, and again for the complex visualization activity intervention. In the development of the activities for this project, we emulated the model-eliciting activities developed by Lesh et al. where students work through a model system and systematically build a mental construct about the problem and situation presented. The questions presented in each activity drew out how students accomplished each step. This method was instrumental in drawing out information about what students visualize as they completed the abstract operations progressively through the activities. There were no set, correct answers in the activities by Lesh et al., so the students had to justify their work and answers for themselves. A key difference in this research was that some questions within the activities accompanying the physical models and within the weekly intervention activities have inherently correct answers the students must work toward and students may have different visualization paths they use to reach these answers. Students' responses reveal how they deconstruct and process the visualization of symmetry operations as a plan to explain a visual task. Within the intervention, students gradually learn to deconstruct images to learn more about the discrete parts in order to build a mental construct of the interrelations within the representation.

3.3.1 Physical Model System Activities

All modified principles from Table 3 were built into activities for the physical models presented here. Each activity contained several tasks made up of one or more questions for students to answer through interaction with the systems. More than one principle was demonstrated in most of the tasks in the activities, similarly to what was done in the activities developed by Lesh et al. For example, the following task from the Proper Rotation Axis system's activity worksheet asks students to address the Model Components principle to deconstruct the system into axes and degrees of rotation in questions A) and B), the Combined Shareability and Reusability to find and keep track of rotation axes in question C), the Self-Assessment when identifying what was challenging in question D), and Construct Documentation when writing down responses to each of these questions.

> *Build adamantane ($C_{10}H_{16}$). A) Locate at least 2 different rotation axes and write their degrees of rotation. B) If you can find more than 2, what degree are they? C) How did you find and keep track of them? D) What was challenging about this molecule?*

The Model Construction principle was included in each model system, as students needed to identify the important components of the systems, define the symmetry operations, and the rules they must follow as exemplified in questions A) and C) below. The model systems helped students work through and document visualization processes that they could later consult to supplement their own mental model system based on what they saw and learned. To address the Reality principle, the activity questions were worded in a way to ensure that students were able to use their practical everyday decision-making skills to determine what is significant in the question and model and break down questions to use skills they'd previously used in chemistry. Question B) from the Permanent Reflection Plane demonstration shows an example of the Reality principle. The Self-Assessment principle is used in question C) when students describe the changes they would make to alter the model to match their expectations. The Construct Documentation principle manifests in each point when students answer the questions in the task.

A) With the plastic inserts open, what do you see? B) How is the real image alike or different from what you expected? C) Describe your observations and thoughts in detail, paying attention to the parts, how they're related, and what changes you'd make to have the model look as you expected.

Students finished a process when they judged their own visualization to be successful. Most of the questions in the activities prompted students to explain what they did and predict other outcomes, to emphasize the Share and Reuse the Strategy principle. With such documentation, students could help another student, describe their process to an instructor, or reuse their own steps again. The activities contained questions that prompted students to reflect on the entirety of the process and recall how they approached the problem and what helped them to succeed.

3.3.2 Weekly Complex Visualization Intervention Activities

The framework was incorporated into the intervention activities explicitly for students to work within the framework regularly over the course of a semester. Each intervention activity required students to directly address questions based on the modified framework. A summary question associated with the content of the presented image accompanied the outlined tasks. Example questions are shown in italics in Table 3. These questions were phrased explicitly so that students learned how to take time to reflect on the visual task in order to promote deconstruction and self-reflection. Instead of combining more than one principle in a question like the physical model activities, each principle was emphasized alone to guide students' thinking along a specific direction. Each student was required to analyze how they should deconstruct the image (Model Construction/Components principle), examine their own memories of similar visual tasks (Compare the Tasks to Reality principle), and reflect upon their own strategies (Share and Reuse the Strategy principle). Incorporating a more structured framework into the activities promoted deeper consideration of students' visualization strategies and helped to bridge visualization and verbalization, making documentation more accessible.

Documentation of visualization is important for both a researcher's and a student's point of view. Once a student gets past a difficult point in a problem-solving process, he or she may not remember what it was that sparked the change in direction. Students that have difficulty visualizing symmetry operations may not have problems once they successfully "see" the operation but may not remember how they got to that point. By arming students with the documentation from when they first figured out an abstract problem and teaching them to acknowledge their own deconstruction strategies, students are expected to be better prepared to approach future problems.

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CHAPTER 4.

METHODOLOGY

4.1 Construction of Physical, 3-D Models

Three physical model systems were developed to help students visualize the motions and structural characteristics of molecules needed when learning symmetry and group theory.[1] The systems provide students with physical and visual frames of reference to facilitate the complex visualization involved. The Permanent Reflection Plane Demonstration provides a clear example of a reflection plane and visual indicators that students may use to support or invalidate the presence of a reflection plane. The 3-D Coordinate Axis system provides an environment that allows students to visualize and physically practice symmetry operations in a relevant molecular context while the Proper Rotation Axis system is designed to provide a physical and visual frame of reference to showcase multiple symmetry elements that students must identify in a molecular model. Each system aims to illustrate specific problems students encounter when first introduced to symmetry and group theory. Corresponding activity worksheets were developed using the Modeling Theory of Learning framework (Chapter 3) and modifying them iteratively based on the feedback received from focus groups of undergraduate inorganic students while interacting with the model systems.[2]

4.1.1 Visual and Tactile Model Design

The model systems presented in this research aimed to provide resources that add to the visual examples that students and instructors have access to. Physical models allow students to explore the structural aspects of molecules from all angles rather than a chosen point of view as in 2-D representations. Students may take control of their mental constructs of the visual and move around a physical model to explore the geometry or halted operation from different angles. In addition, the 3-D Coordinate Axis and the Proper Rotation Axis systems allow students to incorporate their own molecular modeling kits.

4.1.2 Permanent Reflection Plane Demonstration

The Permanent Reflection Plane Demonstration system was designed to demonstrate the difference between a mirror image and a reflection symmetry element while providing students with introductory opportunities to support or invalidate the presence of a reflection plane. To demonstrate what constitutes a reflection plane, a physical plane separates portions of two whole molecules so students may examine both sides simultaneously rather than having access to only one half of an object against a mirror.[3, 4] This system is intended for use when symmetry is first introduced to allow students to form their own construct of a reflection plane and to highlight symmetry terminology. In the demonstration, the model system has two positions, shown in Figure 5. In the first position, two molecule halves are oriented on the glossy physical plane in combination with the reflected images to display two "complete" molecules with the same geometry as water. In position two, the opaque inserts open to reveal that the physical plane is a reflection plane for a water molecule and an arbitrary plane for a molecule with geometry similar to ammonia. Through questions on a worksheet and discussion, students observed that the water molecule has a reflection plane because the image of the front 'hydrogen' is superimposed on the back 'hydrogen'. The physical plane is not a reflection plane for ammonia because the image of its front 'hydrogen' has no corresponding match. This distinction may be used to extrapolate the reflection plane definition to all portions of the molecule such as bonds, halves of atoms within the reflection plane, and larger identical molecular moieties. Water and ammonia molecules were chosen because they are both based on tetrahedral electron domain geometries and were manipulated to look alike in the model's first position in order to demonstrate the difference between a reflection plane and a plane arbitrarily placed through a molecule.

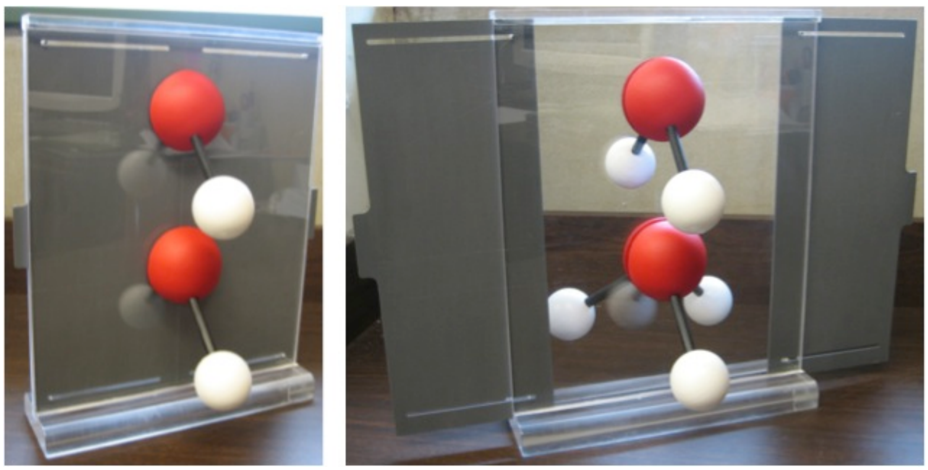


Figure 5. The Permanent Reflection Plane Demo in position 1 (closed) and 2 (open) shows the mirrored images of the front atoms. In position 2, the image of the top molecule half is superimposed onto the back portion.

This model system was designed to promote discussion on identical and indistinguishable atoms, locating multiple reflection planes, atom labeling, and coordinate mapping. By presenting labeling and mapping in a simple model system, students are introduced to abstract concepts before they are actually required to use them in more difficult problems. To avoid showing students what they should note about the model system, students should be instructed to examine the model from all sides in order for them to observe that a reflection plane separates two spatially independent and corresponding, but equal sides of the molecule. The glossy surface of the Plexiglas encourages a comparison to a mirror, so the differences between a mirror image and corresponding atoms related by a reflection plane may be raised as well. Students are encouraged to label the 'hydrogens' when responding to questions from the activity or instructor to give structure to their answers and to reinforce that each hydrogen in water is a physically distinct atom. In Figure 6, the image of A is identical to A and indistinguishable from B. Such language is subtle for students beginning to learn symmetry, but prepares them for the subtleties they may encounter in group theory resources. Coordinate mapping is another point of discussion that may enhance students' construct of a reflection plane. The Plexiglas plane may be referred to as the xy-plane. When water undergoes a reflection operation, each hydrogen atom moves to a coordinate that is exactly the same as where it started, except it's z-coordinate is now negative. The tactile aspect of this demonstration allows students to measure the distances of

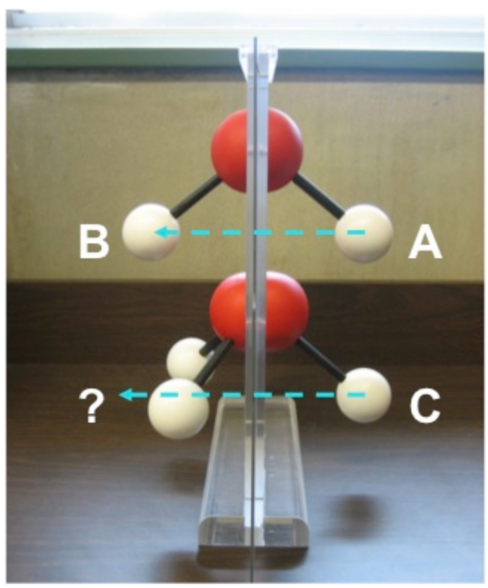


Figure 6. Viewed from the side, the Permanent Reflection Plane demo shows that atom A maps onto atom B through the reflection plane. The plane is not a reflection plane element for the lower molecule because C has no corresponding atom.

the hydrogen atoms from the reflection plane and connect coordinates to a physical example in front of them. Students are able to get a physical sense of what the reflection operation means to accompany the visual examples.

4.1.3 3-D Coordinate Axis System

The 3-D Coordinate Axis system was developed to expand upon the symmetry operations that students could enact with molecular modeling kits and extend the utility of the kits to an inorganic context. It allows them to envision symmetry operations beyond the basic spatial geometry of bonds in a relevant molecular context—instead of manipulating non-molecular objects that students may not deem as important to visualize when solving inorganic problems in class.[5, 6, 7] Reflections, inversions, and improper rotations cannot be enacted on physical models due to the fixed construction of the model kit components. Additionally, an extra hand may be needed to mark a plane, rotate the molecule, and point out differences while holding the model steady before visualizing multiple symmetry elements onto molecular models. This physical model provides students with a three-dimensional workspace where the abstract visualization of symmetry elements is given tangible representation that students carry out themselves. The opportunity for students to work through operations independently makes this system different from other model systems where symmetry operations are demonstrated for students.

This model system enables students to physically and sequentially separate out each motion required in symmetry operations in a flexible, 3-D workspace. Modeling stepwise operations, such as an improper rotation or multiple operations, provides the unique perspective of seeing each step of the motion stopped and displayed simultaneously. In

Figure 6, an improper rotation of allene is modeled in three of the quadrants. Students may carry out the definition of this operation (a rotation and a reflection through the plane perpendicular to that rotation axis) while building a physical reference to observe the outcome of the operation compared to how it was originally oriented. This comparison would serve students when they move to more difficult tasks involving the determination of whether a 2-D image has an improper rotation axis: does the molecule look indistinguishable if the operations were enacted upon it? As shown in Figure 7, students observe both halves of molecules to evaluate reflection planes and may use dry erase markers to document their progress. Students may still explore inversion centers though it's impossible to pull each atom on a model kit through the center and invert it to the other side. As utilized with the improper rotation example, this system holds the initial and final points of a modeled

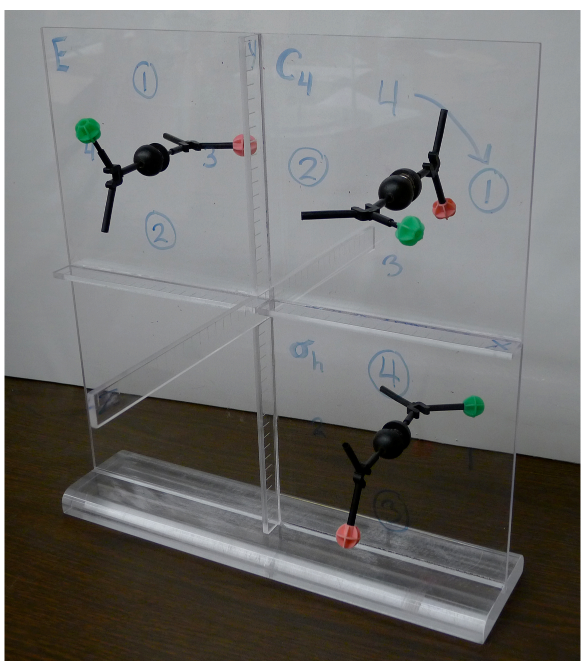


Figure 7. The 3-D Coordinate Axis system displays the steps of an improper rotation while dry erase markers label atoms and document motion.

inversion in place so students can explore the space around it and compare distances to the marked axes. By deconstructing multiple operations into steps and studying how a motion may affect the spatial orientation of the rest of the molecule, this system aims to promote spatial understanding through physical manipulation.

4.1.4 Proper Rotation Axis System

The Proper Rotation Axis system was designed to provide a physical and visual frame of reference for identifying symmetry elements in molecular models. This system can showcase multiple symmetry elements but it is specialized to emphasize the aspects of proper rotation axes with immediate feedback and a constant method to track rotational intervals. Proper rotations are the only symmetry elements that a student can enact upon a physical object without altering the structure of the molecular model and are important for inorganic students to understand because they dictate under which point group a molecule is classified. This system aims to support confidence as students determine degrees of rotation in models since it has designated positions and interchangeable frames to accommodate C_2-C_6 rotation axes to assist students with most of the axes they would encounter.

Once students are able to identify the principle proper rotation axis, the system retains a reference axis to allow students to confirm the degree of rotation from other viewpoints. Students may also use the system to hold the model in that rotation axis environment to look for other symmetry elements, such as additional proper rotation axes and reflection planes. As students look to identify perpendicular C_2 axes, they are encouraged to move around the model system at eye-level to the model, perpendicular to the retained principle rotation axis. This placement helps them accurately discern the angles between rotation axes. Tinkertoy

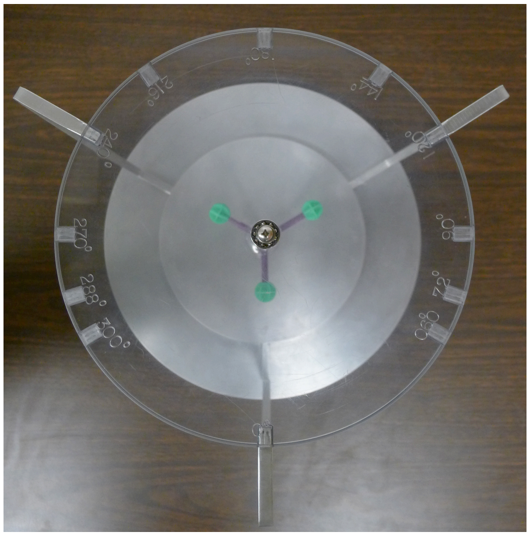


Figure 8. A molecule with a C_3 rotation axis inserted into the system with the atoms aligned to the frames in the correct degree increments.

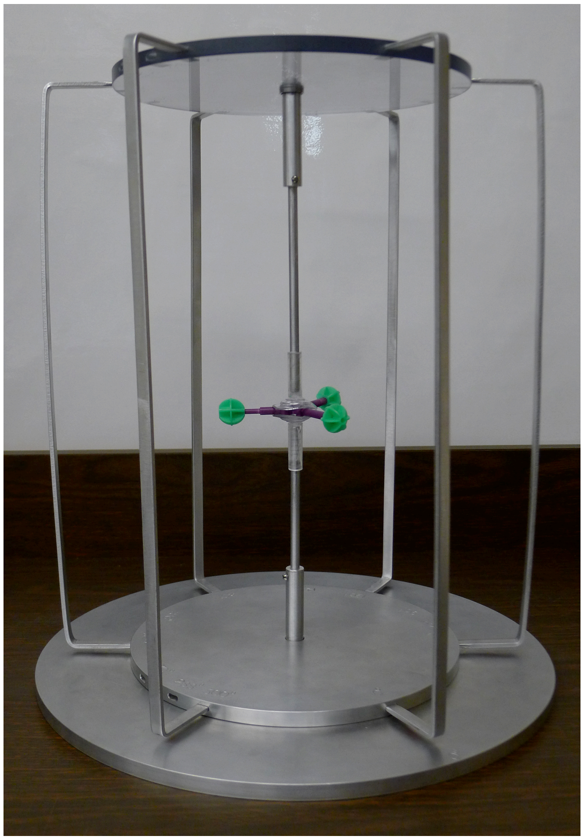


Figure 9. Six frames around a molecule with a C_3 rotation axis outline all the vertical reflection planes simultaneously.

dowels have been used to describe the locations of perpendicular C_2 axes, but the principle rotation axis location is not maintained.[3]

A frame of reference, mental or visual, is needed to track simple rotations of a molecular model. This system outlines the sites where a location on a model takes on an indistinguishable configuration from its original orientation with physical frames to ensure a visual frame of reference as an intermediate step in the visualization (Figure 8). To reinforce the frames' tactile connection to the molecular model's movement, the model system cues students with catches built under the circular base. The catches correspond to the degrees of rotation and alert students that they have completed that amount of rotation as the students rotate the frames around the stationary molecular model. Students may match molecular models to the system designated with a degree of rotation or check their expected degree of rotation by matching the system to their model. If students aren't certain of the degree of rotation, this system supports students with a way to confirm their choice by lining up indistinguishable portions of the model to distinct frames or to invalidate their choice if two different portions of the model each align with their own frames (Figure 9). This model system provides students with a visual and physical affirmation of the rotation operations they complete. Additional information about the materials, cost, and assembly of the three model systems is provided in Appendix A.

4.2 Pilot Study with Focus Groups in Inorganic Help Sessions

4.2.1 Interacting with Model Systems

The physical model systems were made available to students as a resource to the inorganic class work. Examples were prepared as demonstrations for each of the model systems to encourage student interaction and promote interest. In the Fall 2009, optional help sessions were offered to NCSU undergraduate students enrolled in Systematic Inorganic Chemistry I. During the Fall 2010, the optional help sessions were offered again for the same course, but the physical model systems were accompanied by structured activities developed using the theoretical framework based on the Modeling Theory of Learning.[2] Help sessions primarily sought to assist students with the difficulties they had with visualization of symmetry elements, symmetry operations, and determining point groups. Students were encouraged to bring their own model kits and to ask questions about symmetry topics. The model systems and activities were then offered once again to students during the Fall 2011 semester as a supplement to recitations taught by the researcher, but interactions from this semester were similar to what had been observed in the previous two years and did not ultimately change the format of the associated activities. The students that attended these help sessions comprised the focus groups of this research. Questions and topics discussed were recorded during the help sessions and observations about the session and focus groups were recorded immediately following.

During the first pilot study of Fall 2009, the models were primarily used to explain homework questions and problems presented in lecture that students requested repeated explanation. The models were offered to students outside of lecture and independent of instructor and TA office hours. Help sessions were offered at a set time for two hours twice a week unless a student requested a different time. The sessions were advertised to students as help for difficulty seeing the symmetry elements in the form of hands-on experience with models. Students were aware that the models were part of research endeavors and encouraged to offer opinions on improvement. Some students arrived at the help sessions with questions from class they wanted to discuss, and a considerable number of students expressed general confusion regarding symmetry elements. Some examples used for the 3-D Coordinate Axis demonstrated an S_4 improper rotation operation on allene, an inversion on staggered ethane, and an inversion on an octahedral center. The Proper Rotation Axis system was used for tetrahedral and octahedral structures and water to complement students' requested problems. Depending on the nature of the specific question, either the model systems with molecular model kits were used as a resource or the requested examples would be drawn out on paper to best answer students' questions. Over the course of three weeks, fifteen different students attended the sessions or made appointments to meet one-on-one. Groups ranged from one to ten students. Though much knowledge about what problems students encountered with symmetry was gained through the focus groups, the help sessions placed the most emphasis on assisting students with understanding the visual aspects of the topic.

The help sessions during Fall 2010 were more structured in response to the observations from the focus groups in 2009 and the researcher's experience with frequent questions about symmetry and prepared activities. Students were asked to email the researcher prior to attending a help session to organize and control the size of the focus groups and access to the physical model systems. Specific lecture and homework questions would still be addressed in help sessions, but each student would complete an activity while working with the model systems. More detailed observations surrounding the focus groups could be attained while students worked on the activity. Over two weeks of help sessions in

2010, ten different students worked with the model systems in groups ranging from one to five. Two students returned for additional work with the model systems. All student questions were recorded from both years of focus groups and from the lectures pertaining to symmetry and group theory. These questions formed the basis used to develop and refine the activities so the more problematic examples and points of discussion would be emphasized and common misunderstandings about symmetry elements were included.

4.2.2 Accompanying Activities

Student interaction with the model systems required much prompting and frequent questioning from the researcher. These model systems may have utility as teaching and discussion aids for instructors, but not all instructors may have time to phrase questions that will guide students to see the symmetry elements instead of pointing them out right away. Activities were developed to ensure that all students received similar exposure to the model systems and that the examples suited to the model systems were available to all users.

After the initial observations of the 2009 focus groups, the suggested examples for these model systems were constructed into a series of questions and an activity for each model system was developed. Questions where students were asked to show/write where symmetry elements were located were the most successful in getting students to interact with the model systems. For example, the Permanent Reflection Plane Demo questions were worded to help students communicate reflection planes by asking them about the corresponding portions of the molecule on either side of the plane. The 3-D Coordinate Axis system allowed students to explore the details of improper rotation and inversion operations, so questions for this system were designed to give students examples of where the initial, intermediate, and final orientations would be displayed. Questions for the Proper Rotation Axis system asked students to relate reflection planes to rotation axes to get students focused on multiple symmetry operations and coax them into uncovering the patterns in the molecules. Each of the activities posed many of the same questions brought up in the focus groups in order to advance the discussion in a conceptual direction for general application instead of confining symmetry to only the examples in front of students. Each of the example questions on the three activities were examined and modified to conform to the principles of the theoretical framework, in order to aid students in communicating their confusion, thoughts, and arguments. After the 2010 focus groups, the activities were revised to those included in Appendix B. The final activities clarified the questions with the most difficult examples and those that presented observed misconceptions about symmetry operations. Help sessions with activities require more time than those with only discussion, but are necessary to ensure that students get the most out of the model systems to ultimately help refine the connections between their mental visualizations and physical examples.

4.3 Structured Observation Rubrics

Observations from Fall 2009 and Fall 2010 help sessions revealed common questions and problems from focus groups of inorganic students. Questions, examples, and topics discussed were all recorded during and after the sessions, but a more structured measure of students' difficulties and interactions with visual representations was sought to record and classify their responses. Such structure was devised through the development of observation rubrics that enabled organized tracking of students' visualization artifacts in the classroom.

4.3.1 Problems Encountered during the Help Sessions

Upon review of student documentation and the researcher's observations from pilot studies (Fall 20009 and 2010), the data collected from help sessions did not fully represent students' interaction with the model systems and visual problems discussed. The addition of activities to the help sessions aimed to encourage students to write what they were visualizing, but students were unable to articulate any visualization processes, use visual language, or write responses on the activities. Many students were able to answer 'yes/no' to direct, deconstructed questions about where an atom would end up after an operation and some could gesture to the path an atom would take when affected by a symmetry operation. The students who were able to correctly identify symmetry elements and operations could describe incomplete portions of mental imagery using gestures and/or stammering and hesitant phrases. This demonstrated the need for students to communicate their interactions with visual representations through other means or to learn how to more effectively communicate their interactions.

While working in groups to enact a symmetry operation or describe a visual process, students were exposed to how they could think and talk about visual examples. As questions and examples were explained, students were observed using models and similar verbal descriptions of symmetry operations as the researcher. This supported that students learn about visualization through the language, gestures, and general modeling of their instructor and peers. Recorded student questions described common struggles, but the amount of gesturing suggested that students were engaging in visualization in ways that would not be demonstrated by written or spoken visual descriptions and recalled observations by the researcher. Therefore, a structured, well-designed instrument was needed to account for students' non-verbal visual representation interactions.

4.3.2 Lessons Incorporated into Observation Rubrics

The written observations and minimal student documentation guided what information would be pursued in the observation rubrics. Following are examples of how the encountered problems were incorporated.

- *Students answered simple, deconstructed questions with more ease than open-ended visual questions.*

In a 1995 study, Lewandowski studied the language that students used to describe an every day event to see how it indicated visual processes of thinking.[8] Lewandowski noted that one student indicated visual thinking by describing "vivid memories", perceptions, and active verbs. Students in the help sessions had volunteered first-hand perceptions, though they were incomplete thoughts and single words, and visualization artifacts similar to those in Lewandowski's study. These responses were indicative of visualization and using action verbs in a response was incorporated into the observation rubrics (Appendix C). Principles from the modified Modeling Theory of Learning theoretical framework were used to document when students were able to break down questions on their own: describe model components, make a comparison, and describe the steps of an operation.[2]

- *Students used their hands to gesture in place of verbal description and when predicting and reenacting symmetry operations.*

Marshall and Rossman described kinesics as the study of body motion communication.[9] Kinesics provides a view into unconscious thoughts and provides a means for supporting verbal data. Kinesics were represented in the rubrics as gesturing with both hands, one hand, and with a writing utensil. The differentiation was made to separate more engaged, potentially more visual thinking from more passive gestures.

- *Students modeled their interactions with visual representations on their peers and the instructor.*

Because the instructor and researcher helped answer students' questions and modeled how to interact with visual representations, all categories that would be tracked for students were also tracked for the instructor. If students relied solely on the instructor to model visual representation interactions, their class responses and interaction with visual concepts should reveal a pattern similar to the instructor's interactions.

- *Students asked similar questions about symmetry and visualization in lectures and recitations.*

Students frequently came across the same problems, asked the same types of questions, and interacted with the model systems in similar ways. These questions were categorized and incorporated into the rubrics to gauge the questions that accompanied visualization artifacts.

4.3.3 Using Observation Rubrics to Gather Data

For the Fall 2011 semester, two types of field observation rubrics were developed to track the frequency of possible visualization cues from students in lecture and in recitations (Appendix C). Observers in lecture and recitation were positioned in the back of the classrooms to best see the students' hands and what they were writing or drawing without intrusion. The researcher recorded observations in the middle/back of the lecture hall during lectures. In recitations, two assisting graduate students recorded observations using the rubrics from the back corners of the classroom while the researcher taught and briefly noted observations during class, which were expanded after class ended. The rubrics were discussed with the assistants before the onset of the semester to clarify wording and definitions and minimize subjective interpretation.

The observation rubrics were designed to track student questions and student/instructor actions quickly and easily. Both rubrics included a section for observations about students, split into males and females, and for observations about the instructor. Throughout the duration of each class, the observer(s) would tally the instances of events classified by the rubric fields. Each class period's data were associated with a recorded date and content discussed during that class. Attendance was taken for each recitation and a count of students attending was taken for each lecture.

In addition to the observation fields developed, categories were added to track student drawings and interaction with physical models and to track the mechanics of each class period. For lecture, interaction with models had fewer fields because students were limited to their personal models at their desks or partaking in a class demonstration. In recitation, students would have more opportunity for interaction with the physical, 3-D model systems or molecular model kits passed around to the class. In lectures, students' drawings were indistinguishable from taking notes. Fields concerning students' drawings were included only in the recitation observation rubric. Monitoring class mechanics allowed more perspective on how each class was structured and how much students were requested to interact through discussion and in-class problems in contrast to voluntary questions about the presented topics.

The observation rubrics in this research were designed to document the variety of visualization artifacts students may demonstrate. Though the physical model systems were most pertinent during the symmetry portion of the course, the skills students used to learn symmetry were applicable throughout the semester. Many fields in which observations were expected for symmetry alone or sparingly throughout the semester were included to give a comprehensive view of student visualization cues in the entirety of the course. A detailed list of classroom actions was developed to include all artifacts of student visualization and actions potentially related to visualization.

4.4 Complex Visualization Activity Intervention

The insight to students' visualization problems with symmetry supported a need to provide a basis where students could deconstruct visual problems and gain experience in articulating and documenting visualization. The students that attended the help sessions were primarily those that had difficulty visualizing and identifying any symmetry elements. To extend the method of deconstruction to more difficult visualization tasks, an instructional resource that would be valuable to students of all visual spatial skills was developed. Difficult visual examples would be used to encourage visualization or discussion of analytical methods to solve visual problems. These challenging visuals would be administered to students in the form of several complex visualization activities and supplemented with actions throughout the semester to encourage deconstruction and verbalization of complex visual concepts as a method for comprehension of visual topics.

During the Spring 2012 semester, the researcher coordinated with the inorganic chemistry instructor to conduct weekly visualization activities that promoted the use of visual language, modeled the process of deconstruction on complex images, promoted verbalization of visual mental constructs, and emphasized deconstruction as a problem solving method. The researcher taught the three sections of recitations for fourteen weeks and observed lectures to appropriately gauge recitation content. The complex visualization activities were given to students at the beginning of recitations for ten to fifteen minutes. The remainder of the recitation periods was used to discuss past and upcoming topics from lecture and address student questions. To provide a quantitative measure on the intervention's effect on student visualization, two visual spatial skills assessments were employed at the beginning and end of the semester: the Visual-Spatial Chemistry Specific (VSCS) Assessment Tool and the Mental Rotations Test (MRT).[10, 11, 12] To allot recitation time to course topics each week, the fourteen weeks of recitation were scheduled as follows: administer Pre-MRT, administer Pre-VSCS, ten weeks of complex visualization activities, administer Post-MRT, and administer Post-VSCS.

4.4.1 Activity Design

While studying students' visualization obstacles and interaction with the physical model systems (Focus groups of Fall 2009 and 2010), students were not able to volunteer any descriptions about their visualization processes.[1] When prompted to describe the visualization students may have used to solve problems posed by the model systems, students preferred to provide the answer or resulting operations instead of their process to reach that answer. To enhance students' comfort with discussing visualization and potentially using visualization as a tool, the activities within this intervention (implemented Spring 2012) were designed during Fall 2011 to be challenging to the extent that students would not immediately know the answer. The complexity of the visuals and tasks within each activity provided students with room to test different strategies to comprehend the content and time to work through a process to reach this comprehension.

4.4.1.1 Format

The format for all complex visualization activities was based on the Modeling Theory of Learning.[2] This framework was modified for this research to feature three principles to elicit visualization in an inorganic chemistry context from undergraduate students. The basic format and sample questions (in italics) are shown as follows:

1. Summary Question: A content-based question that gives students a purpose when analyzing the image. From Week 4, *"First, show (or describe the locations of) the symmetry operations you need in order to identify the point group. Then, give the point group of the structure."*

2. Model Components
    a. Elements: *What are the simplest parts of the image/problem/object/situation? (Atoms, bonds, edges, faces)*
    b. Relationships: *How are the elements related to each other? (Surroundings, positions, numbers)*
    c. Operations: *How do the elements interact? (Movement, intersections, changes)*
    d. Patterns/Rules: *What patterns and rules do the operations and relationships adhere to (that you observe or infer)?*

3. Compare to Reality: *Connect the visual to reality. Have you ever seen anything like this visual or its parts before? Does it resemble or remind you of anything?*

4. Define the Strategy: *After reading the summary question, what strategy would you use to answer it? If you cannot answer the question, describe the steps you took to make sense of the visuals given.*

The first question on each activity worksheet, referred from hereon as the summary question, would drive students toward a purpose when studying the image. The tasks presented in these questions were designed to promote the development of a process concerning the complex visual. Seven of the ten weeks involved the determination of symmetry elements, point groups, or discrepancies of symmetry elements between two images or portions of images. Finding a point group of a new structure is a procedural problem, no matter the level of proficiency in group theory. These questions could either guide students to look at simpler portions of the images or slow them down to spend more time envisioning the components of the structure presented.

The model component question was broken into the four parts named in the Model Construction/Components principle (Chapter 3, Table 4). Students were prompted to deconstruct the image by: naming the simplest elements of the image, determining the relationships between the elements, finding the dynamic operations that linked elements to each other, and identifying the overall patterns that the elements, relationships, and operations follow throughout the image.

The reality question required students to compare the activity image to anything they'd experienced previously in chemistry or in life in general. This question invoked the Compare to Reality principle in the modified theoretical framework and aimed to promote students' existing visualization skills and connections to familiar imagery. For example, if a student has difficulty comprehending an image of ferrocene but they can compare the cyclopentadienyl ligands to stars (pentagrams), their knowledge of the components of a star may provide them perspective on how to consider the ligands.

Finally, students reflected on their work to define the strategy used to answer the summary question as prescribed in the Share and Reuse the Strategy principle. This question was crucial for students to acknowledge the processes they carried out in analyzing and solving the visual image tasks rather than "seeing" the answer after spending time observing the visual.

It was important that students were asked each of these questions explicitly because the task of visualization and deconstruction takes longer than identifying the answer to the task, as presented in the summary question. Though students wanted to answer the summary question to "get to the point" of the activity, they answered questions that utilized the same framework dimensions each week to teach them to slow down and deconstruct the images. The activities within this intervention strived to show students that they have the tools to understand the complex visual concepts and images they experience in chemistry and teach them to recognize visualization and deconstruction as a strategy to analyze future complex visual problems. The complete activities are included in Appendix D.

4.4.1.2 Scaffolding Visual Complexity

The activities of this intervention featured complex images in order to challenge students with a visual representation that required time and methodical thinking to understand the structure and components presented in the image. However, the activity images and tasks could not be so intimidating that students would not attempt the analysis. To guide students to the point where they would be able to thoughtfully discuss multiple views of intricate chemical structures from recent literature, the activities were scaffolded. In this research, scaffolding refers to providing students with supports that enable them to deal with more complex content and advanced abilities than they would otherwise be able to handle.[13] In every activity, students were supported with deconstruction questions that suggested how to regard the images. Each week of the intervention, students were pushed a bit farther as the activities used a more complex image, a more complex task within the summary question, or both. Livengood et al. similarly made complex spectroscopy material approachable by breaking up concepts and relating it to course content.[14] Scaffolding methods have been reported to help maintain interest, simplify tasks to ensure manageability, keeping students on track, and managing frustration.[15] These advantages helped students progressively tackle tasks concerning visual representations beyond what they experienced in class.

Over the course of the semester, the ten weeks of activities evolved both in complexity of the image and difficulty of the tasks concerning that image. The visual scaffolding component is described in Table 5. Color versions of the images were projected at the front of the class while students worked through the activities printed in black and white.

The Week 1 activity used a non-scientific image and context to introduce students to the deconstruction format, the use of descriptors, and how these questions lead to a process concerning the image. An image of castle ruins was used to provide a representation of the structure and its surroundings. Students could use visual discrimination (perceiving dominant features) and figure ground skills (distinguishing an object from its background) to differentiate the castle from the moat and surrounding land.[16] This image was used in the first week because the researcher predicted that all students would recognize an image of a castle surrounded by a moat no matter their background.

Table 5. Complex visualization activity images and the visual features that describe the visual scaffolding component.

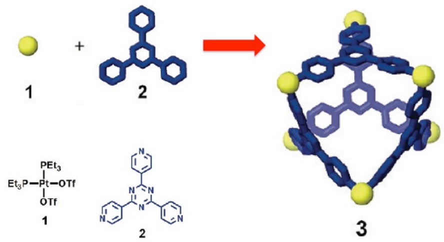
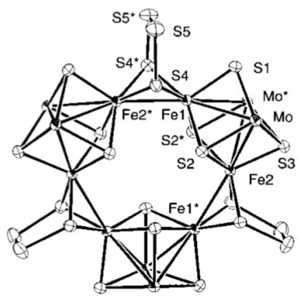
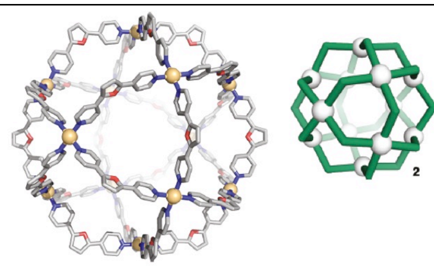
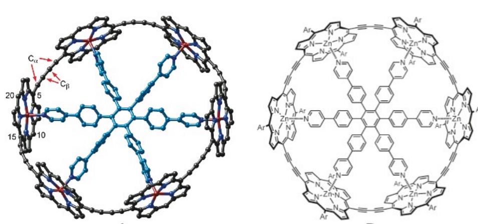
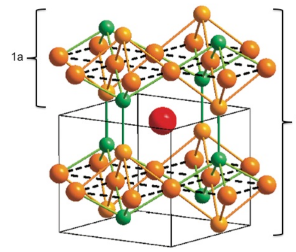
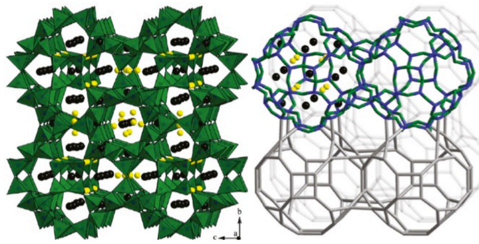
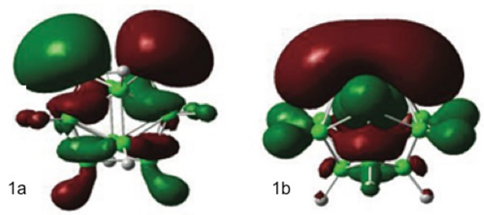
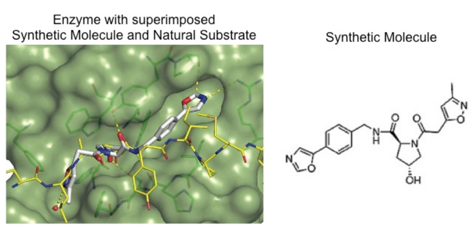
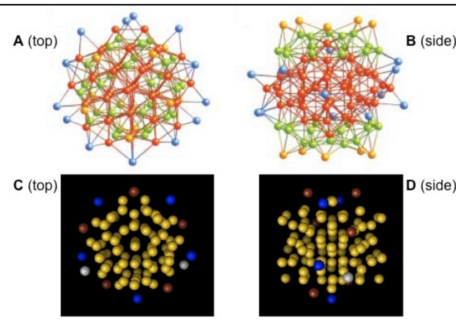
Activity	Image	Visual Scaffolding
Week 1 1/27/12 Caerlaverock	 17	The image features non-scientific, general knowledge content: an aerial view includes multiple areas to allow visual discrimination of the figure (castle) from the background.
Week 2 2/3/12 [6+4] Metal-Organic Supramolecule	 18	A supramolecule is made up of line drawing moeities connected by spheres and is oriented towards the viewer to suggest the principle axis.
Week 3 2/10/12 Cyclic Tricubane Cluster	 19	An ORTEP structure provides more complexity through structure details and partially labeled atom identities. It is still oriented to suggest the principle axis.
Week 4 2/17/12 Self-Assembled $Pt(II)_{12}L_{24}$ Spheres	 20	Two depictions of a large, non-planar supramolecule are given: one with line drawing ligands (left) and one with a bent bar as each ligand (right). The principle rotation axis (C_4) is not oriented towards the viewer.
Week 5 2/24/12 Templated Cyclic Porphyrin Hexamer	 21	Students must discern the discrepancies between two representations of the same structure: one 2-D structure and one ball-and-stick structure with true bond angles. The molecule is primarily planar.

Table 5 (continued)

Week 6 3/2/12 $SrAu_3Ge$ Nets	 22	The structure is formed from two ball-and-stick 'nets' angled into the page to obscure the principle axis. The bonding pattern highlighted by dashed lines suggests the bonding pattern of each net.
Week 7 3/16/12 Microporous Oxonitrido-phosphate	 23	Two representations of a structure are given: one with polyhedra and spherical counterions and one with line drawings (angled/colored and straight) with many atoms removed to highlight the skeletal pattern.
Week 8 3/23/12 $B_{12}H_{10}^{-2}$ Frontier Orbitals	 24	Two different molecular orbitals overlay the ball-and-stick structures of a large molecule. The orbitals are shaded red/green rather than the shaded/unshaded or +/- notation students used in lecture.
Week 9 3/30/12 Binding the VHL Enzyme	 25	The 2-D structure of a non-symmetric synthetic molecule is shown outside a composite image of the line drawing of the synthetic molecule superimposed onto another line drawing in a detailed enzyme environment.
Week 10 4/13/12 Mark's Decahedron	 26, 27	Two representations of the top and side of a many-atom nanoparticle are featured: color-coded ball-and-stick structures (A/B) and unconnected spheres (C/D) color-coded into different groups. Portions of each representation must be visually disregarded from consideration of the overall point group.

The activity images following Week 1 progressed with consideration of molecular representation complexity, image orientation, number of atoms, number of representations, and lecture content. Prominent features that affect the complexity of the images are discussed in Table 5. The Week 2 image introduced chemistry content with a color-coded non-planar molecule. The image was complex in that it had many symmetry operations (T_d point group) but multiple bonds were simplified with line drawings to emphasize geometry and reduce the ligand information students observed. The Week 3 image allowed reinforcement of the symmetry operation identification because the number of atoms was reduced and there was a single principle rotation axis, but it used a more complicated molecular representation with a black and white ORTEP (Oak Ridge Thermal Ellipsoid Plot) structure and atom labeling within the structure.

In addition to the different molecular representations, the image complexity advanced by adding multiple representations within the same week. For Week 4, two representations held the same geometrical information; one was a simplified version of the other. The images in Week 5 were a 2-D structure that showed double bonds and non-carbon atoms and a colored ball-and-stick structure with accurate bond angles. Week 5 marked the point where students were required to visualize not only the internal (symmetry element) traits of the image but to move their visualization to the external task of comparison. The two representations in Week 5 differed enough to result in unique point groups that students had to evaluate.

Weeks 6 and 7 images aimed for yet another aspect of visualization. Both included a part and a whole of the image that could be analyzed with respect to a point group and asked students to study the symmetry of the part before extending their focus to include the whole. Week 6 had only one ball-and-stick representation while Week 7 advanced with multiple representations including a larger, polyhedral structure and the skeletal line drawing of that structure to showcase the geometry. The increase in difficulty and amount of visual information given in Week 7 challenged students to sort through the visual information even if they found the task manageable.

The last advancements of complexity employed application-based activities and a significant jump in difficulty. Weeks 8 and 9 images were carefully chosen to allow students to visualize the symmetry operations they'd been expected to utilize in the past weeks. In lecture, students had been creating and reducing reducible representations. The Week 8 image gave them two molecular orbitals that were more complex than anything they'd encountered. Week 9 put a simple, 2-D structure in a complex environment where students compared and discriminated the molecule from a complex visual environment. Week 10 was not application-based, but the task involved identification of the dominating point group. Students had to visually omit components of the image that detracted from the dominating point group, or continuous symmetry, while the number of atoms increased. The concept of continuous symmetry has been used to teach visualization of symmetry through a quantitative discussion of how much structures differ from perfect symmetry.[28]

The order of the activities was designed to constantly challenge students but supported their visual comprehension of each week's activity by gradually loading more complexity as the semester unfolded instead of taxing students with equally complex images every week. Images advanced in steps that exposed students to differing degrees of complex molecular representation and increasing detail. These activities were designed to slow down students' problem solving as it has been shown that visualization takes more time than analytical methods.[29] Though deconstruction may not be the problem solving strategy all students use to analyze complex images, it requires that students spend time looking at the image at different levels. The activities gave the students opportunities to create thoughtful dimensions of understanding, visual or not, that would be normally overlooked when answering a scientific concept.

4.4.1.3 Task Scaffolding

All questions in the activities required students to interact with the image, but the summary questions specified tasks that gave students a purpose in their analysis of the images. They provided a problem for students to solve so deconstruction questions would have a deliberate intention instead of providing unrelated descriptions of the images. The tasks that accompanied the images were also scaffolded throughout the semester. The summary questions and task scaffolding is described in Table 6; the primary changes in tasks are underlined. With this additional dimension in scaffolding, students needed different problem solving strategies each week rather than learning a single strategy to use on each visualization problem for the semester.

As learned from students' difficulty with describing visual processes in the help sessions, any starting visualization task needed to be open-ended, without a predetermined correct answer. The Week 1 task of describing how to get from one place to another could have many or few steps. This task was designed to let students experiment with descriptive, visual language without intimidating them with a complex image within the chemistry context. Activity tasks never required students to use skills they had not previously been taught in lecture. Lecture content is also presented in Table 6 with the topics utilizing symmetry in bold. The tasks involved challenging examples to explore the depth of the visual components in the course. By Week 2, students had been introduced to the symmetry element definitions and the task used them to guide students through the image. The focus in Week 3 was placed on verbalization and documentation, so the task was not advanced to ease student frustration with the deconstruction questions and visual language. When point groups were discussed in lecture, they also appeared in the activities, as in Week 4. As tools were made available to students during the class, the activity tasks pushed students to use those tools within the visual images. Students may have deconstructed the images in any manner, but the tasks tied the images to inorganic chemistry and gave the activities relevance to what students were studying.

Symmetry elements and point groups were an important visual starting point to use visualization, but more complex tasks prompted students to consider the complex images at different levels. Activities for Weeks 5, 6, and 7 built on symmetry and point groups, but gave students additional tasks beyond identification. Week 5 emphasized the difference between two point groups by asking students to determine the symmetry elements that differed between two representations of the same structure. This demonstrated how a point group changes upon a slight alteration in geometry. The tasks for Weeks 6 and 7 targeted the shift of the center of symmetry in the images. Both weeks, students identified the point groups of the parts and wholes of the molecules and had to determine the elements that caused the two to differ—if they did differ. For this problem, students had to study one image

Table 6. Summary questions, pertinent lecture content and how tasks were scaffolded throughout the intervention.

Activity	Summary Question	Task Scaffolding	Lecture Content Prior to Activity
Week 1 Caerlaverock	Describe how to get from point A to point B.	Students were given an open-ended procedural task to prompt descriptive language.	Nomenclature, structural isomers, quantum mechanics, angular and radial nodes, and Lewis structures
Week 2 [6+4] Metal-Organic Supramolecule	Describe (in words) the locations of all symmetry elements present in molecule **3**. Include all instances of a particular type of symmetry element. Use labels on the portions and parts of molecule **3** to help you put the locations into words.	Students had to <u>utilize new symmetry concepts</u> while using visual language to indicate the location of the elements.	VSEPR, polarity based on geometry, definitions of 5 symmetry elements, draw orbitals with correct angular/radial nodes
Week 3 Cyclic Tricubane Cluster	Describe (in words) the locations of all symmetry elements present in this molecule. Find all instances of a particular type of symmetry element. Use labels on specific parts and groups of parts to help you express the locations into words.	Once again, students had to use symmetry concepts while using visual language to indicate the location of the elements.	Modeling of operations illustrated with a cardboard box and board drawings, demonstration of multiple operations and closure
Week 4 Self-Assembled $Pt(II)_{12}L_{24}$ Spheres	First, show (or describe the locations of) the symmetry operations you need in order to identify the point group. Then, tell me the point group of the structure.	Rather than identify any symmetry elements, students had <u>to evaluate and give the elements needed to identify the point group</u>.	Determination of point groups for classic VSEPR shapes and a few sample molecules, reduction of reducible representations, construction of homonuclear diatomic MO diagrams with little emphasis on orbital images
Week 5 Templated Cyclic Porphyrin Hexamer	a. Give the point group of each figure as it is shown. b. These represent the same structure. What symmetry elements (if any) does the simplified structure (B) have that are not present in the actual structure (A)?	Students had to state the point groups of each representation and <u>determine the symmetry elements that caused the two representations to differ</u>.	Generation of reducible reps from atomic orbitals (drawings of atomic only, drawings of MOs were not discussed), heteronuclear diatomic and polyatomic MO diagrams, completed projection operator for water
Week 6 $SrAu_3Ge$ Nets	a. What is the point group of the top-most net in the figure? b. How, if at all, does the point group change when you consider both nets and the strontium atom? Answer by describing/showing symmetry elements that are gained or lost.	Instead of comparing separate structures, students had to <u>find the point group of half of a structure, the point group of the whole structure</u>, and then <u>state the elements that differ between the two</u>.	MO diagrams for NH_3^{2+} (D_{3h}), NH_3 (C_{3v}), and a MH_3 (D_3) where only central atom atomic orbitals and SALCs were drawn

Table 6 (continued)

Week 7 Microporous Oxonitrido-phosphate	a. What is the point group of a single cage? b. What is the point group of all cages combined? c. List/describe the symmetry elements gained or lost when moving from a single cage to all cages combined. If there's no change, list the elements that you need in order to identify the point group.	Students had to find the point group of one eighth of a structure, the point group of the whole, and then state the elements that differ between the two.	MO review: NH_3 and MH_3, octahedral MO diagrams with review of the location of symmetry elements on an octahedron
Week 8 $B_{12}H_{10}^{-2}$ Frontier Orbitals	Identify the symmetries of the two frontier orbitals. Justify your answer and write the reducible representation for each. a. Give the reducible representation and the symmetry for the MO on the left. b. Give the reducible representation and the symmetry for the MO on the right.	Application: Given the point group, students had to identify the symmetry patterns of the two MOs, then justify their answers with reducible representations of each MO.	SALCs of outer atoms with p-orbitals (ozone), generate a reducible representation of the degrees of freedom of water to find the vibrational modes, and determine the vibrational modes of CO in *mer*-$FeCl_3(CO)_3$
Week 9 Binding the VHL Enzyme	Describe the steps of how the *synthetic molecule* must be manipulated to match its orientation indicated in the enzyme picture. When describing motions of the synthetic molecule, use the rings in the structure as a reference to specifically explain each of your actions (rather than specific atoms). Use either degrees (i.e. 180°) or rotation axis (i.e. C_2) notation in your descriptions.	Application: Students had to describe the steps for moving a molecule into the indicated configuration in the enzyme environment image. Then, they were required to state the extent of rotation on the specified portions of the molecule.	Determine the structural isomer of a molecule with group theory using the vibrational modes of the ligands and ligand field theories (drew LGOs for MH_6)
Week 10 Mark's Decahedron	a. List the symmetry elements required to identify this point group and list the images (A, B, C, D) that helped you determine that specific element. b. What is the dominating point group of the nanoparticle?	To determine the dominating point group of the nanoparticle, students had to describe the omission of a portion of the image to identify the point group of the majority of the image and indicate which image was associated with which symmetry operation.	Applied π-bonding to ligand field theory and constructed an MO diagram for ML_6 by creating the reducible representation for the p orbitals of all six ligands

to find its point group then visually include more of the image. That second step of visual inclusion would cause the center of the structure, and therefore the location where all symmetry elements pass through, to change. The locations of some symmetry elements (reflection planes) remained the same and some moved completely (perpendicular two-fold rotation axes). The activities of these weeks extended beyond what students learned in class, but reinforced the concepts by providing more challenging tasks for students to work within instead of reciting the point group of a many-atom, complex molecule.

Application of symmetry tools students had learned added another angle of task complexity. At this point in lecture, the process of point group determination was no longer discussed explicitly and students were learning to manipulate molecular orbitals. The Week 8 task asked students to identify the symmetries of the HOMO and LUMO of a molecule with C_{2v} symmetry. Asking students to defend their answer with the reducible representations for each orbital compounded this task. Students needed to visualize the C_{2v} symmetry operations and evaluate the character each would generate; they had to judge whether the orbital was changed or unchanged. For Week 9, students had to connect the simplicity of the 2-D structure to the rotated representation in a complex environment. This task was possible to complete analytically and students were instructed to describe the steps and extent of rotation of different parts of the molecule to influence the use of visual skills to solve the problem instead. These application-based tasks acted as a way to continue challenging the students within the activity design while lecture moved to less visually demanding concepts.

In the last activity, students were given a task closely tied to the visual complexity of the image. Rather than finding an exact point group, they were instructed to find the point group of the majority of gold atoms in the structure because some atoms in the image detracted from that point group. During the activity, this concept was referred to as finding the "dominant point group" to better illustrate the task. Students were asked to refer to the image in terms of the color coordinated groups of atoms to suggest the relationships between the groups. They were also asked to describe the motion required to move between the two representations within a specific reference to emphasize multiple views of the structure and give students more information before they chose a dominating point group. This last task was designed to help students appreciate the layers of complexity in the final image. Without the task, the image alone was at risk of being dismissed as too detailed and/or chaotic to see the existing patterns present. Students worked all semester building visual language fluency and had the skill set needed to study the layers of the image. The final task pressed them to spend the time needed to comprehend the representations available to them.

Scaffolding the tasks along with the complexity of visuals used varied the activities to retain students' interest and made each activity challenging. The tasks took into account the content presented in lecture to ensure that students had the background to attempt the activities. Tasks incorporated symmetry in a variety of ways by first introducing symmetry elements, using symmetry elements to justify point groups, comparing the symmetry of two representations, comparing the symmetry of one portion of a structure with the whole, using symmetry in extended application problems, and finally finding deviations from a point group. The task scaffolding built into the intervention allowed students to be guided through highly abstract and visual concepts and gave them a purpose for the critical analysis of complex visuals.

4.4.1.4 Semantic Analysis of Complex Visualization Activities

The visual and task scaffolding design of the weekly visualization activities aimed to help students deconstruct visual problems and learn to communicate mental imagery, but semantic analysis of the activity questions was needed to efficiently relate the objectives of the deconstruction questions. Students were not familiar with describing visualization of chemistry concepts, as evidenced in the help sessions previous to the intervention in Fall 2009/2010. Students frequently volunteered an incorrect guess and preferred to memorize the correct answer rather than use visualization to understand a complicated image. The language of the deconstruction questions required tailoring throughout the semester to guide students to deconstruct the image into its model components and effectively communicate their understanding.

An in-depth semantic analysis was carried out before recitation each week by the researcher and the undergraduate student assisting on the project. Table 7 outlines the major modifications to the activities with respect to semantics. Many of the modifications in the first four weeks were rephrased to help students understand what the questions meant. While working on the activities, students frequently asked aloud what the operation and pattern model component questions were asking. During those initial weeks, the grammar and syntax of the questions was adjusted to clarify the questions aiming to achieve our purposes. When the summary question tasks were scaffolded beyond finding symmetry elements and point groups, the wording of the deconstruction questions changed to reflect and support the new task dimensions (Weeks 5 through 10). The questions were analyzed in detail by the researcher and undergraduate assistant with consideration of the semantic issues encountered in the previous weeks.

Table 7. Semantic analysis of complex visualization activities.

Activity	Semantic Analysis of Complex Visualization Activities
Week 1 Caerlaverock	Based on deconstruction questions used in help sessions, questions were directly modeled on the theoretical framework. The summary question instructed the description of a process.
Week 2 [6+4] Metal-Organic Supramolecule	Adjusted syntax of model component questions and added keywords to translate to a chemistry example.
Week 3 Cyclic Tricubane Cluster	Oral discussion of deconstruction questions and addition of supplementary clarifying deconstruction questions.
Week 4 Self-Assembled $Pt(II)_{12}L_{24}$ Spheres	Removed model component titles (elements, relationships, etc.) and modified the grammar to change deconstruction questions from passive voice to declarations. Added more clarifiers to operation and pattern fields.
Week 5 Templated Cyclic Porphyrin Hexamer	Altered model component questions from descriptions to comparisons to assist with the task scaffolding.
Week 6 $SrAu_3Ge$ Nets	Modified the relationship model component (find relations in one Au/Ge net and how the two Au/Ge nets relate to each other) and the operation model component (which operations will give an indistinguishable position).
Week 7 Microporous Oxonitridophosphate	Modified the relationship model component (how parts relate to each other in one cage and how the collection of cages relate to one another).
Week 8 $B_{12}H_{10}^{-2}$ Frontier Orbitals	All model components asked students to refer to one MO image and in the operation model component, descriptions of were encouraged instead of lists of operations.
Week 9 Binding the VHL Enzyme	Adapted the model component fields to support the task: relationship (how molecule relates to the enzyme pocket), operation (how to move the individual parts of molecule), and pattern (overall motion of the synthetic molecule).
Week 10 Mark's Decahedron	Tailored model components to refer to groups of Au atoms: operation (how A/C images may be moved to get B/D images), and pattern (which Au groups contributed to the dominating point group).

Students were required to document their responses to provide evidence of their visualization processes, as was similarly achieved by Lesh, et al. when developing the Modeling Theory of Learning.[2] Eliciting visual information from students was difficult. As discussed in the Literature Review, visualization and verbalization are separate brain functions.[30] However, documentation is required to monitor changes of visualization skills. In addition, practice developing visual language helps students become adept at understanding visual, descriptive language as it is used to describe visual topics, such as inorganic chemistry.

In combination with the semantic analysis and modifications to the activities, the researcher verbally reinforced the deconstruction questions during instruction. The researcher provided instantaneous feedback and modeled interactions with complex images and visual language during the activities. Students were encouraged to spend time looking at the image and do their best to describe what they were "seeing" and use the activity questions for guidance. Student questions during the activities in combination with their written responses were the primary sources for changes to the activities throughout the semester.

Overall, detailed measures were taken to design the complex visualization activities in a way that would challenge students throughout the duration of the intervention while still teaching them to deconstruct and effectively verbalize how they analyzed the images. The activity format was constant each week to serve as a foundation for students to deconstruct visual concepts and gain practice in expressing the results of their deconstruction. Visual scaffolding pushed students to critically analyze visual representations that were more complex than what they experienced in lecture. It also pushed students to work to understand the visual concepts presented in these representations. The task scaffolding, informed by lecture content, varied the goals of the activities to maintain relevance and students' interest. Both the visual and task scaffolding were supported by thorough semantic analysis of the activities. The lessons offered through student interactions with the visual concepts in symmetry and the deconstruction questions that helped to engage students in discussion of visual concepts led to a meticulous design of a set of activities to challenge students to analyze and discuss complex visualization problems.

4.4.2 Reinforcement of Visualization in Teaching

The principles that guided the design of the visualization activities also guided the researcher's teaching in recitations. The weekly visualization activities were designed to teach students the language of describing their own visualization while applying visualization and deconstruction to difficult images. Inorganic chemistry presents many visually rich concepts beyond symmetry. Deconstructing the concepts to understand the model components, relating the concepts to reality, and acknowledging a problem-solving strategy are practical methods of analysis that were carried out in recitations beyond the ten to fifteen minutes occupied by the visualization activities.

In the Modeling Theory of Learning, deconstruction of ideas into model components was valuable to the students in understanding concepts and to the researchers in observing how students solved problems.[2] To help students work through problems in chemistry that require understanding an image and especially visualization, identifying where they become confused and give up or assume incorrect information is instrumental for the instructional guidance. Observations during the help sessions identified common points where students became confused, but deconstructive questions helped students to recognize that they may have made an incorrect interpretation or find a new path of analysis by reexamining the relationships in the models. When presenting a topic during recitation and inviting student participation and discussion, it was not uncommon for students to decline. The incorporation of model component questions into discussion, especially relationship and pattern components, helped guide students to study the problem more carefully and encouraged more students to get involved.

Providing students with comparisons to reality was used to engage students. Difficult examples were related to previously covered topics and imagery and scenarios from everyday life outside of inorganic chemistry. If a visual representation of chemistry phenomena reminded students of something they were familiar with, they were encouraged to think about how they would regard that familiar example in the chemistry situation. For example, when discussing the molecular geometry of a trigonal bipyramidal structure towards the beginning of the semester, students asked questions about existing symmetry elements even though models were available and bond angles had been discussed. The comparison of the three equatorial atoms to a paper triangle provided students with a basic visual description with which they were familiar to test symmetry operations upon. This example is very simple, but demonstrated to students that they were equipped with the skills and reasoning to approach the problem.

The use of problem-solving strategies is not unique to inorganic chemistry, chemistry, or even learning. During recitations, the researcher often paused discussion to ask students to reflect and summarize how a task was carried out. The later half of the semester involved many topics that utilized the production of molecular orbital diagrams. Students often requested repeated demonstrations of how they were constructed. These requests were always practiced by first asking the class "What do we do first?" Many times, specific answers were noted for later in favor of generalized steps that would help the students draw any MO diagram instead of the specific example under discussion. Extra time was spent to discuss general strategies of all process-based problems to model how students could use reasoning to apply what they know to a new problem.

Extending the principles relayed in the theoretical framework served both to engage students in recitation and model the problem-solving strategies outlined in the visualization activities. The benefits of deconstruction, comparisons to reality, and reflection upon the problem solving process were observed in helping students to discuss visualization and utilized to teach students to work with complex visualization activities. Incorporation of these principles into teaching sought to promote a sophisticated and introspective knowledge of both the course material and how to approach learning new concepts.

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CHAPTER 5.

DATA COLLECTION AND ANALYSIS

5.1 Focus Group Interactions with Physical Models

5.1.1 Common Problems and Questions

During the pilot studies in 2009 and 2010, questions from both lecture and help sessions were recorded to understand and gauge the kinds of problems students were expressing with regards to symmetry and visualization. All questions were reviewed and categorized as repetition, clarification, extension, related new, or example request questions. Students asked for descriptions or answers to be repeated (Repetition) or asked if a term had the same meaning as another term (Clarification). Extension questions included follow-up questions about an example under discussion (Extension). Questions relevant to the topic that had not yet been discussed were grouped as Related New while requests for examples to be demonstrated were categorized as Example Request. Categorizing students' questions helped to pinpoint how the model systems could be used to clarify different aspects of symmetry operations. Table 8 displays examples of recorded student questions from 2009 and 2010 and their classifications. Phrasing and context were taken into consideration to more accurately infer students' goals behind asking specific questions. Student questions and requested topics were categorized based on the context of the lecture or help session and whether the question had previously been explained in the same instructional period.

Table 8. Examples of recorded student questions per category.

Classification	Recorded Student Questions and Requested Topics
Repetition	"Can you go over what you mean by triangular face?"
	"Can you show again where the 4 C_3's are?"
	"So, S_4 is the combination of C_4 and the reflection?"
Clarification	"What's the difference between a C_4 and a C_2 (C_4^2)?"
	"What's five-fold?"
	"Which is the face [shown] on the screen?"
Extension	"I understand the 3 C_4 operations, but why are there 4 C_3's instead of 8?" (*Referring to 8 C_3 operations on the character table.)
	"How can you detect symmetry from an image?"
Related New	Comments relating to understanding dashes and wedges with respect to a horizontal reflection plane
Example Request	"I can't draw an improper rotation. Can you show me?"
	"Will you do an S_n for an octahedron and a tetrahedron?"
	"How do you make a model from the pictures in the book?"

A majority of questions from Fall 2009 and 2010 stemmed from students reported inability to 'see' (visualize) a symmetry element or operation when presented. An example of this recurring challenge during lecture and help sessions is when students asked where the triangular faces on an octahedron were located after they were pointed out on a 2-D image on a projector or on an octahedral molecular model (Repetition). Identification of the three vertices of that face leads to the identification of the three-fold axis in the O_h point group. Even after the vertices were explicitly pointed out, the repetition of students' requests demonstrated that *seeing the location of the vertices did not make the three-fold axis apparent to those students*. Some students did not trust the definition of an improper rotation and many reported the inability to see or draw an improper rotation even if they were able to correctly describe it as a proper rotation followed by a horizontal reflection. It was also common for students to apply a vertical reflection instead of one that was correctly perpendicular to the rotation axis. Symmetry terminology was frequently confusing for students, which is reflected in Table 8. Each semester, students asked if a five-fold axis was the same thing as a C_5 operation. Misunderstanding terminology and the language used to describe the concepts may contribute to students' difficulty comprehending the definition of a symmetry operation.

5.1.2 Role of Kinesics

When interacting with the model systems and discussing symmetry problems, students often gestured with their hands or around molecular models. The frequency that students gestured to ask questions, work through examples, and explain ideas led the project to consider the role of kinesics, any non-verbal gesturing or body language[1], in visualizing and understanding symmetry. Visual information that reaches multiple senses can reduce the cognitive load students use to understand concepts.[2] Using physical models and gesturing while interacting with models or manipulating a model or 2-D image may provide tangible input to complement what students see. This may lead to an externalization of the visualization process to reduce students' cognitive load on their working memory.[3]

The most frequent request from students attending the help sessions was to locate all the symmetry elements of a particular molecule. Students showed much enthusiasm in fitting their own models into the 3-D Coordinate Axis system for this task. Many used Styrofoam spheres and toothpicks along with the model kits provided. Students used the system to methodically enact proper rotations, improper rotations, reflections, and inversions. If students did not have a homework question to show an operation, they requested examples that they could build onto the system. All students in a focus group of ten agreed that it was very useful to track bonds of an octahedron or a D_{4h} molecule (Figure 10) with dry erase markers on the 3-D Coordinate Axis system. Students touched the modeled bonds, pointed out the motion of operations with their hands and writing utensils, and practiced enacting the operations back and forth. All gesturing occurred without prompting or encouragement from the researcher. In this particular large group, students sitting in the back moved in to enact improper rotations on the 3-D Coordinate Axis system and to use the Proper Rotation Axis system to find the C_3 axis of an octahedral structure even though they had just watched their classmates do the same thing. Students touched portions of the molecular models within the systems repeatedly to reaffirm starting positions after they had moved a molecular model.

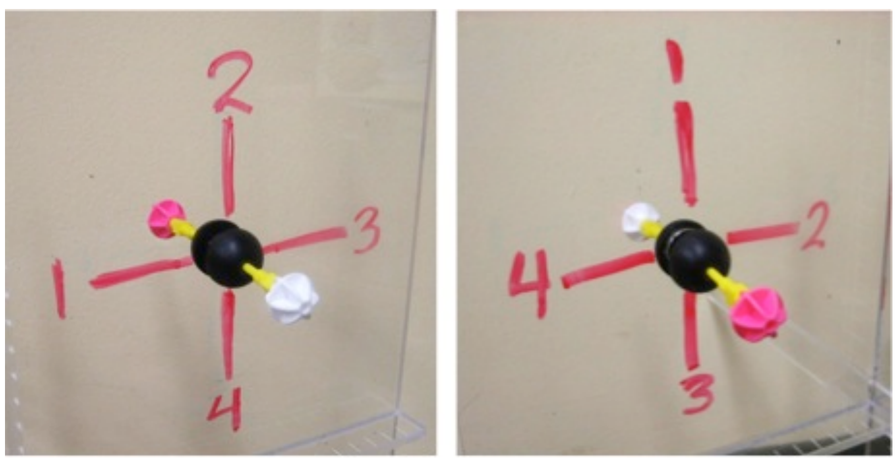


Figure 10. S_4 improper rotation demonstrated on the 3-D Coordinate Axis system.

Student's kinesic interactions with the model systems demonstrated that they methodically tracked symmetry operations on portions of molecules at a time. Using hands and writing utensils, they would hold onto one atom center or bond at a time as they moved it. Reaffirmation of a motion on other parts of the molecule after the students had tracked the first portion supports that they separated the motion of different parts of molecules. If students' gestures around the model systems are an externalization of what they are thinking or visualizing, the tracked motions of individual parts of the molecules may indicate that students used basic deconstruction to begin to understand the symmetry operations as displayed on the model systems.

5.1.3 Obstacles in Verbalization

Students had little difficulty articulating their requests for symmetry examples and demonstrations of problems presented in lecture, but all students had difficulty answering discussion questions about the symmetry operations themselves. Many were able to answer 'yes/no' to direct, one-step questions about where an atom would end up after an operation and some could gesture to the path an atom would take when affected by a symmetry operation. When students were asked questions about the motion of molecules as they underwent symmetry operations, such as "Describe the motion of a particular atom on a molecule as the molecule completes a horizontal reflection", they either did not answer or asked what the question meant. Students from these focus groups could eventually answer the question, however, only when it was broken down into simpler, direct questions.

The discussions from these focus groups were inconclusive as to whether students weren't visualizing symmetry operations, whether they couldn't verbalize their visualizations, or whether they didn't understand the language and terminology used by the researcher. When students are working through complex tasks, helping students articulate and verbalize their thoughts helps them make sense of the tasks and manage their progress.[4] The limited verbal and written responses to requests for descriptions of students' visual processes suggests that an emphasis on student verbalization abilities was needed and, at the least, beneficial to learning symmetry.

5.1.4 Field-Tests of Visualization Activities

As the activities for the model systems were introduced in 2010, students in the help sessions became more involved with the model systems once they were armed with a written guide to interact with the systems. The activities regulated the discussion topics generated across help sessions and provided a written representation to accompany the verbalized concepts.

The 3-D Coordinate Axis activity featured practice with improper rotations, the most frequently requested symmetry operation. When practicing improper rotations on molecules drawn into the activity worksheets, allene (D_{2d}) and staggered ethane (D_{3d}), it was difficult for students to see that the degree of rotation in the improper rotation operation should be different than the degree of the principle rotation axis. Even after enacting an S_4 operation in steps on an allene molecule, students were not able to describe the symmetry elements present in the molecule. When the operations were demonstrated for students or students were assisted in modeling the operations themselves, *they did not document what they observed*. Consistent patterns demonstrated by students included:

a) *Frequently asking for symmetry operations to be demonstrated repeatedly*. When students were asked to follow up on questions about improper rotations or asked to respond to the original question (Describe the steps of enacting an improper rotation with the molecular model on the system), they would instead ask for the operation to be demonstrated again. This reflects on the students' perception that by simply having the instructor repeat a demonstration, they'll be able to visualize what the instructor is illustrating.

b) *Difficulty connecting the definition of an improper rotation to a process or a resulting orientation.*

Students often asked for improper rotations to be shown on octahedral and tetrahedral structures (as shown in class). To assist these students in recalling improper rotations for class, a process based on the operation definition from lecture was discussed to describe an improper rotation on both a drawing of a molecule and the physical model within the system. Students were encouraged to label atoms on both the drawn and physical molecules to help them track where atoms would end up after the initial rotation operation and anticipate the correct placement of atoms after the reflection. During these discussions, students were surprised to learn that the original molecule looked the same (indistinguishable) as the molecule that had undergone the symmetry operation. Consequently, students thereafter requested help labeling atoms. This example supports that showing students how to label atoms in symmetry operations provided students with reassurance of correctly completed operations because students could check the resulting location of each label.

c) *Students avoided any form of documentation.*

During help sessions, students utilized the worksheets to reference the questions, but only marked on them when explicitly instructed. When they were required to write answers to the questions, their responses were incomplete sentences and phrases. Even verbal descriptions had to be requested rather than volunteered. Consequently, the collected activities show no evidence of student visualization. Though students were given structured (activities) and unstructured (requested problems and discussion) opportunities to show their work on visual problems, the documentation obstacle suggested that students did not value a record of what they were learning and instead preferred to work through the questions and examples as they experienced them.

d) *Students needed help to build models and draw pictures of molecules.*

Students did not mark on the molecules drawn on the worksheets, draw pictures, or describe answers to the questions even when encouraged and given time during the help session. Many students had difficulty building models to represent 2-D structures given on the activity as well. In an extreme case, a student was unfamiliar with dash and wedge depth cues and showed agitation and frustration when faced with reproducing a drawing of ethane. The requests for assistance with interpreting and producing 2-D molecular images during the help sessions support that students did not know how to produce visual representations of the molecules and symmetry elements inherent in the structures.

e) *Verbally deconstructing symmetry operations helped generate more student discussion and engagement.*

Any repetition and clarification requests and indications of prolonged confusion were answered by breaking down the question into more basic steps to allow students to answer. Students visibly relaxed when questions were simplified to a familiar level such as, "How many bonds are around the carbon atom on this molecule?" After answering questions centered on observations about the model systems and structures, students tried answering portions of the task questions and asked more questions to clarify what was expected.

Supplementing the activities with simplified questions helped to involve students in the activity and get them to begin verbalization.

The recorded observations from the help sessions showcased common problems students had with learning symmetry. The help sessions also demonstrated that students encountered basic obstacles in understanding visual representations, producing visual representations, and articulating visual descriptions. Documentation from these worksheets gave limited insight to how and if students analyzed the concepts with mental visualization. These focus groups were instrumental for the researcher to grasp the fundamental challenges students were facing and supported the need for better communication of students' confusion and comprehension of symmetry concepts.

5.1.5 Teaching with Structured Visual Deconstruction

The activities associated with the physical model systems were written to highlight how examples of symmetry operations could be deconstructed into portions or layers that students could examine in order to simplify the visually demanding concepts. As deconstructive questions helped foster discussion for topics students sought help with, the researcher structured discussions with the same deconstructive principles presented in the framework.[5] Though deconstruction of the visualization process did not provide direct evidence of student visualization, it helped generate more questions and interactions with the models from students. The following strategies exemplify some of the advantages of using deconstruction in leading student discussion.

a) *Begin with observations of what is given and what it's composed of.*

Many of students' difficulties were first addressed by prompting students to observe images and structures in more detail. Students were encouraged to look for the model components of the visual as was consistent with the Modeling Theory of Learning framework. Students reported not "seeing reflection planes" or not being able to differentiate between reflection planes and C_2 rotation axes perpendicular to the principle rotation axis. Instead of indicating the location of a symmetry element, students were encouraged to consider the definitions of the symmetry operations they learned and examine the environments around the molecule for consistencies with the definitions. An atom repeated three times around a molecule indicated that those bonds were related by a 3-fold rotation. When students took time to identify a single repeating component, they were more receptive to identifying an axis that related all three components.

b) *Identify the relationships between components to find additional operations in different environments about the molecule.*

Acknowledgement of what relationships denote a symmetry element was a powerful strategy for locating elements in a molecule. An example of using relationships to find reflection planes utilized in help sessions featured eclipsed ethane (Figure 11). Students identified the reflection plane in the plane of the paper containing atoms A and B (*trans* to one another) and the three bonds connecting them. To look for similar planes, students were encouraged to look for similar atom relationships in the molecule. Determining relationships was motivated by the Modeling Theory of Learning (relationships model component).[5] Instead of rotating the ethane model looking for more planes, students had a specific relationship to find. From there, students could determine that atoms C/D and E/F indicated other planes because they were related just as atoms A/B were. Perpendicular C_2 rotation axes were located in the same manner, but differentiated from planes by asking students to move the atom labels as if they'd rotated 180°. Envisioning the molecule undergoing the symmetry operation (operations model component) and analyzing the placement of the labels directly use deconstruction to understand the definitions of the operations and how they affect where the labeled atoms end up. This method aimed to help students extend symmetry element identification to more complex molecules.

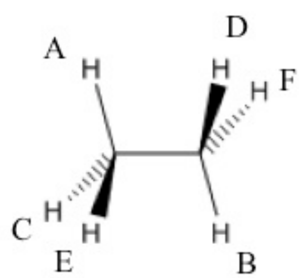


Figure 11. Staggered ethane vertical reflection planes: one containing atoms A and B, one containing C and D, and containing E and F.

c) *Deconstructed steps of challenging questions can reveal mistakes and misconceptions.*

The required deconstruction of symmetry operations provided students with the opportunity to display mistakes they may make while enacting symmetry operations. A recurring mistake was the confusion between a reflection and a two-fold rotation. A typical case from 2010 was a group of three students that were enacting an improper rotation operation on staggered ethane (Problem 1 on the 3-D Coordinate Axis activity). When completing the horizontal reflection on the model system, they rotated the two halves of the molecule front to back so only a single labeled atom on each of the 'halves' was in the correct place. After the students were prompted to confirm where each atom should end up after the reflection operation, they realized that they had not completed a reflection operation. For the remainder of the activity, students were observed checking that the operations they enacted matched their definition of the operation and frequently gesturing where additional reflection planes and rotation axes were located around the molecular model and the symmetry elements framed by the 3-D Coordinate Axis.

The Modeling Theory of Learning framework guided the design of model systems and accompanying instructional materials using deconstruction of complex concepts.[5] The deconstruction principles took on an important role in explaining students' questions about symmetry operations and helping students work with the model systems. Though students at this point were unable to verbalize or document their visual understanding of symmetry, deconstruction helped the researcher communicate the subtleties between different operations and how to initially locate a symmetry operation.

Several impactful lessons were gained from observing students, discussing their difficulties with symmetry visualization, and incorporating deconstruction into model system instruction. Categorization of student questions provided insight to the extent of student comprehension of concepts under discussion. Observing student kinesics may attain potential evidence of deconstructive visualization as students may use questions and gestures to try to understand symmetry topics, however, students exhibited difficulty verbalizing and documenting their understanding. *Deconstruction proved helpful in getting students to discuss intimidating tasks as the first step towards documentation and as a way to model* *skills like drawing visual representations and building models*. As an analytical method, deconstruction provided a path to understand how symmetry elements related different parts of structures. When students slowed visualization down enough to document or verbalize their deconstruction, mistakes and misconceptions were clearly revealed. During the focus group studies, deconstruction showed potential as a powerful strategy to promote visualization and help students interpret and solve visually complex problems.

5.2 Observation Rubrics

5.2.1 Collection of Field Observations

Analysis of observations from lectures from 2009 and 2010 and students' interactions with the model systems showed that students asked different levels of questions (presented in Table 8) that could be indicative of different levels of thinking and engagement with visualization. The use of repeated phrases, copied gestures and the nature of students' questions indicated that there might be a link between how students utilize and demonstrate visualization artifacts and the ways instructors model visualization. Using observation rubrics, this research sought to investigate the following question.

> ***What can classroom observations suggest about the relationship between visualization indicators enacted by the instructor and students' questions and demonstrated visualization artifacts during class?***

To explore connections between the instructor's and students' indicators of visualization during class, questions and actions of students and the instructor were tracked on field observation rubrics tailored to recitation or lecture (Appendix C). The researcher observed Inorganic chemistry lectures during the Fall 2011 and Spring 2012 semesters while the three accompanying recitation sections of Fall 2011 were observed by two assisting graduate students. Both the instructors (in lecture) and the researcher (in recitation) promoted an environment where visualization was encouraged and used to understand and solve problems in the course through visual language, gestures, and the use visual representations. Student questions were the primary source of data obtained through the rubrics and more appropriately represented student engagement with course material than student visualization. As will be shown in the analysis of the data, a more appropriate question would be:

What can classroom observations suggest about the relationship between instructor engagement with visual material and student engagement in class?

The researcher observed each lecture period of Fall 2011 and Spring 2012. Specific student questions and notes about demonstrated examples were recorded in addition to the tallied marks in the observation rubric fields. The five field categories are listed in Table 9 along with the percentage of lectures that each field was observed. The first three fields focused on the students: Student Questions and Responses, Student Kinesics (gesturing), and Interaction with Physical Models (moving, gesturing, or building). Student questions were categorized using the context of class discussion and phrasing of the question, as previously practiced during the pilot studies. The Class Mechanics category was added to keep track of what happened in different classes. The rubric fields were retained from Fall 2011 to Spring 2012 to collect comparable data during the two semesters in order to look for patterns or relations amongst visual representation interactions of each instructor with the students. In

Table 9. The percent of lectures that an instance of each observation was observed during the Fall 2011 and Spring 2012 semesters.

Observation Field	**% Lectures in Fall 2011**	**% Lectures in Spring 2012**
Student Questions & Responses		
Repetition/clarification questions	92	96
Example request	16	8
Specific problem, new to discussion	68	28
Additional question on problem being discussed	80	96
Used action verbs in response	28	12
Described model components	4	0
Made a comparison *(to real-life objects, previous examples)*	4	0
Able to describe steps of operation	0	0
Student Kinesics		
Gesture with both hands in air	12	0
Gesture with one hand in air	12	0
Gesture with pen in air	0	0
Student Interaction with Physical Models		
Manipulate molecular model/homemade kit/pen as model	0	0
Gesture around stationary model (hand or pen)	0	0
Build model at desk	0	0
Instructor Actions		
Used action verbs to describe	96	72
Described model components	28	24
Made a comparison *(to real-life objects, previous examples)*	76	56
Described the steps of an operation	44	88
Gestured with hands (no model or image used)	100	64
Gestured with pen/pointer (no model or image used)	8	0
Manipulated a model as demonstration	28	8
Gestured around physical model	16	8
Made a drawing to explain a concept	92	96
Gestured around 2-D image (hands or pointer)	68	100
Explain a reason and/or goal (*)	Not included	96
Class Mechanics		
Number of problems worked in class	4	56
Time allotted to work problems	4	4
Time allotted to manipulate models	0	0
Time taken for class discussion	0	0
Instances of instructor-generated discussion	0	0
Instances of student-generated discussion	0	0

Spring 2012, one additional field was added to the instructor actions: ‘Use of a reason/goal (*).’ This responded to the need for a category that dealt with the emphasis in lecture of real-world applications. Data was not collected on exam days because exams occupied an entire class period. The number of students in attendance was also tracked for each semester

(Appendix D), but individual attendance, the dates students dropped, and late attendance were not recorded. Because of this, specific actions and questions could not be attributed to individual students.

The observation rubrics were written to be comprehensive in order to observe subtle differences, such as different types of gesturing and questions in different contexts. As shown in Table 9, many fields were not frequently observed throughout the semester. To be able to observe any possible ongoing trend, fields that appeared below 50% were omitted from analysis or combined into a closely related field during the initial grouping. For example, the instructor's manipulation of a model and gestures around that model were combined as 'Model use.' Field combinations are shown in Table 10. Fields that were infrequently observed were shaded and labeled 'N/A.' 'Model use' appeared under the 50% threshold, but was a primary interaction with visual representations during symmetry, so it was retained in the analysis. 'Described the steps of an operation' and 'Use of a reason/goal' appeared more than 50% of the time only for the Spring 2012 instructor. These were not included in the comparative analysis because they were not observed regularly or at all for the Fall semester. In addition, each field averaged two instances per lecture and appeared as a consistent trend, which made it difficult to link to the varying peaks of the 'Total student questions' pattern (Figure D.13). The most important point learned from the data in Table 9 was that students engage in lecture primarily through questions. Students rarely elaborated in their responses to the instructor's questions or independently gestured or used models at their seats. The instructor-based fields show that a variety of visually rich methods were employed by both professors and the differences between them help to describe the different teaching styles. To

Table 10. Frequently demonstrated observation fields within the five categories of the Lecture Observation Rubric with initial and final groupings.

<table>
<tr><th>Observation Field</th><th>Initial Grouping</th><th>Final Grouping</th></tr>
<tr><td colspan="3">Student Questions & Responses</td></tr>
<tr><td>Repetition/clarification questions</td><td rowspan="2">Basic Questions</td><td rowspan="4">Total Student Questions</td></tr>
<tr><td>Example request</td></tr>
<tr><td>Specific problem, new to discussion</td><td rowspan="2">Extension Questions</td></tr>
<tr><td>Additional question on problem being discussed</td></tr>
<tr><td>Used action verbs in response</td><td colspan="2">N/A</td></tr>
<tr><td>Described model components</td><td colspan="2">N/A</td></tr>
<tr><td>Made a comparison (to real-life objects, previous examples)</td><td colspan="2">N/A</td></tr>
<tr><td>Able to describe steps of operation</td><td colspan="2">N/A</td></tr>
<tr><td colspan="3">Kinesics</td></tr>
<tr><td>Gesture with both hands in air</td><td colspan="2">N/A</td></tr>
<tr><td>Gesture with one hand in air</td><td colspan="2">N/A</td></tr>
<tr><td>Gesture with pen in air</td><td colspan="2">N/A</td></tr>
<tr><td colspan="3">Interaction with Physical Models</td></tr>
<tr><td>Manipulate molecular model/homemade kit/pen as model</td><td colspan="2">N/A</td></tr>
<tr><td>Gesture around stationary model (hand or pen)</td><td colspan="2">N/A</td></tr>
<tr><td>Build model at desk</td><td colspan="2">N/A</td></tr>
<tr><td colspan="3">Instructor Actions</td></tr>
<tr><td>Used action verbs to describe</td><td>Visual Language</td><td>Visual Language</td></tr>
<tr><td>Described model components</td><td colspan="2">N/A</td></tr>
<tr><td>Made a comparison (to real-life objects, previous examples)</td><td>Reality Comparison</td><td>Reality Comparison</td></tr>
<tr><td>Described the steps of an operation</td><td colspan="2">N/A</td></tr>
<tr><td>Gestured with hands (no model or image used)</td><td rowspan="2">Gestures</td><td rowspan="2">Gestures</td></tr>
<tr><td>Gestured with pen/pointer (no model or image used)</td></tr>
<tr><td>Manipulated a model as demonstration</td><td rowspan="2">Model Use</td><td rowspan="4">Visual Representation Interaction</td></tr>
<tr><td>Gestured around physical model</td></tr>
<tr><td>Made a drawing to explain a concept</td><td>Drawings</td></tr>
<tr><td>Gestured around 2-D image (hands or pointer)</td><td>Gestures around 2-D</td></tr>
<tr><td>Explain a reason and/or goal</td><td colspan="2">N/A</td></tr>
<tr><td colspan="3">Class Mechanics</td></tr>
<tr><td>Number of problems worked in class</td><td colspan="2">N/A</td></tr>
<tr><td>Time allotted to work problems</td><td colspan="2">N/A</td></tr>
<tr><td>Time allotted to manipulate models</td><td colspan="2">N/A</td></tr>
<tr><td>Time taken for class discussion</td><td colspan="2">N/A</td></tr>
<tr><td>Instances of instructor-generated discussion</td><td colspan="2">N/A</td></tr>
<tr><td>Instances of student-generated discussion</td><td colspan="2">N/A</td></tr>
</table>

gauge if questions are the only way students engage in lecture, it would be interesting to observe the class if gesturing and model use was elicited from the beginning of the semester.

Students may learn how to incorporate these methods of visual representation interaction by putting them into practice early.

Fields were combined to facilitate the emergence of patterns and correlations between consistently represented fields. Table 10 displays how students' repetition and clarification questions were initially combined as basic questions while problems new to the discussion and additional questions along the same topic are grouped together as extension questions. Both basic and extension student questions were evenly observed throughout the semesters. Combining these subsets into 'Total student questions' provided a large enough number of instances that a pattern could be observed from the more prominent peaks. The separation between students' basic and extension questions may be found in Figure D.2, Appendix D. After the initial grouping, there were six frequently represented instructor fields. Analysis of these fields led to the combination, first, of 'Drawings and Model Use', and finally of combining 'Drawings,' 'Model Use,' and 'Gestures around 2-D Images' into 'Visual Representation Interaction.' Final groupings are also displayed in Table 10 and the rationale behind these combinations will be discussed in the following section.

5.2.2 Analysis of Observation Rubrics

The nature of the observation rubrics provided a large amount of data. Each day's fields were totaled and tracked within a spreadsheet specific to the course. The raw lecture data for both the Fall and Spring semesters consisted of field totals observed over twenty-five lecture periods. From the raw data, fields that were consistently observed throughout the semester were examined for trends. The trend of 'Total student questions' was overlaid onto the six instructor-based fields outlined in the initial grouping from Table 10. The pairings of these student-to-instructor trends (Figures D.4-D.9 in Appendix D) were examined for similar patterns. Increases and decreases of instructor actions were sought to match with the increases and decreases in student questions in either the overall trend or in certain portions. To gauge the extent of correlation, total student questions were plotted against the analyzed instructor fields to obtain a coefficient of determination (R^2) for each pairing. Each R^2 value is listed on the corresponding figure in Appendix D.

Table 11. Descriptions and examples of the analyzed instructor rubric fields.

Instructor-Based Field	Description & Example
Visual Language	Includes use of action verbs or vivid description of a concept: "spinning," "crossing a node," "bond projects straight out toward Joe's face"
Reality Comparison	Comparison to real world or previous chemistry examples: "like a doughnut with cones above and below," "four fork tines are quadruply degenerate" **A comparison may be discussed briefly or extensively, but each comparison is only counted once.*
Gestures	Instructor use of hands or writing utensils specifically to describe a topic, but not while expressing emotion or natural accompaniments to speech: gesturing distance of an electron from the nucleus, not waving hand to ask a student to elaborate on a response
Model Use	Any manipulation (turning, building a model) of a 3-D object or gesturing around that object: moving a labeled atom to illustrate a reflection, pointing to the angle formed between bonds
Drawings	A unique drawing to describe a concept or illustrate a problem: a molecule with symmetry elements indicated, one orientation of a molecule, one MO diagram, each drawing of an MO or LGO **Alterations to a drawing were not counted as an additional instance.*
Gestures around 2-D Images	Gestures around a projection, chart, or drawing on the board to supplement discussion: using hands to show the location of a plane on a molecule projected on a screen, gesturing the path of an atom's inversion on a blackboard drawing

As discussed in the previous section, 'Total student questions' was chosen to compare to each of the instructor fields because the combination of the questions resulted in large enough numbers to discern a distinct pattern, especially in Spring 2012, where basic and extension questions followed a very similar pattern (Figure D.2). This research sought relationships between visualization indicators of students and the instructor. Separation of basic and extension questions did not necessitate the separation of visual and non-visual questions. The rubric fields are briefly described on the observation rubrics presented in Appendix C, but to illustrate the visual nature of the instructor categories under analysis, Table 11 provides examples of each field/grouping.

Upon qualitative analysis of the paired student/instructor trends, characteristics of some of the instructor field trends suggested that further grouping might provide more similar patterns. In Figure D.7, 'Model use' consists of primarily a single peak in the first half of the semester for both Fall 2011 and Spring 2012 that corresponds with a significant peak in 'Total student questions'. This peak corresponded with the introduction of symmetry operations and lead into group theory. In Figure D.9, the 'Drawings' trend lacks a peak in the same location as the 'Model use' peak. To help students visualize symmetry operations in three dimensions, the data in Figure D.9 demonstrates that both professors opted to use models as instructional visuals rather than two-dimensional drawings. Figure D.10 in Appendix D combines the data from 'Drawings' and 'Model use,' which provided a pattern that better resembled 'Total student questions.' Because 'Model use' was a combination of manipulation and gestures around a 3-D object, 'Gestures around 2-D images' was also combined to the actions in Figure D.10. This addition resulted in the most qualitatively similar patterns and the highest R^2 values of all pairings analyzed for both Fall and Spring. These three categories showcase how the instructors used visual representations to explain concepts to students, rather than verbal descriptions of visuals. This combination was generalized to 'Instructor interaction with visual representations' and the pairings are shown in Figures 12 and 13. The similarity between 'Total student questions' and 'Instructor visual

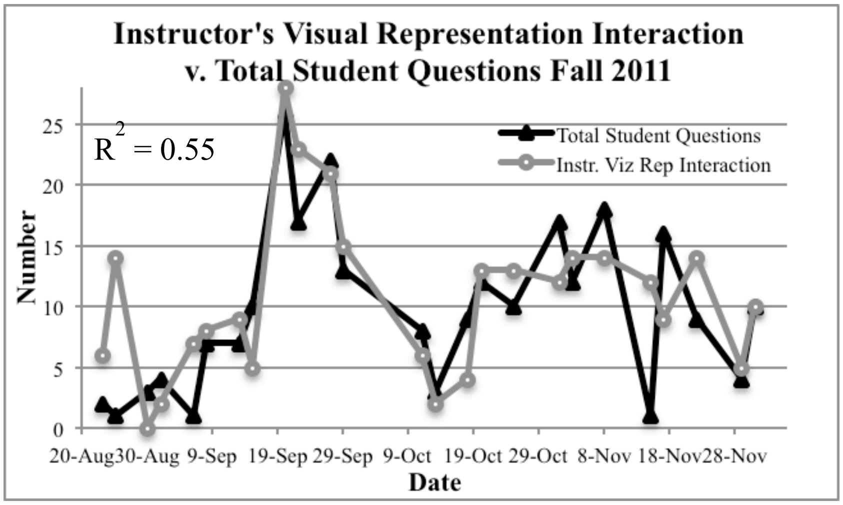


Figure 12. Total Student Questions in Fall 2011 compared to Total Instructor Visual Representation Interactions.

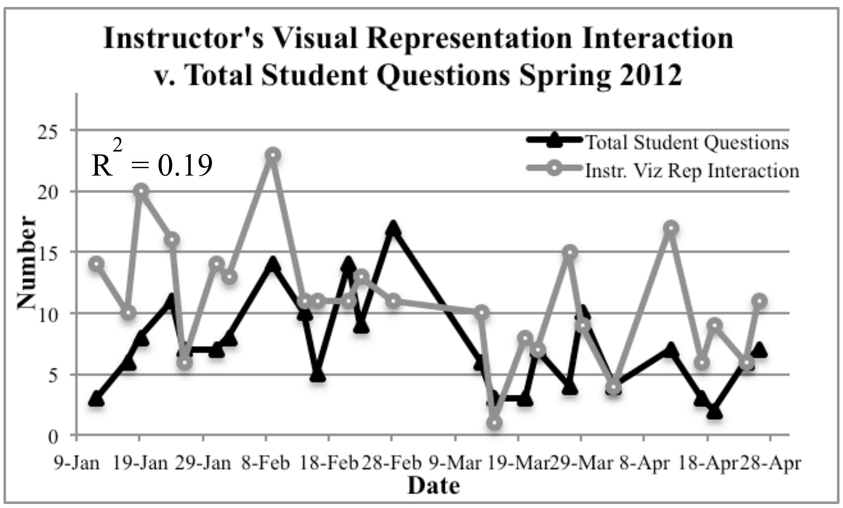


Figure 13. Total Student Questions in Spring 2012 compared to Total Instructor Visual Representation Interactions.

representation interaction' suggests that an instructor's actions in class that extend beyond a variety of verbal methods is answered with student questions. Table 9 shows that the various types of questions were the only way students participated in class. Class notes were not monitored in this research, so questions were the most appropriate measure of student engagement. The similar patterns in Figures 12 and 13 show that increased interaction with visual representations in class was answered with increased student engagement in class.

The combined instructor fields from Fall appeared to follow a very similar pattern to the total student questions and additional ways to display these patterns were sought. The points of each instructor field were plotted against the points of 'Total student questions' and a coefficient of determination was calculated, shown on each comparison plot (Figures D.4-D.10, 12, and 13). Though not as tight a correlation, the plot of Spring data also show patterns of correspondence between the instructor's visual representation interactions and the number of student questions. The correlation plots used to calculate the R^2 values for Figures 12 and 13 are included in Appendix D (Figure D.11). R^2 values for the other comparisons were calculated in the same manner. The overall low values of the coefficients of determination suggest that this statistical test may not best describe this data. The R^2 values within Figures D.4, D.6, D.7, D.8, and D.10 are larger for the Fall semester than the Spring, though all are 0.31 or below. The R^2 values for the pairings shown in Figures 12 and 13 were the highest in each semester's compared data (0.55 for Fall and 0.19 for Spring). The values alone point to no correlation, but the qualitatively similar patterns shown in Figure 12 suggest the presence of some relationship between students' total questions and the instructor's interaction with visual representations. The amount of student questions may be interpreted as a measure of students' involvement and engagement in class. Therefore, these comparisons demonstrate a relationship between student engagement and the instructor's engagement with the material through interaction with visual representations.

A number of uncontrollable factors such as students' attendance and perceived difficulty of the material by students led to the decision of using the class as the unit of analysis rather than normalizing the data by attendance and using each student as the unit of analysis. Within a semester, attendance varied (Figure D.1), student engagement varied, and questions were not evenly distributed across all students. For example, in Fall 2011, the number of students present varied from thirty-eight to forty-nine. Questions would most frequently come from about fifteen different students. Normalizing the number of questions between different days would falsely adjust the data, as the students asking questions were usually present. Furthermore, the number of questions per lecture cannot scale directly with the number of students present. A small class may provide a discussion format and foster many questions, but this may not scale to a larger lecture that consists solely of student questions and no presentation of new material from the instructor. Considering the class differences, the Fall and Spring classes were both lectures that encouraged student questions, were conducted under the same amount of time and meeting periods, and were of intermediate size (fifty-six and thirty-seven students enrolled at the end of the semester, respectively). To illustrate the challenge of normalization, total student questions and total questions normalized by class enrollment at the end of the semester for Fall 2011 and Spring 2012 are shown in Appendix D, Figure D.13. Both semesters had the same number of lectures and availability of class time. Normalization suggests that both classes were similarly populated with questions, when the number of questions alone shows that more students voiced questions in more of the lectures in the Fall than did in the Spring. One more notable observation from the data is when questions arose. Figure D.12 shows that the total number of student questions in Fall 2011 increased right before both exams while questions increased before the second exam of the Spring 2012 semester. This may be another artifact of teaching styles, but because the connection between questions and exam timing isn't replicated on each test in the Spring, a correlation is inconclusive.

5.2.3 Limitations of Observation Rubrics

The goal of the observation rubrics was to investigate any pattern relating students' questions and visualization artifacts with the instructor's interactions with visual representations. Rather than an expected variety of visualization indicators, only student questions formed the basis of analysis of the observation rubrics because that was the only consistently observed field demonstrated by students. The visualization context of students' questions could not be segregated from contexts such as comprehension and mishearing. Any conclusions that are drawn from the data must consider student engagement and interaction in class rather than visualization. To gauge whether students exhibit gains from instructor visualization modeling, additional student artifacts, such as drawings, model building, and descriptions must be elicited. Lectures were not a setting that fostered much independent model use or gesturing from students.

The observation rubrics from recitations had more limitations than those from lecture. Two graduate assistants observed the three recitation sections during Fall 2011. The researcher held periodic discussions of the observation fields with the assistants throughout the semester, but these discussions revealed that each assistant's understanding of the fields drifted from original instructions which was reflected in frequently different numbers of observations each week. One assistant paid closer attention to instructor actions while one recorded partial data on students' questions. The absence of observations in some fields by one of the assistants left no way to gauge which of the differing observations was more accurate and prohibited any estimates of interrater reliability to be made. Much effort was put into constructing comprehensive observation rubrics that could collect a significant amount of data efficiently. Despite the planning, the outlined fields left room for enough interpretation to prevent agreement between observers. Because of these limits, the relationships observed in both semesters of lecture were not observed in recitation.

The extent to which the fall and spring semesters may be compared is limited by a variety of factors. First, the students of each sample are different. Demographics were not controlled and several students who started in or failed the Fall semester reenrolled in the Spring semester. Fifty-six students received final grades for Fall 2011 and thirty-seven received final grades in Spring 2012. The two Inorganic classes observed taught primarily the same topics, but differed in a number of aspects. Fall 2011 was taught by a professor in his eighteenth year at NCSU. Spring 2012 was the second year of teaching at NCSU for the second professor. The Fall instructor made a point to actively address female involvement in class and recognized his attempts to be very enthusiastic during lecture to engage students. The Spring instructor described his teaching style to be less visually-based since he was familiar with the previous instructor's style. These differences are reflected in the instructor action trends included in Appendix D. Figure D.3 shows a much larger separation of male and female students' questions in the Spring than in the Fall. The plots are not normalized, but both classes were roughly one third female (Fall: 18/56 female, Spring: 10/37 female). Figures D.4 and D.6 show that the Fall instructor used more visual language and more gesturing, respectively. Table 9 shows that the Spring instructor utilized the more practical applications included in the rubric, which are evident through the higher percentage of lectures where the steps of a process and the reason or goal of a concept or specific method were described. The lectures were also arranged by topics covered. Students' questions by related topics were plotted and are shown in Figure D.14. Though the culture of different classes could not be controlled and varied between semesters, the Fall 2011 class was observed to contain more students that participated in class while the Spring 2012 class had two male students that frequently dominated and sidetracked discussion. This aspect of the Spring class may have contributed to the larger gap between male and female students. Though many of these limitations were uncontrollable, the researcher aimed for consistent interpretation of the rubric to allow for any similarities and relationships to be observed.

5.2.4 Interpretation of Observation Rubric Findings

The observation rubrics developed in this project were informed by students' questions and interactions with the physical model systems in the pilot studies. In lecture, the rubrics were used in a strictly observational role, rather than an interactive role that could encourage students to draw, gesture, or use models. The lack of visualization artifacts from the students supports that visualization artifacts must be elicited with increased exchange between instructor and students. The lack of visualization artifacts shown in Table 9 indicates that artifacts will not be volunteered in a more passive lecture setting. Students engaged in the lectures observed in this research through questions. These questions ranged from repetition to thoughtful insight, but almost always took the form of a question rather than a volunteered statement and students focused on what the instructor said and did in class rather than working on understanding visual concepts during class by using models or gesturing.

Though the detailed data collected through the observation rubrics did not provide insight to students' visualization use, the observation process helped focus attention to how students and instructors interacted with visual representations in these particular Inorganic chemistry courses. Correlations between the instructor's actions and how the class as a whole responded were investigated. An examination of the R^2 values for each pairing of student-instructor data indicated weak or no statistical correlations. The highest R^2 values for both fall and spring were between 'Total student questions' and 'Instructor's interaction with visual representations' in Figures 12 and 13. The qualitatively similar patterns followed in these pairings, especially within Figure 12, suggest that there is a notable relationship and perhaps the coefficient of determination is not the most appropriate statistical test to employ. The similar trends in Figure 12 imply that increased instructor engagement with visual material will result in increased student engagement with the class content in the form of questions posed to the instructor. Upon examination of the analyzed data presented here, the combination of the instructor's interaction with visual representations (drawings, use of models, and gestures around each of these and overhead projections) portrays the best exchange between students and the instructor. As the instructor models advanced interaction with visual information, students ask more questions to try to understand and learn those interactions. This conclusion speaks to the value of utilizing visual representations and supports a potential approach to increasing student involvement in class.

In this research, two different instructors were observed teaching a similar course. Though each had a unique teaching style, both elicited primarily questions as evidence of student engagement. Student interaction through questions alone may be due to their expectations of lecture as a passive event, their preference of lecture as a passive event, or their unfamiliarity in using kinesics and models to comprehend visual concepts. Observations of a single instructor teaching a lecture and a more interactive small class may demonstrate if students utilize additional visualization indicators in a more casual, interactive setting. In the courses observed in this research, the instructors' interactions with visual representations were indispensible because of the visually rich topics under discussion. Students' engagement may have been prompted by the understanding that they should model that interaction to comprehend the visual material. To explore whether an instructor's interaction with visual representations would also incite engagement in other chemistry courses, observations could be made in General, Organic, Analytical, and Physical chemistry courses to see if the relationship demonstrated in this work is retained. To elicit additional visualization indicators, perhaps the incorporation of reproducing models, drawing representations, and gesturing around models into a teaching style would elicit additional visualization indicators from students. In addition to providing time in class to work problems, students may be required to draw structures, build a model, or indicate motion on a preexisting model. The relationship between student engagement and an instructor's interaction with visual representations suggests that utilizing visual representations could enhance student participation in class. Examining the effect of emphasizing an instructor's interaction with visual representations in large lectures and online courses where it is difficult for all students to see an instructor's actions may provide more insight to the relationship demonstrated in this research.

5.3 Complex Visualization Activity Intervention

The intervention utilized the principles from the Modeling Theory of Learning displayed via several methods to encourage students to use visualization: complex visualization activities, deconstruction, and visual language.[5] To describe the impact these measures had on students' visualization skills, students' scores on standardized visualization tests were examined and the activity worksheets were analyzed.

5.3.1 Standardized Visualization Assessments

5.3.1.1 VSCS and MRT Descriptions and Results

To examine how the efforts of a one-semester intervention were reflected in standardized visualization tools, students enrolled in the Spring 2012 semester were asked to take the Visual-Spatial Chemistry Specific (VSCS) assessment tool and the Mental Rotations Test (MRT) at the beginning and end of the semester.[6, 7] The first tests were given before any intervention materials were used or discussed. The final tests were given after all ten weeks of activities were completed.

Administration of the MRT and VSCS was conducted based on best practices suggested by the corresponding authors. For example, students were given four minutes to complete each section of the MRT and scores were graded as suggested by M. Peters.[8] Out of twenty-four questions, a question earns one point if both stimulus figures that match the target are correctly identified. No credit was given for blank, incorrect, or half-correct answers. The maximum score for this instrument was twenty-four. The VSCS tool was modified for this group of students since the students did not have access to a class web application, such as WebAssign. Therefore, the computerized memory questions were omitted from the VSCS. A correct answer for each of the remaining twenty-nine questions earned one point. The maximum score for this instrument was twenty-nine. Results for the two assessments are summarized in Table 12. Two students were omitted from the analysis due to their limited attendance. One of those students attended only one week of activity recitations while the other student attended only four weeks intermittently.

Table 12. Summary of pre- and post-intervention visualization assessment scores.

		General	Males	Females	5-7 Weeks	8-10 Weeks
Pre-VSCS	Number of Students	21	7	14	12	7
	Average	**21.81**	**22.29**	**20.86**	**22.50**	**21.14**
	Standard Deviation	2.77	2.55	3.13	2.50	3.34
Post-VSCS	Number of Students	21	7	14	12	7
	Average	**22.57**	**22.71**	**22.29**	**23.67**	**21.29**
	Standard Deviation	3.34	3.89	2.06	2.27	4.68
Pre-MRT	Number of Students	23	7	16	11	10
	Average	**15.70**	**16.25**	**14.43**	**15.73**	**15.50**
	Standard Deviation	5.29	4.91	6.29	4.98	6.00
Post-MRT	Number of Students	23	7	16	11	10
	Average	**19.43**	**19.31**	**19.71**	**19.27**	**19.10**
	Standard Deviation	2.64	2.50	3.15	2.37	3.00

5.3.1.2 Statistical Tests

The significance of the differences and changes in scores for both the VSCS assessment and MRT were compared in a number of ways. The F-test determines if two variances (squares of the standard deviation) are statistically different.[9] The t-test determines if the means of two sets of measurements are statistically different. For all statistical tests, the calculated value was deemed significantly different if it was greater than the tabulated value at the 95% confidence level. A paired t-test was used to gauge improvement for each student on pre- and post-assessments. F-, t- and paired t-tests were calculated using the statistical Data Analysis Toolpak within Excel from Microsoft Office 2007.

The pre- and post-assessment score differences for the VSCS ranged from negative five to six with the exception of one student (023), who scored twelve points lower in the post-assessment. The large difference prompted investigation of this data point as an outlier. Two outlier tests were applied to this data point: Dixon's *Q* test and Grubbs' test. The *Q* test is recommended for sets with a small number of observations. Grubbs' test assumes a normal distribution and may be used when only a single point is in question. Both tests disqualified the retention of this data point.

$$Q = \frac{|\text{suspect - nearest}|}{(\text{largest - smallest})}$$

$$Q = \frac{|-12 - -5|}{(6 - -12)}$$

$Q_{calc} = 0.389$

$Q_{tab} = 0.337$ for 21 observations[10]

For a one-sided test where the suspect point is the minimum, the following Grubbs equation was used.

$$\text{G} = \frac{(\text{mean - minimum})}{\text{standard deviation}}$$

$$\text{G} = \frac{(0.762 - -12)}{4.09}$$

G = 3.12

$G_{tab} = 2.58$ for 21 observations[11]

Table 13. Summary of visualization test results.

	Pre-VSCS	Post-VSCS	Pre-MRT	Post-MRT
General Improvement	Significantly Improved**		Significantly Improved	
Male vs. Female Means	Not Sig	Not Sig	Not Sig	Not Sig
Female Improvement	Not Significant		Significantly Improved	
Male Improvement	Not Significant		Significantly Improved	
8-10 vs. 5-7 Week Means	Not Sig	Not Sig	Not Sig	Not Sig
8-10 Improvement	Not Significant		Significantly Improved	
5-7 Improvement	Not Significant		Significantly Improved	

Table 13 summarizes the results of the various t-tests (for comparing the means of two groups) and the paired t-tests (for comparing improvements of a group). Data were analyzed and compared by gender or by recitation attendance. When the improvements of all the groups were measured through paired t-tests, all groups showed significant improvement for the MRT and insignificant improvement for the VSCS. When student 023 was determined to be an outlier through the previously mentioned analyses, only the cumulative, general class improvement changed from not significant to significant improvement (**). This student belonged to the Male and 8-10 week attendance sub-groups, but data analysis of these groups with 023 removed did not change the other results.

The methods used in this intervention sought to teach students how to critically analyze complex visual representations and reflect on their personal problem solving processes. It should be noted that the VSCS tool gauges a variety of visual-perceptual skills and the MRT measures mental rotation specifically. The VSCS tool is new, but specific to chemistry. The MRT is an established assessment used in educational research. These assessments were used to investigate if the measures taken throughout the intervention would align or could be detected with either assessment. All divided groups and the class as a whole improved, as shown in Table 12. The span of score differences and standard deviation when all students are pooled for general improvement accounts for the change from non-significant to significant improvement. The significant general improvement in *both* assessments demonstrates that students practiced visualization within the intervention methods enough to be detected by two instruments that measured skills that were not directly addressed during the intervention.

5.3.2 Complex Visualization Activity Data Analysis

Several factors were taken into consideration while examining students' documentation of deconstruction on the weekly visualization activities. The framework principles outlined opportunities for students to deconstruct the image and task presented each week.[5] The summary question gave students a problem that could be graded as right or wrong within a chemistry context (with exception to the first week). Then, there were underlying, subtle aims that students may or may not fulfill such as demonstrating visual language, using deconstruction to solve the visual problem, and extending the symmetry-based visual skills they learned during the semester to more advanced problems. This section outlines the different phases of activity analysis and results from each phase.

5.3.2.1 Analysis of Weekly Activities

Activities were analyzed weekly by the researcher and an assisting undergraduate student. Before evaluating the activities, a rubric was developed for each activity and a collaborative grading scheme was used: grading side-by-side and together deciding the validity of unique deconstruction statements. Specific cases and examples were noted on the rubrics for each week to corroborate valid deconstruction statements. It was observed that student deconstruction statements in the earlier activities were not always found in the corresponding sections of each activity. For example, responses describing image patterns were not always discussed by students in the pattern model component question. Student responses were used to model accurate deconstruction responses through feedback on the activities. As the semester progressed, deconstruction statements were more frequently found within the correct corresponding question, but students continued to provide responses that did not answer the particular deconstruction question.

5.3.2.2 Detailed Analysis of Summary Question Responses

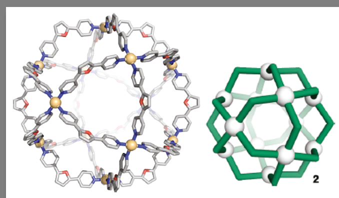
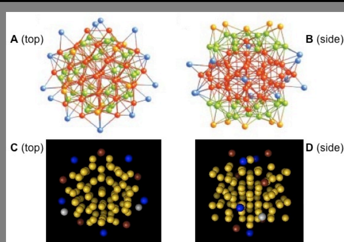
During the second phase of activity analysis, the question of how well students answered the tasks in the summary questions was explored. This meant not only evaluating the summary question responses for partial credit, but also examining all the other questions for indications of disregarded guesses, misinterpretations, and partial thoughts to gauge where students may have gone wrong. For example, a student may not have received points in the first phase for a statement that used the wrong descriptor, but had a drawing of the correct concept. This student would have been closer to understanding the visual than a student that did not attempt the question at all. Students' summary questions were frequently reexamined and their responses to deconstruction questions were also inspected for evidence of answers to the summary question. Examples of categorized student responses for each week are listed in Appendix F.

Upon closer examination of how students answered the summary questions, two activities stood out by posing particularly challenging obstacles to students: Weeks 4 and 10.

When students first saw the activity images, their comments and questions demonstrated that certain characteristics were noticed immediately. The most immediate characteristics may vary between people. While grading students' activity worksheets from Week 4 and Week 10, the visuals had characteristics that, when observed first, led students to a wrong answer when responding to the summary question. What students reported visualizing was certainly there and not incorrect, but the predominant aspects that students documented as deconstructed parts either misled students to the wrong point group or prevented students from further analyzing the image for additional evidence towards the answer. The cues in the images that misled students may have been overcome if students spent additional time on the visual and compared multiple views. Weeks 4 and 10 were the only instances where a number of students documented interpreting the image differently than the majority.

The images, correct interpretations, and misleading visualization evidence are shown in Table 14. Evidence of students' misguided interpretations is displayed in the underlined portions of Misleading Visualization. Student identification numbers are in parentheses. For Week 4, a few students saw four large rings connected, but bypassed the shapes made by the intersections. The four rings are certainly there, but do not lead the students to the correct point group. Some student responses suggested that students didn't spend enough time looking at the image and these recorded observations may have led to the wrong point group assignment. Examples include statements such as "all faces were identical and triangular," "C_4 rotation axes were located on Pt atoms" (instead of through faces), and descriptions that the faces were hexagonal, octagonal, and pentagonal shapes. During Week 10, students used a single view of the nanoparticle to use the colored atoms in the belt in defining a C_5 rotation

Table 14. Evidence of misleading visualization that led students to an incorrect answer.

Activity Images	Key Interpretations	Misleading Visualization
 Week 4[12]	• The C_3 rotation axis is oriented directly in the center. • Three 4-sided and three 3-sided faces surround the center space.	• "There are three main hexagonal rings. The outer 2 rings are small and are only bonded by three atoms on each ring, while the innermost middle ring is bonded by 6 atoms on the edges of the hexagonal structure. The outer 2 rings are in staggered formation for the atoms." (013) • "4 hexagonal rings connected together vertically and horizontally to form a 3-D structure. Rings evenly spaced and connected together by the spheres." (020) • "12 Pt atoms, 24 L atoms, 3 per bond, 4 hexagonal shapes that cross w/ each other." (022)
 Week 10[13, 14]	• From the two side views (B, D), atoms within the belt are not in the same plane. • The gold atoms of views C and D retain regular spacing in both views.	• "Without the white, D_5d. From 'C', C_5 from center in, C_2's from 1 brown or blue straight across to between other two." (010) • "Red at points of pentagon and yellow is in shape of a pentagon and blue are points of a pentagon out of phase by 180" (011) • "Blue atoms and red atoms in C are in a C_5 rotation axis, and is used to find the main rotation axis." (013) • "I used the 5 red and 5 blue atoms as a reference for the C_5 symmetry." (025)

axis. Looking at an alternate view in "D" could demonstrate that these atoms were not in the same plane, leading them to the wrong conclusion that these atoms contributed to the particle's dominating symmetry. This misleading visual cue most frequently led students to rule out the possibility of a horizontal reflection plane. These two examples depict the subtleties and unpredictable complexities encountered during this study.

Though the evidence from Table 14 showcases statements that led to incorrect answers, there were many instances where students identified correct rotation axes and accurately described reflection planes by drawing shapes on the diagrams and referring to coordinate axes. Students used depth cues like wedges to show that a rectangular plane was going into the paper through an image. Though these descriptions and drawings were not necessary to determine the point group or visualize the symmetry, they effectively communicated what students envisioned while solving these problems and how students interpreted the image at the point where they diverged from a correct problem-solving path was made apparent. The format of the activity provided the opportunity for students to elaborate and gave a unique insight to alternate and unexpected views of the activity image that would have otherwise been unavailable.

5.3.3 Evidence of Extended Analytical Parameters

As the Spring 2012 semester progressed, students demonstrated better familiarity with deconstruction questions and completing the activities. The third phase of analysis sought specific evidence of the persisting themes: analytical deconstruction, identification of a valid pattern or rule within the image, ability to describe a personalized and useful strategy, and ability to extend symmetry skills. A rubric defining these parameters and used to grade each week may be found in Appendix E.

Figure 14 shows the percentage of students that demonstrated these parameters throughout the intervention. Week 1 is omitted due to its role as an introduction to the layout of the activity and the non-contextual content. Many students documented more than one parameter and more than one instance of each parameter each week. Presenting the parameters with percent presence demonstrates how many individual students showed more advanced deconstruction each week. The following sections will refer to this figure.

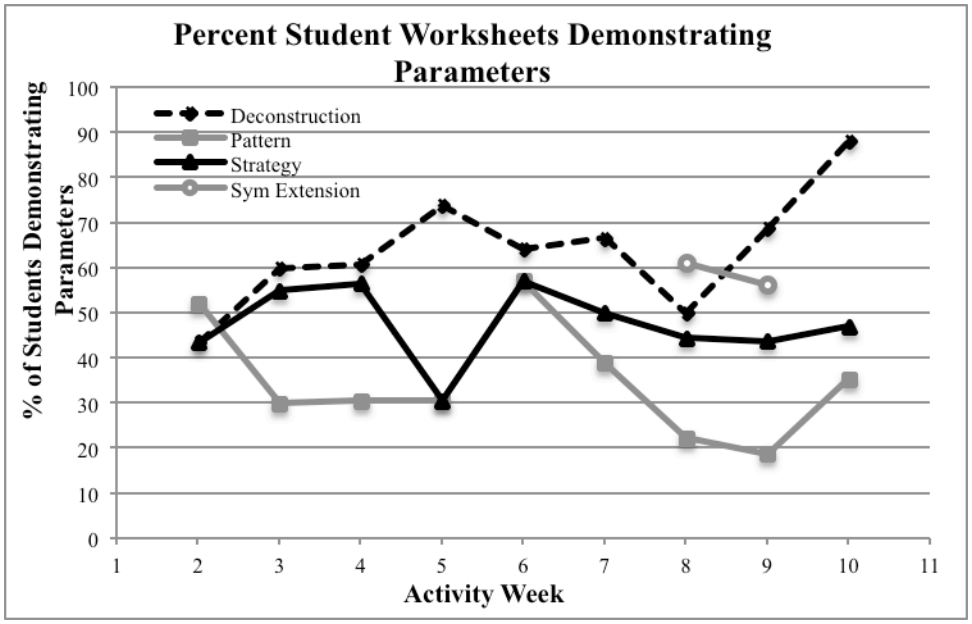


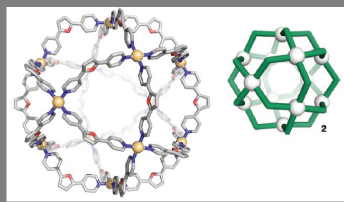
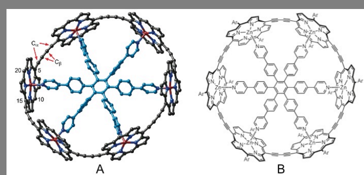
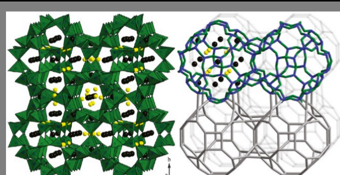
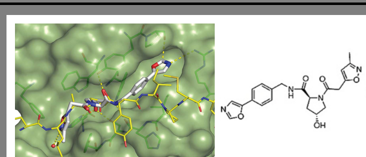
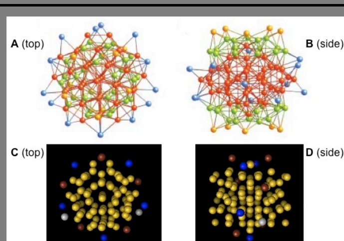
Figure 14. The percentage of students' activity worksheets that demonstrated a presence of each of the extended analytical parameters each week of the intervention.

5.3.3.1 Analytical Deconstruction

The complex visualization activities were written to guide students through varying levels of deconstruction to understand the presented image. Instead of answering each question directly, many students demonstrated thoughtful analysis of how the relationships depicted in the images represented 3-D structures. Analytical deconstruction of the image within the activity was separated out as a more advanced theme because students repeatedly documented their use of deconstruction to actively comprehend the image. The rubric in Appendix E provides guidelines to separate evidence of deconstruction that helped students analyze the image from answers to the deconstruction questions for the sake of completing the activity.

Table 15 displays several illustrative examples of analytical deconstruction. The underlined phrases show instances where students focused on a certain aspect of the image to note relevant observations, support their summary question answer, or describe the portions of the image they used in their problem-solving process. A complete repository of analytical deconstruction evidence may be found within the data for each of the ten weeks in Appendix F. As shown in Figure 14, the overall percentage of students demonstrating analytical deconstruction increased over the course of the semester. Week 8 demonstrated a larger drop, but this may be due to the change in the activity questions of that week. Week 8 was the first application-based activity and the task was no longer aligned with deconstructing the image to identify symmetrical portions of the structure. Fewer examples of deconstruction analysis in the initial weeks were expected as students became familiar with the activities and deconstruction questions. Week 4 frequently included illustrative descriptions of deconstruction, as discussed in the examples of misleading visualization in Table 14. Students' responses in Table 15 from Week 4 show that students are able to pinpoint crucial compound relationships that will lead to the students' determination of symmetry elements and a point group. Students' observations about the non-planar components of the spokes in Week 5's structure show the different information students were able to deduce from that observation. The side-by-side comparison may have made the differences apparent and easier to document for students. This may be why there is an increased number of deconstruction statements for that week in Figure 14. Students' responses from Week 7 show that they were able to navigate the relationship of shapes in the complicated image. The examples from Week 9 show the specific parts of the images students focused on to orient themselves in the

Table 15. Examples of student deconstruction as an analytical tool.

Activity Images	Task	Evidence of Deconstruction
 Week 4[12]	List the symmetry elements needed to determine the point group	• "Circular atoms are corners that connect chains of rings. Each triangle-like section is surrounded by a square-like section at each side and triangle at each corner." (009) • "The triangles on each side are out of phase by 180°. So, they move together symmetrically by C_3 but also allow the possibility of S_6. (011)
 Week 5[15]	Find the point groups of each structure and name the symmetry elements that cause the two to differ	• "A forms 3 unique [axes] with the rings, B forms 6 [axes]." (003) • "Figure A has restricted sym[metry] operations because it has tilted rings. Figure B is easier to rotate since it's planar." (017) • "A is less planar→ benzene rings twist. B each 1/6 of the circle is the same A, parts of circle have different angles. " (026)
 Week 7[16]	Find the point group of a single cage, then of the collection of cages, and state the symmetry elements that differ between the two	• "There are four cages, they are all the same, they are bound in a square plane each with two adjacent sides bound to another, (If you look through a triangle, the one opposite it through the center, the opposite triangle is out of phase by 180°)" (011) • "The square faces are connected by the octagonal faces in the corner cages. These cages have two different types of atoms. Each corner cage is connected to each other by the center cage." (017)
 Week 9[17]	Describe how the synthetic molecule must be manipulated to match its orientation indicated in the enzyme pocket.	• "The corners of the pentagonal ends bond to the enzyme (the nitrogen groups) and the two hetero groups interact" (004) • "turn synthetic 180° on x and 90° on y [drawn coord axis], bend bond between ring 1 and carbonyl, put ring 2 in boat conformation, turn ring 4 60° from ring 3 along bond" (026)
 Week 10[13, 14]	Examine the image closely to find the dominating point group of the structure and find the atoms that detracted from the higher symmetry.	• "Red at points of pentagon and yellow is in shape of pentagon and blue are points of a pentagon out of phase by 180°, white ones destroy C_5 & C_2 [perpendicular]," (011) • "A central column of Au atoms, an inner pentagonal shaped structure consisting of 10 columns of gold atoms." (023)

application task. The two examples from Week 10 demonstrate these students' ability to focus on a specific portion and clearly analyze that portion's role in the pattern.

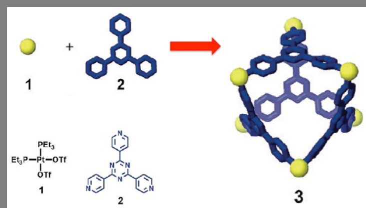
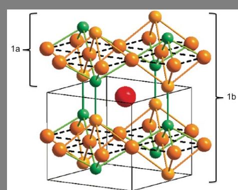
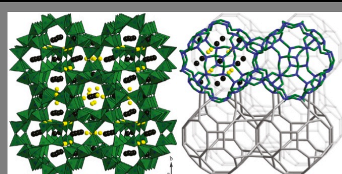
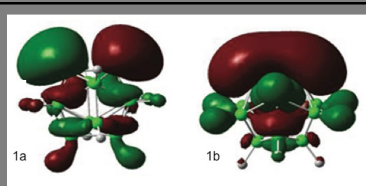
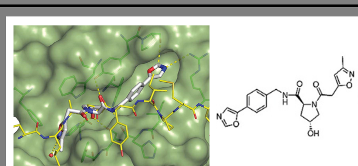
Throughout the semester, students documented their understanding of the images and the tasks associated by deconstructing their observations and documenting those of relevance. Many students showed the ability to make complex connections and were able to articulate their analyses of the images clearly and with detail. This intervention sought to teach students to use deconstruction as a strategy to solve problems and comprehend complex visual representations. In these statements throughout the semester, students showed that they were using deconstruction at a variety of levels and more students were demonstrating advanced deconstruction at the end of the intervention.

5.3.3.2 Valid Pattern Identification

As students analyzed the images each week, the deconstruction questions of the activity aimed to lead into and support the pattern or rule of the visual. Comprehension of patterns within an image signifies an understanding of the information presented in that visual representation. In the activities whose summary question asked students for the point group, the summary question aligned with the pattern question. In the last three weeks, students' language and phrasing were examined for evidence of an understanding of the pattern layout in the image. The rubric in Appendix E details acceptable and unacceptable indicators for pattern identification and was used to categorize students' responses as evidence found in the data for each week of activities in Appendix F.

Table 16 provides examples of responses categorized as valid pattern identification. Patterns and rules were modeled during recitation and in written feedback on the activities,

Table 16. Evidence of successful identification of patterns and rules.

Activity Images	Descriptions of Patterns/Rules
 Week 2[18]	• "The (1) is always attached to 2 (2) molecules, connecting the (2). No (1) is connected to the same two (2) molecules" (009) • "the 3 exterior rings of 2 are each attached to molecule 1" (012) • "Each group of six-membered rings is organized in an upside-down Y formation. The outside edges of these molecules are linked to a ball-shaped molecule, which links each formation together." (013)
 Week 6[19]	• "[The] tops and bottoms of the square prisms alternate between Au and Ge. Each has one corner in the center, so the center is surrounded by a square." (011) • "The green atoms alternate up and down positions in the net." (013) • "Ge bonded to Au in each net and then bonded to the other net in the same way. For every one Ge, there are 4 bonds to Au**.**" (022)
 Week 7[16]	• "Each contain same # of spheres of both colors, each has a square through the middle" (003) • "Individual cage patterns in c. Collection of cages has C_2 on x & z axes and C_4 on y axis. Plus reflection planes through z & y axes." (009) • "The same shapes and order of shapes are all around the cage. Small cage with 4 cages around it**.** With the collection, it has a lot of the same patterns. Has one shape with 4 identical shapes surrounding it." (015)
 Week 8[20]	• "The one on the right is symmetric. The one of the left has a mirror plane along the axis of rotation." (012) • "1a)→yz plane sign change reflection plane, 1b)→ yz plane sign consistency across yz reflection plane" (019) • "In 1A the orbitals are anti-symmetric with respect to the primary axis. In 1B the orbitals are symmetric with respect to the x-axis." (023)
 Week 9[17]	• "A total 90° rotation along the molecule and flip 180° along axis perpendicular to molecule." (005) • "A 180° rotation ([perpendicular] to the plane of the molecule) so that methyl of synthetic points down" (016)

but students found this question difficult throughout the intervention. Illustrative phrases are underlined and students' identification numbers are in parentheses. The percent of students that documented a valid pattern each week is shown in Figure 14. There is not a consistent trend in the description of patterns. Of the four parameters, it contains the lowest percentages (19% at Week 9). The highest percentages of students stating valid patterns were in Weeks 2, 6, and 7. During these weeks, Examples from Week 2 show that students tried to describe patterns as rules, but many students struggled to describe an overall pattern. Table 16 shows students' attempts to describe the role that portions of the image played in the overall structure. There were more examples for the simplified internal comparison in Week 6 than for the internal comparison of Week 7. Looking for the differences between point groups of each of these portions may have made students more attentive to patterns that would suggest symmetry elements. Weeks 8 and 9 may have had such low pattern description because of the nature of the application task. The patterns categorized in these weeks described the overall layout of the image, which was contrary to the specific use of the image to answer the task. Responses for those weeks revealed students' voluntary visual analyses of the images in a different perspective than that required for the task. The examples in Table 16 reveal what patterns students observed in the image to guide their analyses.

The goal of the pattern deconstruction question was to promote students' recognition of the overall layout of the structures portrayed in the images. This goal was closely aligned to the task of determining symmetry elements and point groups. Students may have had difficulty conceptually separating the two tasks, which resulted in many lists of symmetry elements and repeated statements of the relationships they observed. The valid patterns described by the rubric in Appendix E showed students' thought about the structure as a whole. Though the set of pattern responses are not all exemplary and the number of students who documented patterns varied throughout the intervention, they do attest to students' effort in comprehending the complex visuals. Additional modeling of patterns and an emphasis on understanding the overall layout of images may benefit students' ability to articulate patterns and rules.

5.3.3.3 Description of Personalized Strategies

The final deconstruction question of each activity was to describe the strategy used to answer the summary question or to how students made sense of the question about the image. Documenting a personalized strategy was emphasized so students would gain recognition of the processes they themselves used. Missteps, clarifying statements, and incomplete initial steps were all counted because these demonstrated that the students reflected on how they solved the problem rather than reporting a strategy they should have used. The rubric in Appendix E was used to categorize students' responses as evidence found in the data for each week of activities in Appendix F. This rubric advises how to differentiate from personalized strategies from strategies that are too generalized to be of assistance in future tasks. A well-articulated strategy may better prepare students to solve similar problem solving strategies in the future. The percentage of students that reported a personalized strategy each week is shown in Figure 14.

Table 17 displays examples of student strategies that when considered within the context of their activities, could assist students as a strategy beyond the specific instance alone. Many examples from the first three weeks were students' repeated answers of the summary questions, relationships or patterns, or short observations of what students deemed important (as in the Week 2 examples). The strategies noted for Weeks 4 and 5 show that

Table 17. Evidence of successful communication of strategies to solve the summary question.

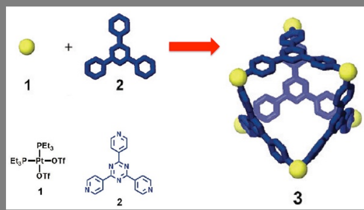
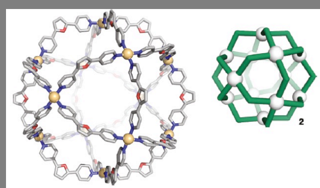
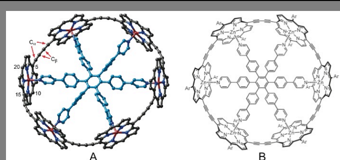
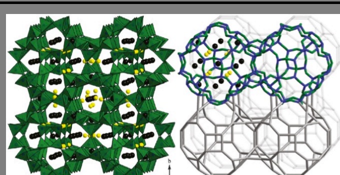
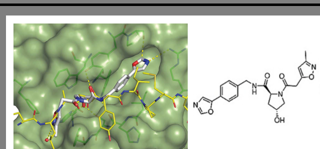
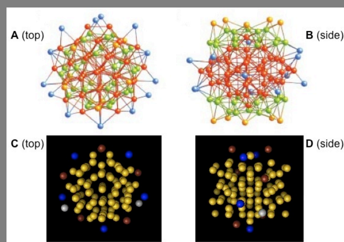
Activity Images	Evidence of Strategy Communication
 Week 2[18]	• "I would look at the symmetry of the parts and use that to determine the symmetry of the whole. Also, it's mostly the symmetry of (2) that matters for this molecule." (009) • "Structure one was a good reference for where each of the structure 2 molecules came together. They allowed me to see that this was a 3D structure." (016)
 Week 4[12]	• "1) Designate a set of axes, 2) Identify possible rotations [through] the center of each face, 3) Identify the highest order (C_n) and the number of C_n present, 4) Figure out if the structure can be inverted [through] its center." (001) • "First find principle axis, then any C_2 operations [perpendicular] to principle axis, then find reflection planes." (005) • "I would relate the molecule to the representation of a cube and use that to help me find the elements of symmetry." (009)
 Week 5[15]	• "Start at center (high symmetry) look for parts that reduce **[it]** such as a starts as C_6 then gets reduced to C_3." (011) • "Get the symmetry operations and find point group for structure B, the representation, first. Afterwards, see whether the operations can apply to the actual structure." (013) • "Use the center ring to put my primary rotation axis. Use ligands as the other points for the axis. [Watch] how the angle of the benzene rings changes as the structure is rotated." (017)
 Week 7[16]	• "Identify symmetry operations, choose a central axis, choose # of cages to use, use flow chart to determine point group." (006) • "Looked for symmetrical shapes in each cage. Tried different rotations and concentrated on where the yellow and black atoms went and if their angles changed." (016)
 Week 9[17]	• "Compare 2D structure to structure in picture, list differences, determine how those differences occur, use a model to determine possible movements." (006) • "Fit the overall structure together, then match some of the colored edges of the ring to atoms in the structure and rotate." (013) • "Pick an end and determine where it is in the picture with the enzyme, then determine what you must do to the molecule so that end will be in a new position." (022)

Table 17 (continued)

 **Week 10**[13, 14]	• "Use blue & red points to find dominating pattern. Then use white points to narrow down the pattern & [exclude] certain symmetries." (009) • "Try to find a MAIN rotation axis, because if it works for the most part, it can be used as the primary axis. Small parts that might prove the point group wrong could be used to identify other possible symmetries or find a different point group." (013) • "Looked like a [drawing of a pentagon] C_5 at first, then look at rotation to D and realize that atoms are not all in same horizontal plane" (019)

students personalized the process of determining the point group beyond statements of "Used the symmetry flow chart." One student (009) even related the Week 4 image to a cube, a more familiar object than the image given. A student (017) in Week 5 described the use of visualization as a strategy by watching how the structure changed upon rotation. Week 7 shows decisions students made or attempts to understand the image. Strategies for the last two weeks suggest how students oriented their understanding of the images. They matched the representations of the synthetic molecule for Week 9 and described the portions of the images that led them to conclusions for Week 10.

The visuals and tasks given in the activities were set at a difficult level for students. Inclusion of the strategy question sought to help prepare students for future visualization tasks and to encourage reflection on their work. Throughout the intervention, the percentage of students that described a personalized strategy remained fairly constant, ranging from 43-57% of students, with the exception of one week that dropped to 30%. This suggests that the intervention did not have as significant an impact as intended on the emphasis of reflection. Processes used to approach and solve problems in recitation may not have translated as personal reflection since modeling took place within an instructional role. The activity format did not require students to recall methods used in previous activities. Students may have approached each week like a new problem rather than thinking back on their struggles of prior weeks. Tying the activities together with an additional question or changes in semantics may have increased the importance of this question for students. Despite the absence of any apparent trend, the personalized statements and descriptions of the student strategies shown in Table 17 provide evidence that students were able to verbalize and document how they understood and solved the tasks. The documented responses also provide additional insight that enriches the summary question response and answers to the deconstruction questions.

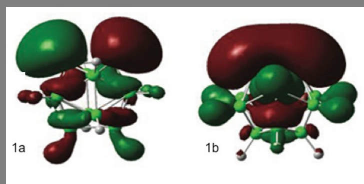
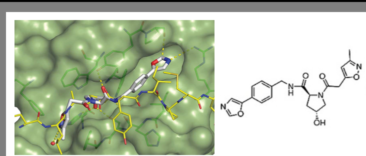
5.3.3.4 Extension of Symmetry

The final theme observed within the weekly activities was the extension of symmetry. Students extended the use of the symmetry concepts they had practiced throughout the intervention by using symmetry operations as a tool to explain envisioned motion of the structure represented in the image. Students demonstrated this extension through constructive application of descriptive words and symmetry terminology. The initial activities of the intervention placed much emphasis on determining and describing symmetry elements and point groups. As the semester progressed, students were expected to use symmetry to find patterns in the images but the focus of the tasks shifted to observing the details within the complex visuals. Weeks 8 and 9 were application-based activities and provided an opportunity for students to solve a task beyond what they would be expected to do in class. The rubric in Appendix E describes the requirements for symmetry extension and was used to categorize students' responses as evidence found in the data for the Week 8 and 9 activities in Appendix F. Figure 14 shows that 61% of students demonstrated the extension of symmetry in Week 8 and 56% in Week 9.

In Week 8, students were instructed to identify the symmetry labels of the molecular orbitals and justify their answers by writing the reducible representations. They wrote reducible representations in class, but they had only assigned symmetry to a d orbital on one homework question. Students were informed that the molecule belonged to the C_{2v} point group and given the character table. To choose the correct symmetry, students needed to reconcile the orbital pattern with the symmetry elements in the character table. Students could evaluate whether an operation produced symmetric or anti-symmetric configurations by envisioning the image undergoing a symmetry operation or analytically tracking where different orbitals would end up after an operation. The documentation of students' symmetry element visualization demonstrated the extension of symmetry. Table 18 features examples of how students described envisioning symmetry operations onto the images. Key phrases are underlined. Students justified their answers with documentation that they mentally manipulated the images in order to support or discount a symmetry operation. These examples demonstrated the success of the intervention by showcasing how the majority of students that week (61%) were able to describe the use of visualization to solve a process.

For Week 9, students were instructed to describe how the 2-D representation of a synthetic molecule must be manipulated so it would fit into the enzyme pocket, oriented the same as a line drawing of the same molecule in the figure on the left. Students were encouraged to describe motion of the molecule with degrees (180°) or symmetry notation (C_2). The image of the enzyme environment depicted a number of overlapping structures: the

Table 18. Evidence of symmetry extension to application-based activities.

Activity Images	Extension	Student Evidence
 Week 8[20]	Evidence of the application of visualized symmetry operations	• "I would rotate the molecule based upon an axis that extends through the 'top' and 'bottom' of the molecule." (004) • [coord axis drawing] "C_2 rotates around z axis, $\sigma_{v(xz)}$ mirror plane xz, $\sigma_{v(yz)}$ mirror plane yz" (012) • "A C_2 about the center of the big red glob orbital through molecule [drawing of rotation around a vertical axis]" (016)
	Evaluation of a symmetric or anti-symmetric result of a symmetry operation	• "A C_2 would be able to rotate the 1b structure on its y-axis, but the different charge makes C_2 an unusable operation in the 1a structure. σ_v is present in both structures, and the 1b structure can be reflected on the xy and yz plane while the 1a structure can only be reflected on the xy plane." (013) • "If you split them into ½ (through the plane coming out of the board) you get the same pattern on both sides: 1a) but they are in different colors, 1b) they have the same color" (018)
 Week 9[17]	Correct description of overall motion into the enzyme pocket	• "Rotate molecule 90° along axis that follows the chain. Then flip it 180° along axis into the page." (005) • "Rotate 90° (in the plane of the molecule across longer end of the molecule)… and then rotate 180° along axis [perpendicular] to the molecule (out of the bond)" (016) • "Two C_2's must be performed, one on the z axis, one on the x as drawn above. This will turn the molecule so it is oriented correctly into the binding pocket." (022) • "Turn synthetic 180° on x and 90° on y [drawn coord axis], bend bond between ring 1 and carbonyl, put ring 2 in boat conformation, turn ring 4 60° from ring 3 along bond" (026)

line drawing of the synthetic molecule, the natural substrate that binds to the enzyme, and a shaded enzyme environment with relevant molecular moieties contained within the shading. Students had to identify which structure represented the 2-D synthetic molecule before they could determine the overall motion of the synthetic molecule from its given orientation. Almost all students were able to correctly identify and describe how the synthetic molecule should fit into the enzyme pocket. They used a mix of degrees and rotation axes to describe their movement, but demonstrated symmetry extension by describing the location of the axes around rotation would occur (i.e. coming out of the page, through the length of the molecule) and other symmetry elements that helped them communicate motion. Many students incorporated drawings of coordinate axes, rotation axes, and reflection planes into their descriptions to add orientation and context to their responses. Examples of overall motion into the enzyme pocket and contextualized motion are given in Table 18.

Extension of symmetry was determined when students used symmetry as a tool to describe visualized motion of the images to communicate visualization. Though the Week 8 task required an understanding of symmetry, students were not required to enact the operations on the structures in the images. Not only did they demonstrate a working knowledge of symmetric and anti-symmetric MO patterns, they communicated visualized manipulation of the structures to explain the symmetric or anti-symmetric result. The synthetic molecule of Week 9 had no symmetry elements (besides identity), but students successfully applied proper rotations to manipulate a molecule to a specific location. An examination of students' use of symmetry in these two activities showed sophisticated use of visual language in interpreting the visuals of the application activities and in their abilities to approach complex problems.

5.3.3.5 Interrater Reliability of the Deconstruction Parameter Grading Rubric

To gauge how well the analytical deconstruction parameters translated to being captured by independent raters, a measure of interrater reliability was sought. Stemler and Tsai argued that the various statistical tests used to provide interrater reliability ratings fit one of three categories: consensus, consistency, and measurement estimates.[20] A consensus estimate is used to demonstrate that a traditionally subjective construct may be agreed upon by independent judges and is most useful when data are nominal in nature (the differences between the categories of data are qualitative). A consistency estimate does not require judges to come to a consensus on the interpretation of the defined rating scale, but the judges must rate consistently in their personal understanding of the scale. This type of estimate is most useful when the data are continuous in nature, but may be applicable to qualitative data if categories in the rating scale represent an underlying continuum. Finally, a measurement estimate uses all information available from all judges (including disagreement) to create a summary rating. This estimate is usually more numerically complex and used when there is a large amount of data, multiple judges, and impractical to compute by hand. In this research, the data gathered from students' complex visualization activities are qualitative and the analytical deconstruction parameters were defined by a rubric. The qualitative data and limited availability of judges ruled out a measurement estimate. An interrater reliability rating was sought to determine if the defined parameters would be observed by an additional judge besides the researcher instead of determining how consistently the researcher and additional judge graded each parameter. The additional judge was trained with the rubric in Appendix E and one week of activities. A consistency estimate would have been more appropriate if students' responses were rated with a scale of how well they represented the parameters. Because each weekly activity was scaffolded, students' performance of deconstruction was not expected to progressively improve in sophistication. They were expected to demonstrate the ability to deconstruct as the tasks became more difficult. A consensus estimate to gauge the presence of these parameters was best suited to this research.

Stemler and Tsai described three common methods of calculating consensus estimates: percent agreement, Cohen's kappa, and odds ratio.[21] Percent agreement is popular, intuitive to explain, and involves simple calculations, but may result in artificially inflated numbers. An odds ratio is common for dichotomous ratings (like in this research), but conveying the results is less intuitive. Cohen's kappa was chosen because it considers how often the judges agreed, but corrects for whether the two judges might be expected to agree by chance. By consistently correcting for coincidence, this measure of interrater reliability is considered to be a more conservative calculation. Cohen's kappa was calculated for each parameter of three of the remaining eight activity weeks to provide the ~30% overlap in grading that is recommended as best practice.[21] Week 1 was omitted from parameter comparison because it was used to introduce deconstruction to students and Week 8 was used to train an additional grader using the rubric in Appendix E, as it contained all four parameters. These values are summarized in Table 19.

Each of the Cohen's kappa values was determined as described by Cohen.[22] Values for Cohen's kappa may range from -1 (complete disagreement) to +1 (complete agreement) while a value of 0 suggests that graders do not agree any more than would be predicted by chance alone. Though this estimate of interrater reliability is conservative, the values calculated to measure the consensus between the researcher and the assisting graduate student were all positive. Landis and Koch outlined arbitrary guidelines to interpret kappa values to aid in discussion:[23]

Kappa Statistic	*Strength of Agreement*
<0.00	Poor
0.00-0.20	Slight
0.21-0.40	Fair
0.41-0.60	Moderate
0.61-0.80	Substantial
0.81-1.00	Almost Perfect

Based on these guidelines, the values calculated for the consensus estimates on the grading rubric for the analytical deconstruction parameters ranged from fair to almost perfect, with the majority (nine out of thirteen) of the values as moderate.

Table 19. Cohen's kappa values to gauge consensus interrater reliability for the four analytical deconstruction parameters.

	Deconstruction	**Pattern**	**Strategy**	**Sym Extension**
Week 3	0.55	0.26	0.29	N/A
Week 6	0.36	0.55	0.59	N/A
Week 9	0.47	0.67	1.00	0.43
Combined	0.46	0.50	0.60	N/A

This intervention aimed to promote mindful and reflective consideration of complex visualization problems. Structured deconstruction was used to help students understand symmetry operations and discuss problems. The physical model systems and weekly activities provided vehicles to promote students deconstruction independently. A significant benefit of deconstructive questions was the documentation of students' misleading visualization. The questions provided access to student problems that would have gone unseen without the variety of questions about how students visualized different components of the image. In an effort to teach students to look at the overall pattern found in complex images and to reflect upon their own strategies of analysis, students demonstrated the ability to do both and provided evidence of such throughout the semester in a variety of complex visuals. Through these activities, students practiced analytical visualization and deconstruction to solve tasks posed to them and, in turn, showed significant improvement in two visualization skill assessments and the ability to extend their symmetry skills to visually complex application problems.

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CHAPTER 6.

IMPLICATIONS AND CONCLUSIONS

This research sought to investigate students' development of visualization strategies by providing a platform for students to accurately communicate their analyses of visual problems. The methods used to assist students in this process involved physical model systems that provided students with visual and physical frames of reference, activities to accompany the model systems to allow students to elaborate on what they saw and felt, classroom observation rubrics to investigate how students used visualization in the classroom, and an intervention consisting of ten weeks of complex visualization activities for students to document the deconstruction of complex images and modeled guidance of the deconstruction of complex visuals and concepts in inorganic chemistry. Data collected included recorded observations from the pilot studies, the frequency of student questions and instructor actions from lecture observation rubrics, and student documentation of visual, analytical deconstruction on the complex visualization activities from the intervention. In developing methods to help students recognize their own processes and in analyzing students' interactions with visual representations, this research sought to examine closely the following:

1. ***To what extent do students document their visual comprehension?***

In this work, visual comprehension was defined as the ability to analyze images with a discerning eye to zero in on the details that define the overall pattern—the understanding of the layout of the image and the structure portrayed. Chemistry concepts presented in visual representations display facets of chemical phenomena that may not be immediately apparent to students. When topics such as symmetry rely on visual representations to provide examples of chemistry concepts, it's important that students are able to comprehend the examples intended to assist them.

The pilot studies utilized physical model systems and developed activities. They demonstrated that students did not voluntarily document any observations, findings, or evidence of analysis or comprehension in working through visual problems. Even with prompting from the instructor, an overwhelming majority of students had a difficult time articulating and documenting visual tasks. The collected activities from the pilot studies had little to no documented observations from students. Without documentation or verbalization from the students, it was not apparent if they used visualization. A major challenge involved in verbalizing visual concepts and processes is translation. Gazzaniga's split-brain studies demonstrated that verbalization is not coincident with visualization and some transfer must occur in the brain to understand visual information received verbally or to communicate mental imagery.[1] Quintana et al. recommended encouraging students to verbalize their thoughts as they worked with complex tasks to help students acknowledge their steps in problem solving and manage their progress.[2] These sources support that purposeful translation of thoughts, visualization, and processes into verbal representations helps to reinforce the thoughts in students' minds and memories. The practice of moving a thought from the visual or abstract into the verbal, which may be articulated or written down anchors the thought in another location in the brain. From these pilot studies, it became clear that students needed targeted opportunities to reinforce this translation. The semester-long intervention was developed to model structured deconstruction of complex visual problems and provide students with complex visualization activities where they could put into practice articulating and documenting their visual analyses at a variety of deconstruction levels.

After the ten weeks of activities in the fourteen-week intervention, students showed the ability to document responses to deconstruction questions that did not obviously nor directly answer the task presented. They elaborated on their visual comprehension of the image in responses that were classified as analytical deconstruction, valid pattern identification, and symmetry extension. In addition, in taking time to successfully answer these questions, students demonstrated that they came to comprehend the image through their ability to discuss the relationships and patterns within the represented structure.

The extent to which students elaborated on their visual comprehension beyond directly answering the tasks in the summary questions varied between students and for each student between activity weeks. Figure 14 displays the percent of students each week that demonstrated the different deconstruction parameters, but it was not uncommon for students to demonstrate analytical deconstruction, symmetry extension, and sometimes pattern description multiple times in a single activity. This may be a result of particular students comprehending particular images better than other images. The images were scaffolded with a specific, described method, but a different researcher may have ordered the same images differently if different aspects of the representations stood out. The evidence of alternative interpretations of the images from Weeks 4 and 10 in Table 14 show that students interpreted the same images differently. It may also be a result of student engagement and enthusiasm for the activity and recitation. The extent of variation of student engagement cannot be determined or controlled.

An examination of the percentage of students that demonstrated the four parameters (Figure 14) showed that over the course of this intervention, analytical deconstruction increased, pattern identification decreased overall, description of a personalized strategy remained fairly consistent with the exception of one drop, and more than half of the students were able to extend symmetry concepts and language into the application-based activities. Analytical deconstruction, as defined and detailed in the rubric in Appendix E, was useful for students. The activity format required students to use direct, methodical deconstruction, but students reached beyond and documented compound relationships and details from the images that stood out in students' minds. Ten weeks of deconstructing complex visuals provided students a platform to analyze the visuals, but also to be creative in observing more in the images than what was strictly practical to solve the task.

The overall decrease in pattern determination may be rooted in the scaffolded complexity of the images and/or the complexity of describing patterns from the relationships and operations. Students frequently expressed frustration on the pattern model component question by writing question marks and admitting "I don't know." Successful pattern identification in the images required students to step back from the details of the image to understand how the simplest parts worked together to form the layout of the structure represented. This shows an advanced understanding and careful thought. In addition to the other deconstruction questions and answering the summary question, perhaps the expectation of such a sophisticated analysis placed a high cognitive demand on students in the timespan of ten to fifteen minutes. As the intervention progressed, the images became more complex. This may explain the increase in Week 6, which portrayed a countable number of clearly colored atoms, and the decrease to Weeks 7 through 10, all of which contained a much higher number of atoms and complex arrangements and content. The additional complexity in the activities may have placed students' priorities on comprehending the details in the images before articulating the overall layout.

The consistency of the percentage of students each week that reported personalized strategies might suggest that students did not come to value reflection more throughout the intervention or that it was also a consequence of the activity scaffolding. The decrease seen in strategy description in Figure 14 at Week 5 and the gradual decrease after Week 6 may have been affected by the change in task. Week 5 introduced comparison. Weeks 6 and 7 also required comparison, but the Week 7 image was very complex and many strategies reported steps to make sense of the image. The tasks for Weeks 8, 9, and 10 were each different again after that. The quality of students' personalized strategies in Table 17 demonstrates that the complexity of understanding the images and answering the tasks was a more likely factor than students' indifference toward reflection. The personalization of students' documentation of their methods speaks to students' enthusiasm for making themselves understood. Though analytical deconstruction was the primary focus of these activities, the strategy question offered students a platform to promote connection to their analysis and an invitation to the instructor to observe their process. The Modeling Theory of Learning promoted documentation because instructors could gain insight to students' problem-solving processes, but students' report of personalized strategies on the activities demonstrated that students welcomed the instructor to this insight.[3]

The extension of symmetry was an unexpected parameter demonstrated by students in the application-based activities. The activities were developed to utilize the same deconstruction students had used throughout the intervention and were designed to relate to the symmetry-based activities, but students proved to be adept in utilizing symmetry elements and operations to orient the images and describe their visualized actions. The use of these elements as tools to visualize motion and provide a context to describe that visualization demonstrates students' ability to use learned concepts to document their visual comprehension.

The parameters discussed here are complex means by which to describe students' visual comprehension during the intervention. A close examination of each demonstrates that students were able to convey their analyses of the complex images beyond the outlines of the activity format and show creativity in the connections and alternative interpretations of the images. An increase in the percentage presence in student activities was not observed for all parameters, but factors such as image and task complexity, student engagement, and time on task all had influence on students' documentation.

2. ***What measures are required for students to effectively communicate their problem solving processes?***

During the pilot study, students were reluctant to write down and to verbalize the processes used to analyze problems presented with the physical model systems. No documentation of students' strategies was collected during this phase of the research. Regularly providing students with the opportunity to deconstruct and relate what they did showed that students were capable of describing personalized strategies and they continued to do so throughout the intervention. An increase in the percentage of students reporting personalized strategies was not observed during the intervention, but as addressed for the previous research question, many factors were involved in students' documentation and students *were* able to relate their strategies given a platform to do so, which was not observed during the pilot studies. Students could not verbalize or document how they completed a visual problem or how they came to comprehend the visuals in the pilot studies.

The classroom observation rubrics sought to investigate how visualization artifacts manifested during class, as students listened and interacted with the class material presented to them. The data from the rubrics consisted almost completely of student questions (Table 9) and showed that evidence of visualization must be elicited from students. The relationship between student questions and the combination of the instructors' drawings, model use, and gesturing around models and 2-D images suggests the powerful impact of instructor modeling on how engaged students are in class, no matter the material being presented or the type of student in class (as shown in Figures 12 and 13). This leads to an important supplementary research question that may be related to what is required for students to communicate their processes:

> ***What can classroom observations suggest about the relationship between instructor engagement with visual material and student engagement in class?***

Despite the differences between two instructors and between the cultures of two classrooms, the instructors' interactions with the variety of visual representations used in class follow a similar pattern as the total number of student questions asked in class. An instructor's demonstration of how to use visual representations with respect to chemistry phenomena increases student engagement in the lecture setting. Combined with the evidence of student documentation during the intervention, this relationship underlines the significance of modeling not only interaction with visual concepts, but also the reasoning and strategies involved in modeling.

From the pilot study to the intervention, the opportunity for students to communicate their visual problem-solving processes was adjusted. In the pilot study, students would work on problems for about an hour once or twice. For the intervention, students were given a platform consisting of questions based on the Modeling Theory of Learning framework to analytically deconstruct an image/problem.[3] For ten to fifteen minutes during recitation sessions, students were instructed to write out analyses of images and answer challenging deconstruction questions that extended beyond what they practiced in class. The activities within the intervention period provided more documentation (communication) than was possible to obtain during the pilot study, and students' responses provided insight into the elements required for them to effectively communicate their problem solving processes. These elements include:

- *Modeling.* Modeling was crucial in teaching students the difference between the question fields on the activity and in promoting an atmosphere of familiarity and trust in using descriptive language. Modeling deconstruction throughout the intervention sought to show students its utility and relevance on a variety of problems. Students continued to provide insightful deconstruction throughout the intervention as the activities and images evolved as well as verbally articulating deconstruction during class discussion. Modeling also plays an important role in student engagement.

- *Commitment to communication.* There should be a deliberate, consistent, and sustained instructional effort on the use of documentation of students' analyses and strategies. Documentation of deconstruction and insight to students' strategies and alternative interpretations were only available through the intervention. The pilot studies did not result in any usable student documentation.
- *Time dedicated to the promotion of visualization skills.* Students may need additional time to modify their analyses as they work, since the dedicated time to the activity in this intervention made students spend time on a single problem. Many answers were left incomplete and blank each week. The number of unattempted questions each week is documented in Appendix F. Though time was limited for each problem within the intervention, the little time dedicated to visual deconstruction over the course of ten weeks provided an array of documented responses compared to the lack of responses in the short-term help sessions of the pilot studies.

3. ***What kind of evidence of visualization deconstruction (if any) do students show after a one-semester intervention tailored to address visualization strategies?***

Students were tasked with outlining the various levels of deconstruction per the Modeling Theory of Learning.[3] Through the consistent question format each week, students learned how to address the different levels through guidance and consistent feedback on their activities and from modeling the approach of problems in recitation. Beyond the levels of deconstruction outlined by the framework, students documented more advanced analytical deconstruction throughout the intervention.

To characterize the more advanced deconstruction, a rubric was developed that outlined the observed deconstruction parameters (Appendix E). The dimensions of this rubric were derived from students' documented responses that extended beyond what the activity format directly elicited. Student responses conforming to the specifications of the rubric were recorded and subsequently, the interrater reliability of the analysis of responses was gauged with Cohen's kappa to provide consensus estimates for each of the four parameters. Cohen's kappa provides a conservative measure of agreement that corrects for coincidence and the agreement between the researcher and an assisting graduate student using the rubric in Appendix E was moderate, overall. Instances of the parameters were tracked for all students each week and the percent of students that demonstrated these parameters each week was plotted (Figure 14). Student responses had to attain a higher level of analysis described in the rubric in order to be considered evidence of these advanced deconstruction parameters. Within their responses, students had to consider insightful compound relationships, identify relationships as a pattern appearing throughout the image, and describe their personal strategies in understanding and solving the image and task for each activity. Through the specific accounts of analytical deconstruction, students revealed what facets of the images made an impact on how they viewed the image. Table 15 gives several examples of how they documented which shapes, atoms, and orientations supported the symmetry elements and point groups the students argued.

Their self-described strategies (with one exception in Week 5 of Figure 14) were fairly constant over the course of the intervention. They maintained reflection even though the tasks and images increased in difficulty. The qualities of the personalized strategies outlined in the rubric ranged from detailed, global strategies of everything students did to answer the summary question to descriptions of single observations that set them on their path of deconstructing the image. Personalized responses indicated reflection. The documented strategies may have differed if students were not given the task until they had deconstructed the image or if they were required to communicate their strategies before solving the task. Strategies may have been written as a plan rather than an account of what happened.

Instances of both the analytical deconstruction and description of patterns provided insight into students' processes, which revealed common mistakes, novel comparisons, and what aspects of the images were most prominent in students' analyses. Documented responses from Weeks 4 and 10 contained examples of students' visual comprehension that were unanticipated. Their analyses of the images that misled them to an incorrect conclusion (perhaps due to incomplete deconstruction or observation of the image) provided an opportunity for analytical deconstruction in another direction than the levels outlined in the activity format. Instead of observing the geometry of the spaces in the self-assembled sphere of Week 4, some students saw the four large hoops that intersected. In Week 10, the last activity of the intervention, many students incorrectly used the outer belt of thirteen Au atoms to indicate symmetry, but they supported their arguments by describing locations of the symmetry elements and the envisioned locations of where these atoms would end up. As the images and tasks concerning these images became more complex throughout the intervention, students documented that they analytically deconstructed the images with contextual descriptions and used symmetry concepts and terminology and visual language to make their analyses understood.

Throughout this work, evidence of student visualization and visual comprehension were sought through complex problems that could be addressed through deconstruction. Initial attempts to elicit students' verbalization of visual comprehension proved that additional modeling, dedication to documentation, and time were required to gain insight to how students solved complex visual problems. Deconstruction was utilized as a method to provide structure and time to students' consideration of complex visual problems. Utilizing a structured format on the visualization activities guided students' deconstruction at the levels of simplest parts, relationships, operations, and patterns. The requirement of deconstruction in addition to solving the summary question task gave students the opportunity to spend more time considering the complex visual problems than they would have otherwise spent. This research proved that a deliberate focus on verbalization of visual comprehension provided insight to how students regarded specific images, their creative interpretations, and understanding of the patterns that describe the layout, and helped more students communicate higher levels of analytical deconstruction as the intervention progressed.

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3. Lesh, R.; Hoover, M.; Hole, B.; Kelly, A.; Post, T. Principles for Developing Thought-Revealing Activities for Students and Teachers. In *Handbook of Research Design in Mathematics and Science Education*; Kelly, A., Lesh, R., Eds.; Lawrence Erlbaum: Mahwah, NJ, 2000; pp 591-646.

APPENDICES

APPENDIX A. Physical Model Construction Information

Physical Model Construction Information

All model systems were designed and constructed to be durable for long-term use in classrooms by using Plexiglas and aluminum as the major building components. This section contains an outline of the major materials used and their costs. Costs of materials supplied by the NCSU Machine Shop reflect the prices available to the machine shop though these materials may be found through other suppliers.

Permanent Reflection Plane Demonstration

Table A.1. Outline of Supplies and Costs for the Permanent Reflection Plane Demo.

Part	Supplies	Supplier	Dimension	Amount	Cost	Subtotal
Base	1-inch clear Plexiglas	NCSU Machine Shop	1"x3"x10"	0.208 ft^2	\$21.91/ft^2	\$4.56
Top	3/8-inch clear Plexiglas	NCSU Machine Shop	3/8"x1"x10"	0.0694 ft^2	\$5.86/ft^2	\$0.41
Front & Back	1/4-inch clear Plexiglas	NCSU Machine Shop	2*(1/4"x 10"x12")	1.666 ft^2	\$4.87/ft^2	\$8.11
Inserts	1/16-inch gray PVC sheet	NCSU Machine Shop	1/16"x11"x 12"	0.917 ft^2	\$1.58/ft^2	\$1.45
Large Atoms	2 1/2-inch wood ball	AC Moore	2 1/2" diameter	2	\$3.39 each	\$6.78
Small Atoms	1 3/4-inch wood ball	AC Moore	1 3/4" diameter	5	\$0.69 each	\$3.45
Bonds	5/16-inch wood dowel	Ace Hardware	5/16"x4'	1	\$1.29 each	\$1.29
					Total	\$26.05

This model consists of a shiny layer (clear Plexiglas) covering an opaque, removable layer (gray PVC) that reveals the back halves of the molecules. The base Plexiglas measures 10 in. x 3 in. x 1 in. The vertical planes and connecting top piece are 1/4 in. thick. The only movable parts in the system, the opaque inserts, are 1/16 in. thick. To keep the inserts attached to the system, there are pins on the top and bottom of either side that runs through both Plexiglas layers. A track has been cut out of the PVC inserts to allow them to move past these pins. The whole model system stands 13 in. tall, is 10 in. wide, and the molecules extend it to 7 in. deep so that it can be used in lecture classrooms.

All wooden spheres used as “atoms” were purchased at a craft store. Bonds were cut from wooden dowels. A screw was drilled through the Plexiglas planes (front and back for both water and ammonia) before assembly. The wooden halves were painted and then screwed onto the Plexiglas. The center spheres were glued in place on the Plexiglas before attaching the bonds and smaller atoms. Wooden pieces were connected with wood glue.

3-D Coordinate Axis System

Table A.2. Outline of Supplies and Costs for the 3-D Coordinate Axis System.

Part	Supplies	Supplier	Dimension	Amount	Cost	Subtotal
Base	1-inch clear Plexiglas	NCSU Machine Shop	1"x4"x16"	0.444 ft^2	$21.91/$ft^2$	$9.73
Field	1/4-inch clear Plexiglas	NCSU Machine Shop	1/4"x16"x16 1/4"	1.806 ft^2	$4.87/$ft^2$	$8.80
Vert Axis	1/4-inch clear Plexiglas	NCSU Machine Shop	2*(1/4"x7/8"x7 1/2")	0.0912 ft^2	$4.87/$ft^2$	$0.44
Horiz Axis	1/4-inch clear Plexiglas	NCSU Machine Shop	2*(1/4"x7/8"x7 7/8")	0.0958 ft^2	$4.87/$ft^2$	$0.47
Perp Axis	1/4-inch clear Plexiglas	NCSU Machine Shop	1/4"x7/8"x16"	0.0972 ft^2	$4.87/$ft^2$	$0.47
Magnets	Rare Earth Disc Magnet #2VAE9	Grainger	0.5" dia, 0.75" thick	18	$1.30 each	$23.40
Glue	Aleene's Jewelry & Metal Glue	AC Moore		1	$6.37	$6.37
Flexible Tubing	1/4-inch Tygon Tubing	NCSU Chem Stockroom	1/4" outer dia, 1/8" inner dia	1 ft	$1.93/ ft	$1.93
Connectors	1-inch wood balls 16/pk	AC Moore	1" diameter	1 pack	$3.29/pack	$3.29
					Total	$54.90

To allow students to incorporate existing models, a field to hold the models and connectors to hold them to the field were needed (Figure A.1). Anticipating years of use, 1/4-in. Plexiglas was used for the plane (16 in. x16 in.) and coordinate axes (16 in. deep) of the system field. The base is 1-in. thick Plexiglas. The coordinate axes were etched with centimeter marks to allow students to mark relative distances while working.

Figure A.1. The Plexiglas field of the system. The marked axis perpendicular to the plane may be removed for storage.

The atom connectors (Figure A.2) allow students to attach and incorporate their models into the system. If the flat plane of the field is considered to be the reflection plane, students should be able to envision an atom or bond going through the Plexiglas plane. The atom connectors were made from 1-in. wooden spheres from a craft store because they were lightweight and easy to cut and shape. One, two or three 0.266-in. holes were drilled through sphere halves to allow for planar, tetrahedral, and octahedral geometries. To hold model kit bonds, 0.25-in. (outer diameter) clear Tygon tubing was cut to fit the holes. Jewelry cement (Aleene's Jewelry and Metal Cement) was used to secure the tubing at the flat side of the half-sphere and the flat side to the smooth magnet surface. In order for the tubing to grip model kit connectors, the tubing must remain flexible and unglued at the rounded side of the half-sphere since the jewelry cement leaches into the tubing to bind it to the wood and solidifies it. These connector dimensions were fit to two models: the Molecular Visions Inorganic-O kit from Darling Models, Inc. sold at NCSU bookstores, and a homemade kit of toothpicks and Styrofoam spheres often used by inorganic students. Both plastic model kits had connectors about 3 mm in diameter and fit the Tygon tubing well. The toothpicks may be adapted to the system by using two picks in the bond anchored in the atom connector.

Magnets were chosen based on how much weight they could hold through the Plexiglas system. Ultimately, neodymium disc magnets from Grainger were chosen. For tetrahedral and octahedral connections: #2VAE9 Thickness 0.125 in., Dia 0.500 in., Size 0.1 oz., Max Pull 4.9 lb., Stability Temp 300 °F, Sintered Neodymium, Nickel-plated. For linear connections: #2VAE6 Thickness 0.118 in., Dia 0.709 in., Size 0.1 oz., Max Pull 6.5 lb., Stability Temp 300 °F, Sintered Neodymium, Nickel-plated. The same jewelry cement was used to attach the magnets. The stronger magnet held a 30-g construction of model pieces that extended 8 in. from the plane, but also pulled away from the wooden connector with any adhesive besides the jewelry cement.

Dry erase markers are very valuable to illustrate in-plane bonds, label atoms/operations/axes, and keep track of students' thoughts on the visualized motion of bonds. If marker is left on the Plexiglas for more than a week, appropriate cleaner will be needed to remove it.

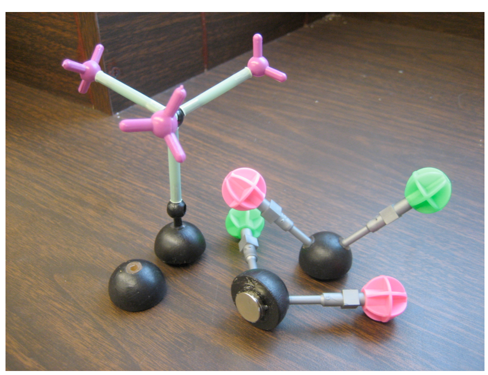


Figure A.2. Different model kits used in the atom connectors show the Tygon tubing (visible on a linear connector) while the neodymium magnet is revealed on the bottom of a tetrahedral connector.

Proper Rotation Axis System

Table A.3. Outline of Supplies and Costs for the Proper Rotation Axis System.

Part	Supplies	Supplier	Dimension	Amount	Cost	Subtotal
Base Disc	3/8-inch Aluminum	NCSU Machine Shop	14" diameter	1.07 ft^2	$56.57/ft^2$	$60.50
Bottom Disc	3/8-inch Aluminum	NCSU Machine Shop	9" diameter	0.442 ft^2	$56.57/ft^2$	$24.99
Top Disc	3/8-inch clear Plexiglas	NCSU Machine Shop	9" diameter	0.442 ft^2	$5.86/ft^2$	$2.59
Frames	1/8-inch Aluminum	NCSU Machine Shop	6*(1/8"x5/16"x20")	0.260 ft^2	$10.75/ft^2$	$2.80
Center Axis	1/4-inch dia Aluminum dowel	NCSU Machine Shop	2*6" pieces, 2*3" pieces	1.5 ft	$0.30/ft	$0.45
Axis Holders	1/2-inch dia Aluminum dowel	NCSU Machine Shop	2*(3" pieces)	0.5 ft	$0.95/ft	$0.48
Bearing	Steel bearings	NCSU Machine Shop	5/8" outer dia, 5/16" inner dia	2	$7.25 each	$14.50
Model Grips	Small Suction Cups	Ace Hardware	1 1/4" diameter	2	$0.79 each	$1.58
					Total	$107.89

A practical solution to fit common rotation axes C_2-C_6 was to design one flexible system instead of five. To take full advantage of a 3-D model of a proper rotation axis, students should be able to see, touch, and feel how a molecule can be rotated into indistinguishable positions. The system was built large (14 in. diameter, 15 in. tall) in order to allow many models and objects to be examined. The entire system breaks down to be stored flat (Figure A.3). The system is made primarily from aluminum to give it strength, but the top disc is Plexiglas so students may look down the principle rotation axis.

Frames connect the top to the base and outline the indistinguishable positions of the rotations. The rotation stops for C_2-C_6 operations are set into the top and bottom discs. The frames fit into these stops to correspond to the degree of rotation. Students will need to determine which stops are needed for a particular degree of rotation. To connect the molecule's movement to physical input, the system makes a 'click', or catch, to cue that the original position of the molecule has passed a certain degree. A pin was set into the large, base disc (Figure A.4) and layered with another (bottom) disc with indents at each of the degrees needed for each stop in proper rotations C_2-C_6. The same indents are set into the Plexiglas (top) disc. Both the top and bottom discs are necessary fixtures in each rotation axis set-up because they hold the frames together, and in turn, the frames hold the top disc up (Figure A.5). The base disc and center axis remain stationary as the top/bottom discs and frames all rotate around the model held in the center. Free rotation of the frames around a stationary center axis is made possible by two bearings surrounding the top disc. Aluminum dowels were tooled to fit smaller dowels and screws to secure them to the top and base discs.

The dissembled pieces laid out in Figure A.6 show the sequence of how these parts come together to form the center axis.

Figure A.3. All pieces of the Proper Rotation Axis System, clockwise from upper left: base disc with pin, Plexiglas top disc, two security screws, four aluminum dowels (two sizes), PVC tubes, suction cups, six aluminum frames, bottom disc.

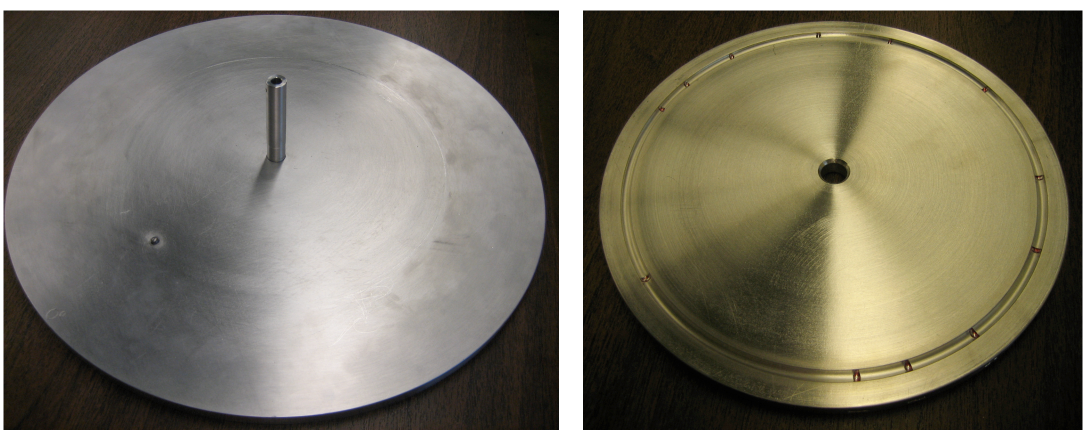


Figure A.4. Bottom two discs of the Proper Rotation Axis system. Left: the large, base disc has a pin that lines up with a 0° mark. Right: the underside of the bottom disc shows the indents along the track for the pin of the base disc.

Figure A.5. The top Plexiglas and bottom aluminum discs feature matching degree indents. The aluminum frames hole the Plexiglas disc upright.

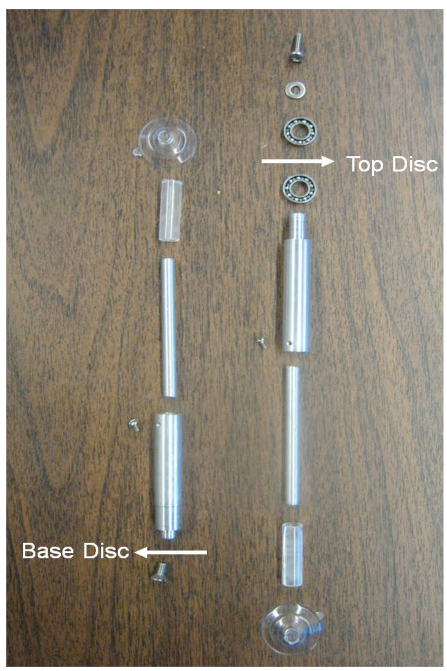


Figure A.6. The dissembled components of the center axis.

The split center axis is made up of four removable pieces to meet in the center and hold a flat model or extend to hold a model 7 in. tall. Suction cups were fit into clear, PVC tubing to grip the model kit pieces. The PVC tubes fit around aluminum dowels that may be interchanged to fit the models. All pieces can be mixed and matched to fit the particular model (Figure A.7). On the left, depending on the size of the model, the aluminum dowels can be adjusted to provide tension around the model and hold it in place. On the right, once the dowels, PVC tubes, and suction cups are in place, the dowels may be moved to squeeze the model and held in place with the security screws. Starting with the frames, attaching the top and bottom discs is the easiest way to insert the model and provides the most stability. Each frame should be inserted as far as it will go or the center axis will not align correctly.

The model is inserted between the two permanent center axis holders. Once in place, screw the small security screw on the bottom attachment tightly to stabilize the axis inserts. Slide on the suction cup holders of the chosen length. Insert the top attachment, then the model and brace them against the model as you tighten the upper security screw.

The vertical axis inserts should line up with the principle rotation axis of the molecule. For example, with BF_3, the boron atom should be sandwiched between the two suction cups and each fluoride should line up with a frame. Check that the molecule doesn't rotate or become misaligned as you spin the bottom disc. The system will catch at several locations, but students should pay attention to the catches that match up with the frames. Notice that the bonds matched up with the frames will match the following frames if the correct proper rotation axis was set up.

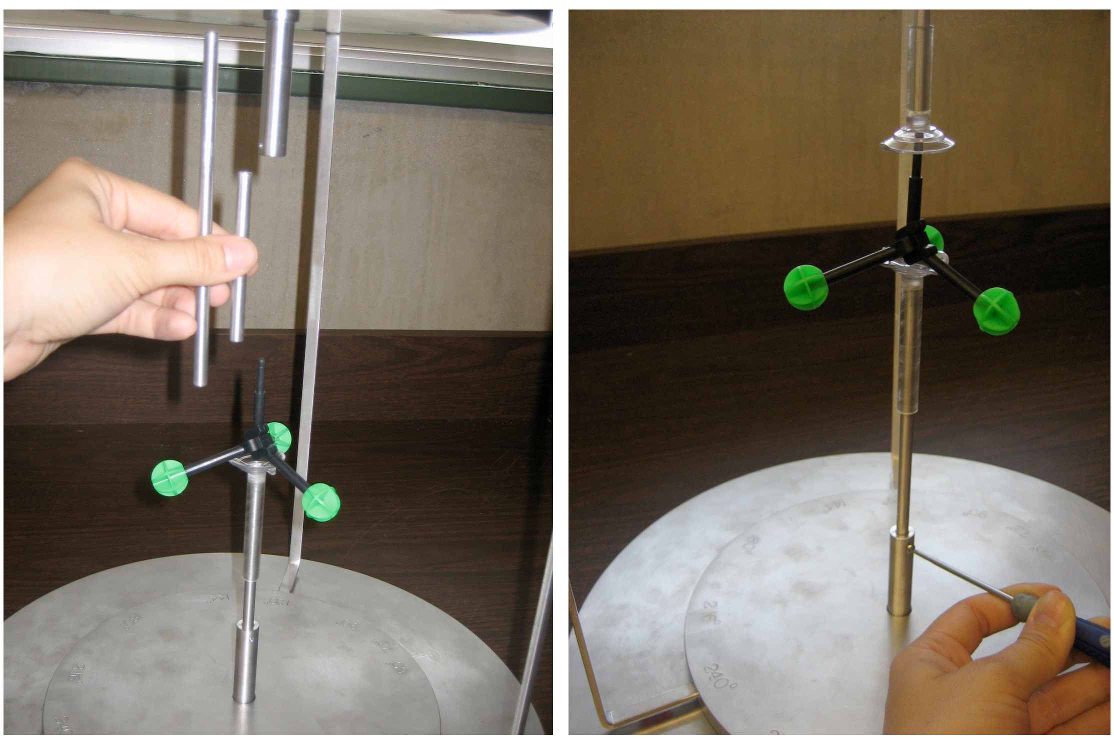


Figure A.7. Fitting a molecular model into the Proper Rotation Axis system.

How to Assemble and Use the Proper Rotation Axis System

This section gives more detail and may be used as a handout for students. Alternatively, it may be already set-up for students to use with their own model kits.

Though this model system is large and seemingly mechanical, once you understand how the pieces fit together, it's easy to interchange the parts to make it fit a particular molecular model. Complete assembly is described below. Interchanging between different degrees of rotation is much simpler than starting from everything dissembled. Set-up is described using a C_3 axis for ammonia for a more illustrative explanation.

From Scratch

1. Begin with the largest aluminum disc. It will have a small cylinder sticking up from the middle and will be stamped with only a 0° mark. Stack the smaller aluminum disc on top of the first, threading the small cylinder on the disc through the hole in the smaller disc. Line up the 0° marks. Twisting the smaller disc should reveal the catches at each of the degrees marked on the plate.
2. To determine how many frames you should insert into the smaller disc, you need to consult the model of your molecule. Looking at the ammonia model, if it's held by the position the lone pair occupies, all three hydrogen atoms can rotate the same way around your fingertips. If you hold the model by one of the hydrogen atoms and spin it, the bonds don't quite look the same. This is what you look for in a rotation axis. Since there are three of the same bonds, you need three frames.
3. The frames should be distributed evenly around the disc once you know how many you need. Divide 360° by how many frames and set a frame at each progression of that number until you get to the original 0°. This system is set up to work with C_2, C_3, C_4, C_5, and C_6.

   C_2: 0°, 180°
   C_3: 0°, 120°, 240°
   C_4: 0°, 90°, 180°, 270°
   C_5: 0°, 72°, 144°, 216°, 288°
   C_6: 0°, 60°, 120°, 180°, 240°, 300°
4. The frames are stamped on one end with "BOTTOM". They are filed down differently on the bottom than on the top. Fit the bottom ends into the slots marked by the correct angles. Start attaching each of these frames with the same corresponding angles on the top, Plexiglas disc. The rotating cylinder on the Plexiglas disc should point down. All 0° marks should still be aligned with that first frame. The frames need to go in all the way to get the center axis to align as well.
5. After all the frames are secure and as tight as they can be, hold up your model to the system and decide which lengths of aluminum dowels would best fit your model. Take into consideration that the dowel can go into the full length of the cylinder, but the plastic suction cup covers may go down only so far. See if you can shorten the bonds on your

model and use the shorter aluminum dowels if it won't fit. Adjust the lower half of the center axis first and tighten its security screw. Insert the upper half of the center axis and fit in the model—align the center axis with the place on your molecule where you can spin it and all the portions that spin around look the same. While bracing the upper and lower suction cups against the model, tighten the upper security screw.

6. It's important that the center axis be secure, but not too tight. It needs to be tight enough to remain stationary as the discs are rotated and loose enough that the model is not distorted. Check that the molecule doesn't rotate or become misaligned as you spin the bottom disc. The system will catch at several locations, but pay attention to the catches that match up with the frames. Notice that the bonds you matched up with the frames will match the following frames if you have the correct proper rotation axis set up.

From Previously Set-Up

1. Moving around the pieces can put strain on your models, so make sure that none are being braced in the center axis before changing anything. If the model system has already been set up, you'll still need to decide if you need to change the frames around before inserting your model. If you need a different number of frames than were previously set up, put those into the bottom and have them ready to stabilize the top disc once you remove the other frames from their initial positions.
2. Follow the 'From Scratch' instructions on inserting a model into a middle frame (start at Step 5, above).

APPENDIX B. Associated Activities for Physical Model Systems

Name: _______________________

Permanent Reflection Plane Demonstration

(Omit suggested rubric in italics before handing out)

Reflection planes are an important part of group theory and symmetry and there are more to these planes than just mirror images. In this demo, the clear Plexiglas is the reflection plane in discussion. Be as specific in your answers as possible to iron out a reflection plane definition for yourself.

By the time you finish this worksheet, you'll be able to…

- Work out a concrete, usable definition of a reflection plane.
- Give reasons for the presence or absence of a reflection plane.
- Be familiar with the ideas of atoms in 3-D space, atom labeling, and differentiating between atoms on either side of a reflection plane.

1) Describe what you understand by the term "reflection plane" in a molecular context. Use parts of the molecule and actions to help you.

To probe how they can describe reflection plane and hopefully, they'll use the term mirror or mirror image.

2) With the plastic inserts closed, what do you see? Please write as much detail as you can about the different parts, their positions, textures, size, etc.

Perfect: Two half-spheres with spheres on sticks jutting down at an angle. The surface of the 'plane' is shiny so I can see the spheres and sticks reflected in it. Acceptable: Descriptions about what the model looks like.

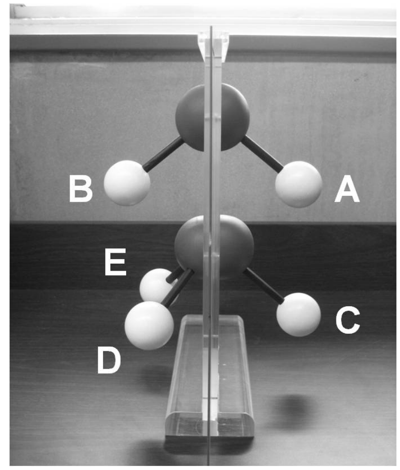
3) What molecule is suggested from what you see? Compare what you are seeing to anything you've previously learned or seen before.

With the reflection, both could be water, with oxygen as red and the hydrogen atoms as white. Compare to other molecules, a mirror, a boomerang…

4) With the plastic inserts open, what do you see? How is the real image alike or different from what you expected? Describe your observations and thoughts in detail, paying attention to the parts, how they're related, and what changes you'd make to have the model look as you expected.

There are more sphere halves. The top back looks the same on both sides, but the bottom back is different than on the front. Students should notice lengths, angles, the reflection of the front atoms and maybe observe that there are too many atoms on the back bottom.

5) If all atoms are given unique labels, as shown in the picture, how do A and B relate to each other? How does C relate to D and E?



A and B are separated equally by the Plexiglas. C is right in between D and E. A/B are on the some horizontal level and C/D/E are all on the same horizontal level.

6) What are the **requirements or rules** for a reflection plane based on what you've seen and written down? Has your definition of a reflection plane changed? How?

In order for there to be a reflection plane, the atoms on both sides of the plane have to match (in all locations in space except on the axis perpendicular to the reflection plane. From focus groups: "My definition has changed since I am focusing on locations of the atoms in space and that each side needs to have a match on the other side."

7) If you could insert more pieces of Plexiglas into this demo to show all the reflection planes at once, where would they go? Describe your reasons for placement using the labels in the picture above. What assumptions or rules did you use?

Put the planes where the orientation of bonds and atoms have exact matches, in different directions, on both sides: one through A/B/top red sphere, one through C/bottom red sphere/between D and E, one through D/bottom red sphere/between C and E, and one through E/bottom red sphere/between C and D.

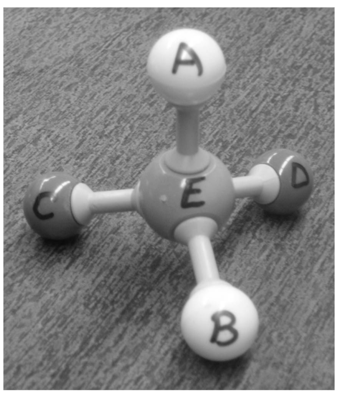
8) Describe what a reflection plane is by how it affects your sense of touch.

"When starting at the reflection plane, each hand feels the same placement and parts of the molecule as it moves outward. If the plane wasn't there, you would feel details of a molecule until you got to a certain point where you'd keep touching in the same direction, but it would feel like you'd turned the molecule around and felt the way backwards, feeling shapes in backwards order from how it started." In the least, students need to say that starting in the middle it's the same, but different directions.

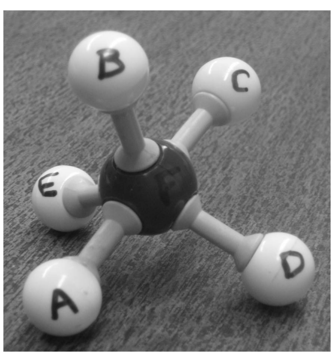
9) Describe what a reflection plane for someone who can neither see nor touch the model (as if you were speaking with the person over the phone)? What words would you use to give examples (i.e. shapes, directions, comparisons)? Try using x, y, and z coordinates in your descriptions.

> *This can be much like #8. Whatever coordinates they choose for the reflection plane, the coordinate they DID NOT choose is the only one that varies in the two sides (i.e. if a reflection plane lies on the xy-plane, the z-coordinate is the only one that changes. It will be especially beneficial for a reusable strategy if the student uses an example OTHER than the model presented.*

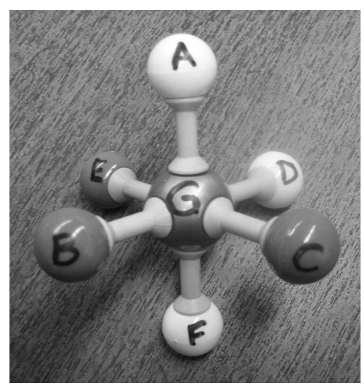
For 10-12, refer to the physical model that matches the one shown in the picture. Use the space to list or sketch as many reflection planes as you can, using the letters marked on the atoms. Differently shaded atoms are different elements.

10)


A/E/B, C/E/D

11)


B/F/D/E, A/B/C/F, A/D/C/F, A/E/D/F

12)


A/D/F/G/B, C/B/E/G/D

Name: ______________________

3-D Coordinate Axis System

(Omit suggested rubric in italics before handing out)

At times, an extra set of hands may be helpful when working with molecular modeling kits. This system acts as a 3-dimensional space to carry out the operations you've learned in class and track what you've done. Keep in mind how you moved your molecules and why you did it the way you did throughout the activity.

Here's what you need to know to start:

The magnetic centers cross the Plexiglas reflection plane may be used as atoms in the molecule or be ignored if a whole bond passes through the reflection plane. Model kits with attachments of ~3mm will work well. If double bonds and lone pairs aren't working with the model kit you have, try matching the geometry of the bonds to the model kit pieces available. Mark the bonds with scotch tape if the double bonds or lone pairs are not on the principle axis. Make this system work for you!

It's helpful to label atoms to keep track of their movement throughout operations. You can use colored atoms, colored stickers, tape, paperclips, whatever you have available, or use dry erase markers to write on the Plexiglas next to the atoms. Just make sure you document what is and isn't a label before you begin.

Working in groups to discuss what you're doing will help you put words to the strategies needed in the activity. Each group member must complete their own worksheet and enact the symmetry operations on the 3-D Coordinate Axis system.

This activity should be used when you are ready to work on some activities and/or homework. The symmetry elements are listed below for your convenience and review.

A **reflection plane (σ)** is a plane separating two halves of a molecule in which all portions of one side map directly onto all portions of the other side. 'Map' means that their coordinates are exactly the same except for the coordinate perpendicular to the reflection plane, which is equal, but opposite in sign. For example, if the reflection plane lies in the xy-plane, all the x- and y-coordinates of the two halves are the same. But, the z-coordinates of one side are positive while the z-coordinates of the other side are negative.

A **proper rotation (C_n)** occurs when a molecule can be rotated around an axis that runs through it. If it rotates all 360° without coming to an orientation that looks exactly like it did when you started, then it has a proper rotation of degree one (C_1). If it comes to a position that looks like its original orientation, this is an indistinguishable position. Count how many of these will happen before you get to where you started. Counting these and the endpoint when you reach your starting position will give you the degree of rotation (n).

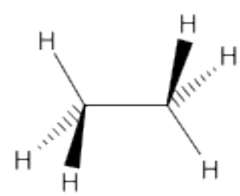
An **improper rotation (S_n)** occurs when a molecule undergoes a proper rotation with the same degree as the S_n indicated and is followed by a reflection through a plane perpendicular to the axis it was just rotated around.

An **inversion (i)** is when every atom and bond in the molecule travels a distance and direction to the center of the molecule and continues in that same distance and direction out the other side of the center, which is called the inversion center. A molecule has a center of inversion when you can map each atom onto another atom of the same element that is exactly on the opposite side and equidistant of the center of the molecule.

By the time you finish this worksheet, you'll be able to…

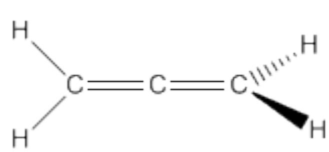
- Build and work with physical models of symmetry elements.
- Carry out different proper and improper rotations and determine the degree of rotation.
- Carry out multiple symmetry operations on a molecule and compare each step to the original orientation.
- Defend and discuss your reasons for carrying out the operations in the manner you did.

1) Staggered ethane has an improper rotation. List, describe, or draw the steps of putting ethane on the model system and carrying out the operation.



Put two tetrahedra into two atom connectors. Have one with a bond straight up and the one on the other side with a bond straight down. First, rotate both tetrahedral 60° to the same side of the room. Then, flip the two halves so all atoms have been reflected through the system.

2) What is the degree of improper rotation (S_n) for allene (C_3H_4). Please describe all your work: what did you try, how did it work, how did you change your previous answer? Did your group members have different first guesses than you did?



For this molecule, there are two H's that point vertically and two that lie horizontally. To get them to map onto one another, the molecule has to be 'prepped' for reflection. It needs to be rotated 90°, then reflected through the plane (i.e. so the top H is still on top).

3) Recall or look-up and build the general geometries you learned in General Chemistry with electron domains ranging from 2 to 6. Which kind of geometries around the center atom can have an S_n symmetry element? Please write any problems, missed attempts, and successes you had answering this question.

> *S_n symmetry: linear, trigonal planar, tetrahedral, trigonal bipyramidal, octahedral, square planar. No: bent, trigonal pyramidal, see-saw, t-shaped, square pyramidal.*

4) Write down how you'd identify an improper rotation in a molecule.

> *Anything that has a σ_h has an improper rotation that is the same degree as its proper rotation. If it looks like it could reflect, but is just a little off, try an improper rotation, i.e. a tetrahedron.*

5) Write your argument on why or why not methane has an inversion center. What do you look for in a molecule when you're looking for an inversion center?

> *Methane has to be held in a certain way to consider the improper rotation and students may have missed it for #3. The rotation axis used does not align with any bonds. A possible strategy could be to imagine a horizontal reflection plane and how they would rotate it to get it ready for the reflection step.*

6) Construct a model of benzene in two quadrants to show the before and after of an inversion operation. Use labels on the atoms to show which atoms end up where and explain how you got to your final decision. Sketch what you did and any labels or drawings you made on the system. What are the original and resulting x-, y-, and z-coordinates of the moving atoms?

> *Best built with 3 sp^2 pieces on each side with the reflection plane cutting through bonds rather than atoms (to fit to the connectors). Label the hydrogens on the before and after models. Finding the coordinates may be difficult, but they should be the same on both sides except for the axis perpendicular to the plane—those coordinates should be equal and opposite.*

Name: ______________________

Proper Rotation Axis System

(Omit suggested rubric in italics before handing out)

A proper rotation, or a rotation around an object's principle axis, is at the heart of group theory. Any symmetry decision trees or flowcharts are centered on finding the "C_n" and the presence of additional C_n's. The Proper Rotation Axis system is made to be used with any kind of molecular model kit or system. It can be used for degrees of rotation that range from 2 to 6 (C_2-C_6 axes). For help on putting the system together and other mechanical issues, see "How to Work with Proper Rotation Axes."

By the time you finish this worksheet, you'll be able to…

- Build frames of reference coordinating to the proper rotation axes of molecular models.
- Connect the visual frames and physical rotation catches to the geometry of molecules.
- Confirm suspected proper rotation axes in molecular models with the model system.
- Locate and defend the presence of multiple rotation axes at the same time.
- Locate reflection planes in a molecular model after finding the proper rotation axes.

1) What parts of the molecule do you need to pay attention to in a proper rotation? What happens as an atom rotates around its principle axis? What rules could you set for a proper rotation?

Students should look for similar, repeating bonds. As a specific atom rotates around its principle axis, it will encounter locations that are indistinguishable from the original position. Any atoms or bonds on the rotation axis remain stationary while the surrounding atoms and bonds move uniformly around it.

2) Build ferrocene into the rotation system. Describe how you decided the system should fit around it. Try a different way of fitting the ferrocene model into the system, discuss any changes and relevance.

Once a model is put together, decide if it will be staggered or eclipsed. 5 frames should be set up in the system. Specify if the frames align with the C's on the cyclopentadiene ligands or the bonds. Changes shouldn't matter—each rotation of 72° will result in an indistinguishable position.

3) How many different n-fold axes can you find in ferrocene? What do you do to find other symmetry elements: more proper rotations, reflection planes, improper rotations, inversions?

The principle rotation axis is C_5 and there are 5 C_2 rotation axes perpendicular to the principle rotation axis (CW and CCW to match the character table). There are reflection planes containing the principle axis and a horizontal plane in the eclipsed form. They're doing well if they notice the inversion center and improper rotation axis here (S_{10}).

4) Build NH_3 and BH_3. How do the models of these differ? What influence do their structures have on proper rotation axes? Give an argument for which symmetry element is most affected by their differences.

The different structures have no effect on the principle rotation axis (C_3), but BH_3's structure has a perpendicular C_2's and a σ_h. Both have σ_v's. Students can argue their symmetry element of choice, but they should see that BH_3 has more symmetry because it has the horizontal reflection plane.

5) Using a model of a basic octahedron in the system, how many different rotation axes can you find? Please list or sketch the axes you found, how you found them, and how you kept track of what you found. What could help you find these faster if you were asked the same question later?

There are 4 C_3 axes (8 if counting CW/CCW), 6 C_2 axes, and 3 C_4 axes (6 if counting CW/CCW and 3 C_2 ($=C_4^2$) in the same location). A C_3 goes through a triangular face, through the center atom only. Use labels to keep track of found axes and use the system to find the most difficult to see axis (probably C_3 or C_2).

6) Build adamantane ($C_{10}H_{16}$). Locate at least 2 different rotation axes and write their degrees of rotation. If you can find more than 2, what degree are they? How did you find and keep track of them? What was challenging about this molecule?

Adamantane has Td symmetry. They may find two different C_3 rotations first, but it may be harder to find a C_2 axis. There are 4 C_3's and 3 C_2's. Labeling helps tracking the different axes. Only 1 C-H bond aligns with each C_3 and no bonds are contained in the C_2.

7) a. Build $[PtCl_4]^{2-}$. What is its geometry? How did you choose a rotation axis to set it up?

$[PtCl_4]^{2-}$ is square planar and can be set up based on C_2 or C_4 to align it with each bond or flipping the whole molecule 180°.

b. If a dihedral reflection plane passes only through the center atom, how many dihedral planes are present? How do the planes relate to any rotation axes you've found? Describe or sketch any other reflection planes. What advice would you give for locating reflection planes?

There are two σ_d's, 2 σ_v's and a σ_h. The dihedral planes contain the principle rotation axis and C_2 axes perpendicular to the principle C_4. When a proper rotation or reflection plane is located, it may be a good indication that other symmetry elements are contained in the same spot. Look for ways the molecule can be flipped/rotated to get an indistinguishable position.

8) Set up NH_3 in the system. Add frames to the system until you've outlined all of this molecule's reflection planes. What do you observe? How do you differentiate between vertical and dihedral planes in this example? Were there any reflection planes you couldn't represent for NH_3? Which ones?

They should just double the frames so all six are distributed around NH_3. The pairs of opposite frames outline all vertical reflection planes in NH_3. In this case there is no difference between vertical and dihedral planes. The horizontal reflection plane can't be shown, but NH_3 doesn't have that symmetry element anyway.

APPENDIX C. Lecture and Recitation Observation Rubrics

Lecture Observation Rubric

Lecture Date: ________________________

Researcher Keeping Tally: ________________________

Keep a tally in the columns on the right for how often each action presents itself for both males and females.

	Male Students	Female Students
Student Questions & Responses		
Repetition/clarification questions		
Example request		
Specific problem, new to discussion		
Additional question on problem being discussed		
Used action verbs in response		
Described model components		
Made a comparison *(to real-life objects, previous examples)*		
Able to describe steps of operation		
Kinesics		
Gesture with both hands in air		
Gesture with one hand in air		
Gesture with pen in air		
Interaction with Physical Models		
Manipulate molecular model/homemade kit/pen as model		
Gesture around stationary model (hand or pen)		
Build model at desk		

Instructor Actions	
Used action verbs to describe	
Described model components	
Made a comparison *(to real-life objects, previous examples)*	
Described the steps of an operation	
Gestured with hands (no model or image used)	
Gestured with pen/pointer (no model or image used)	
Manipulated a model as demonstration	
Gestured around physical model	
Gestured around 2-D image (hands or pointer)	
Made a drawing to explain a concept	
Use of a reason/goal	
Class Mechanics	
Number of problems worked in class	
Time allotted to work problems	
Time allotted to manipulate models	
Time taken for class discussion	
Instances of instructor-generated discussion	
Instances of student-generated discussion	

Lecture Observation Rubric Descriptors

The field descriptors were referred to throughout the Fall 2011 and Spring 2012 semesters.

Student Questions & Responses	
Repetition/clarification questions	*Can you repeat that? Can you describe ____ again?*
Example request	*Can you show an example of [specific operation]?*
Specific problem, new to discussion	Independent question brought by student.
Additional question on problem being discussed	Follow-up questions--extending the conversation.
Used action verbs in response	Spinning, moves, flips, goes, makes, turning, doing.
Described model components	From framework, taught in recitation.
Made a comparison *(to real-life objects, previous examples)*	Any comparison will be fine to show visual thinking.
Able to describe steps of operation	May take extra time, but instrumental to use in more difficult problems and to teach their peers.
Kinesics	
Gesture with both hands in air	Self-explanatory.
Gesture with one hand in air	Self-explanatory.
Gesture with pen in air	Similar to writing/drawing in the air.
Interaction with Physical Models	
Manipulate molecular model/homemade kit/pen as model	Different from gesturing w/ pen, USING the pen as object.
Gesture around stationary model (hand or pen)	Holding the model still or on the desk.
Build model at desk	Assembly of commercial or homemade model.
Instructor Actions	
Used action verbs to describe	Describes something happening or doing, not the states of appearance.
Described model components	Elements, relationships, operations, patterns/rules.
Made a comparison	Self-explanatory.
Described the steps of an operation	Emphasis of what comes next or a summary.
Gestured with hands	No model or image used.
Gestured with pen/pointer	No model or image used.
Manipulated a model as demonstration	One mark for each concept—each sym element is a concept
Gestured around physical model	Held model stationary while moving hands around it.
Gestured around 2-D image (hands or pointer)	Around images on the overhead or board drawings.
Made a drawing to explain a concept	One mark for each drawing, additional marks for additional point made.
Use of a reason/goal	Stated reason/application of studying a concept.
Class Mechanics	
Number of problems worked in class	Instructor gives problem, students work on their own.
Time allotted to work problems	Keep a running tally on this per class period.
Time allotted to manipulate models	Keep a running tally on this per class period.
Time taken for class discussion	Keep a running tally on this per class period.
Instances of instructor-generated discussion	Instructor prompted students for explanations/examples.
Instances of student-generated discussion	Started maybe when prof says, "That's a good question…"

Recitation Observation Rubric

Researcher Keeping Tally: ________________________ **Recitation Date: ___________________**

Keep a tally in the columns on the right for how often each action presents itself for both males and females.

	Male Students	**Female Students**
Student Questions & Responses		
Repetition/clarification q*uestions*		
Example request		
Specific problem, new to discussion		
Additional question on problem being discussed		
Used action verbs in response		
Described model components		
Made a comparison *(to real-life objects, previous examples)*		
Able to describe steps of operation		
Kinesics		
Gesture with both hands in air		
Gesture with one hand in air		
Gesture with pen in air		
Drawing		
Draw in lieu of using a physical model		
Copy a drawing after board demonstration		
Draw on the board (volunteer or chosen)		
Interaction with Physical Models		
Manipulate molecular model/homemade kit/pen as model		
Gesture around stationary model (hand or pen)		
Fit model to any system		
Manipulate Ref Plane system		
Manipulate 3-D Coord system with model		
Write on 3-D Coord system (1 tally per problem attempt)		
Label atoms on 3-D Coord system		
Manipulate Proper Rot system		
Compare free model to one in a system		

Instructor Actions	
Used action verbs to describe	
Described model components	
Made a comparison *(to real-life objects, previous examples)*	
Described the steps of an operation	
Gestured with hands (no model or image used)	
Gestured with pen/pointer (no model or image used)	
Manipulated a model as demonstration	
Gestured around physical model	
Gestured around 2-D image (hands or pointer)	
Draw on board to explain	
Class Mechanics	
Number of problems worked in class	
Time allotted to work problems	
Time allotted to manipulate models	
Time taken for class discussion	
Instances of instructor-generated discussion	
Instances of student-generated discussion	

Additional Observations/Student Questions:

Recitation Observation Rubric Descriptors

Assisting graduate students were given the descriptors at the beginning of Fall 2011.

Student Questions & Responses	
Repetition/clarification q*uestions*	*Can you repeat that? Can you describe ____ again?*
Example request	*Can you show an example of [specific operation]?*
Specific problem, new to discussion	Independent question brought by student.
Additional question on problem being discussed	Follow-up questions--extending the conversation.
Used action verbs in response	Spinning, moves, flips, goes, makes, turning, doing.
Described model components	From framework, taught in recitation.
Made a comparison *(to real-life objects, previous examples)*	ANY comparison will be fine, start thinking visually.
Able to describe steps of operation	May take extra time, but instrumental to use in more difficult problems and to teach their peers.
Kinesics	
Gesture with both hands in air	Group by question as they happen.
Gesture with one hand in air	Group by question as they happen.
Gesture with pen in air	Similar to writing/drawing in the air.
Drawing	
Draw in lieu of using a physical model	When models are available, student chooses to sketch.
Copy a drawing after board demonstration	Obvious copying, usually furiously.
Draw on the board (volunteer or chosen)	Student drawing on the board.
Interaction with Physical Models	
Manipulate molecular model/homemade kit/pen as model	Different from gesturing w/ pen, USING the pen as object.
Gesture around stationary model (hand or pen)	Holding the model still or on the desk.
Fit model to any system	System: Research materials/model systems
Manipulate Ref Plane system	Permanent Reflection Plane demonstration
Manipulate 3-D Coor system with model	3-D Coordinate Axis system
Write on 3-D Coor system (1 tally per problem attempt)	3-D Coordinate Axis system
Label atoms on 3-D Coor system	3-D Coordinate Axis system
Manipulate Proper Rot system	Proper Rotation Axis system
Compare free model to one in a system	Needs two models being used at the same time.

Instructor Actions	
Used action verbs to describe	Describes something happening or doing, not the states of appearance.
Described model components	Elements, relationships, operations, patterns/rules.
Made a comparison *(to real-life objects, previous examples)*	Self-explanatory.
Described the steps of an operation	Emphasis of what comes next or a summary.
Gestured with hands (no model or image used)	No model or image used.
Gestured with pen/pointer (no model or image used)	No model or image used.
Manipulated a model as demonstration	One mark for each concept—each sym element is a concept
Gestured around physical model	Model remains still, gesturing occurs in space around it.
Gestured around 2-D image (hands or pointer)	Projector or chalkboard.
Draw on board to explain	One mark for each drawing, additional marks for additional point made.
Class Mechanics	
Number of problems worked in class	Instructor gives problem, students work on their own.
Time allotted to work problems	Keep a running tally on this per class period.
Time allotted to manipulate models	Keep a running tally on this per class period.
Time taken for class discussion	Keep a running tally on this per class period.
Instances of instructor-generated discussion	Instructor prompted students for explanations/examples.
Instances of student-generated discussion	Started maybe when prof says "That's a good question…"
Additional Observations/Student Questions:	Recorded questions you can hear, important observations, discussed topics.

APPENDIX D. Analyzed Observation Rubric Data

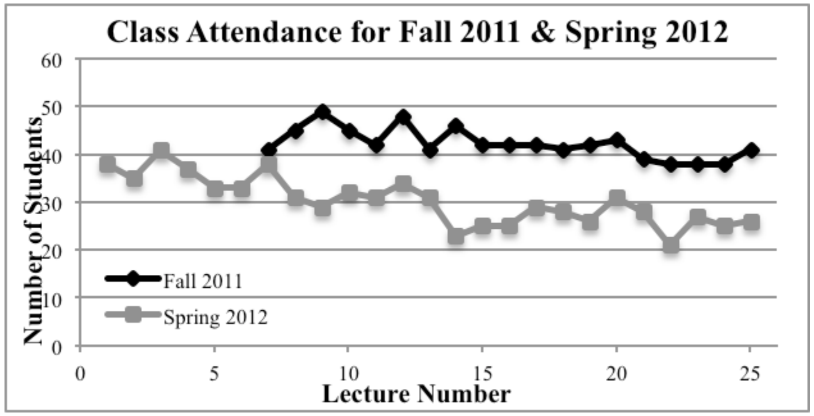


Figure D.1. Number of students attending each lecture of Fall 2011 and Spring 2012 excluding exam days.

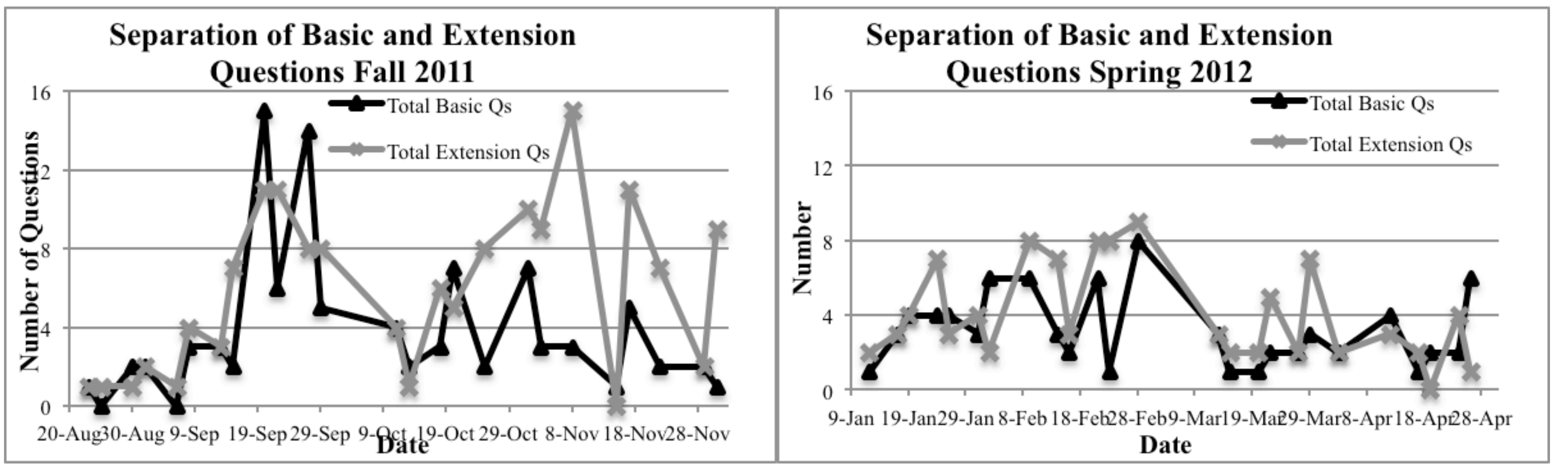


Figure D.2. The total number of student questions separated into basic and extension questions for Fall 2011 and Spring 2012.

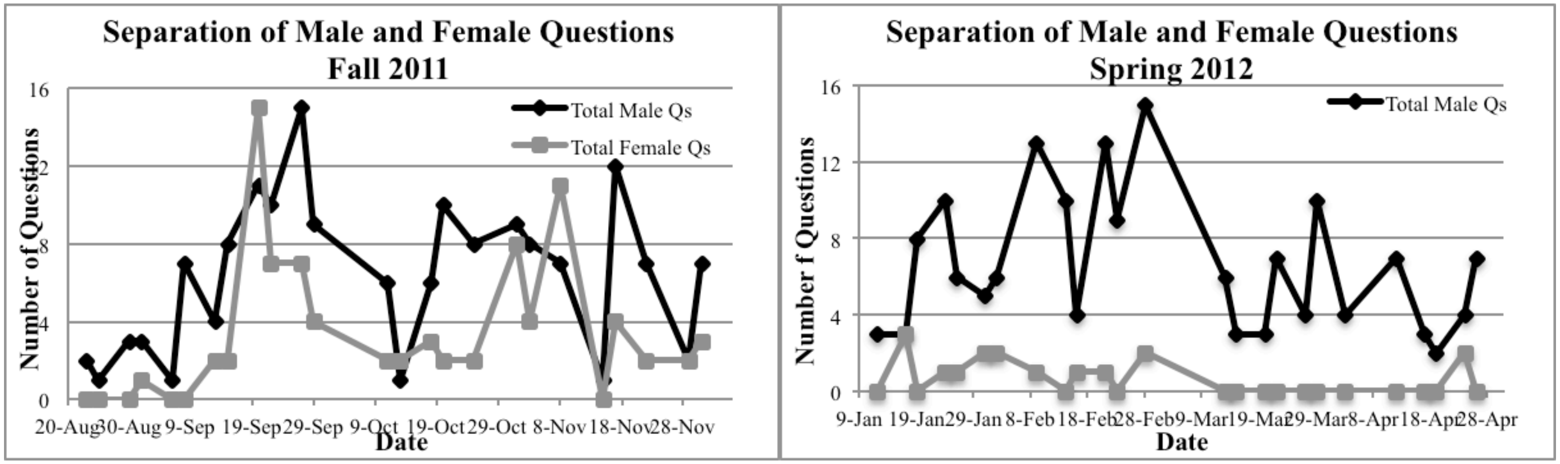


Figure D.3. The total number of student questions separated between male and female students for Fall 2011 and Spring 2012.

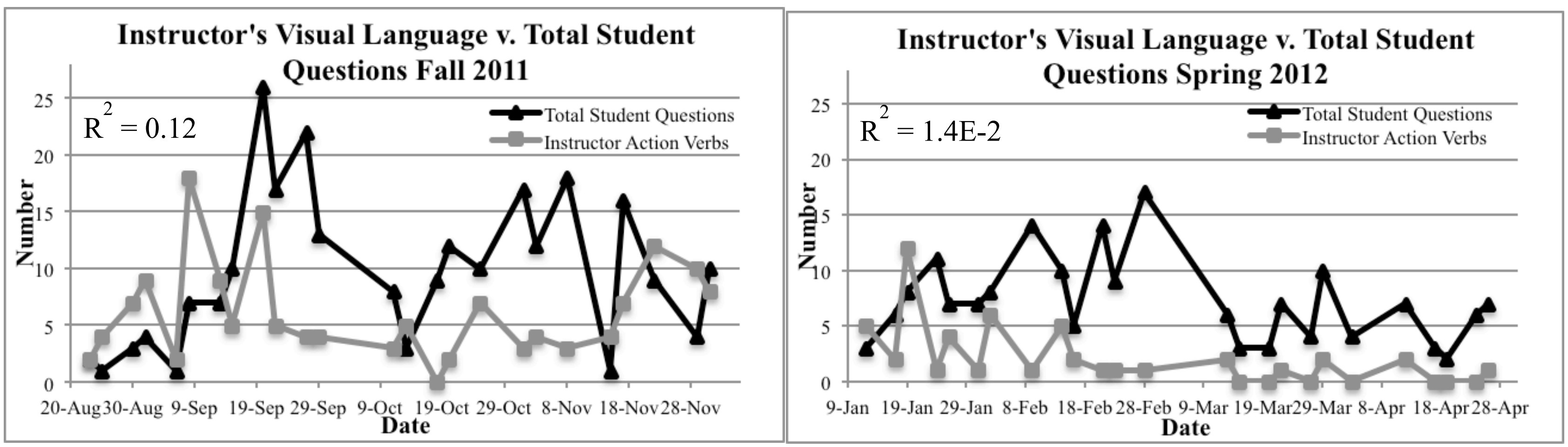


Figure D.4. Total student questions overlaid onto the instructor's use of visual language for fall (left) and spring (right).

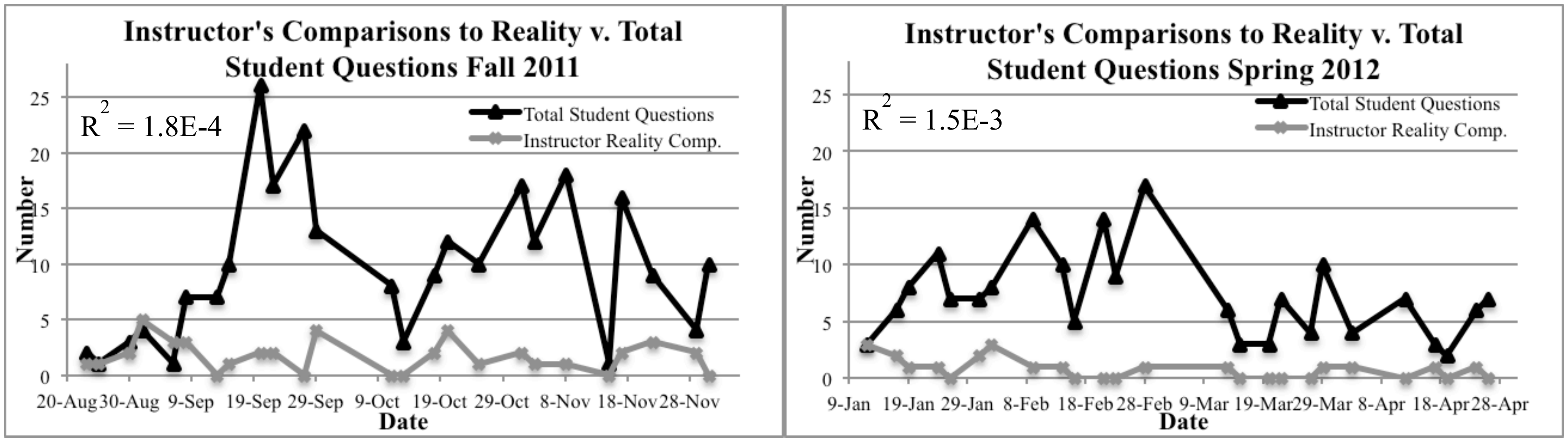


Figure D.5. Total student questions overlaid onto the instructor's comparisons to real life or past class for fall (left) and spring (right).

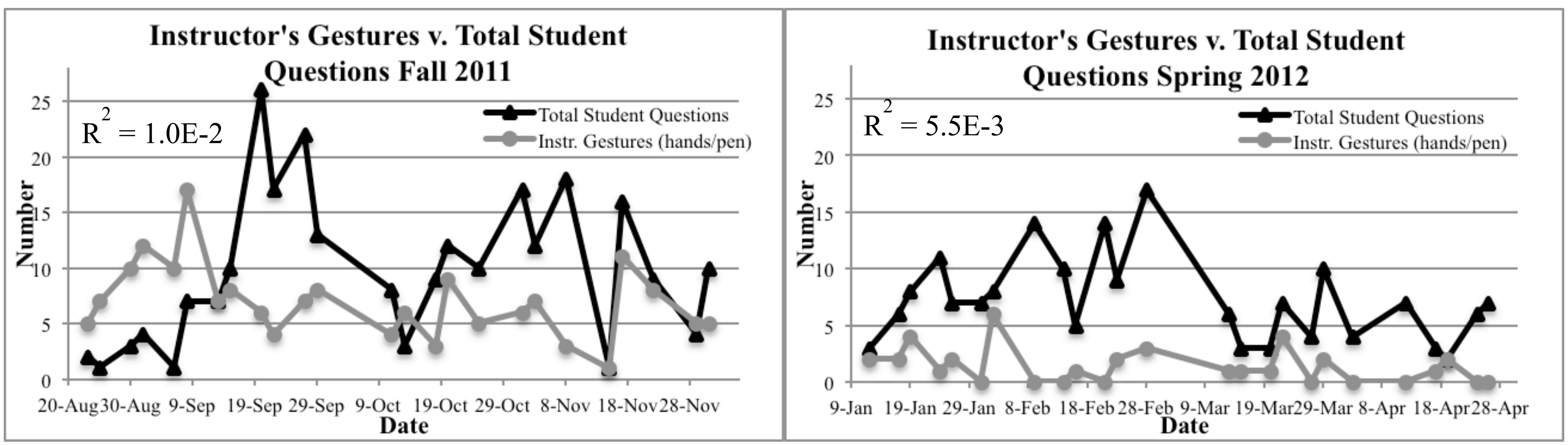


Figure D.6. Total student questions overlaid onto instructor's explanatory gestures for fall (left) and spring (right).

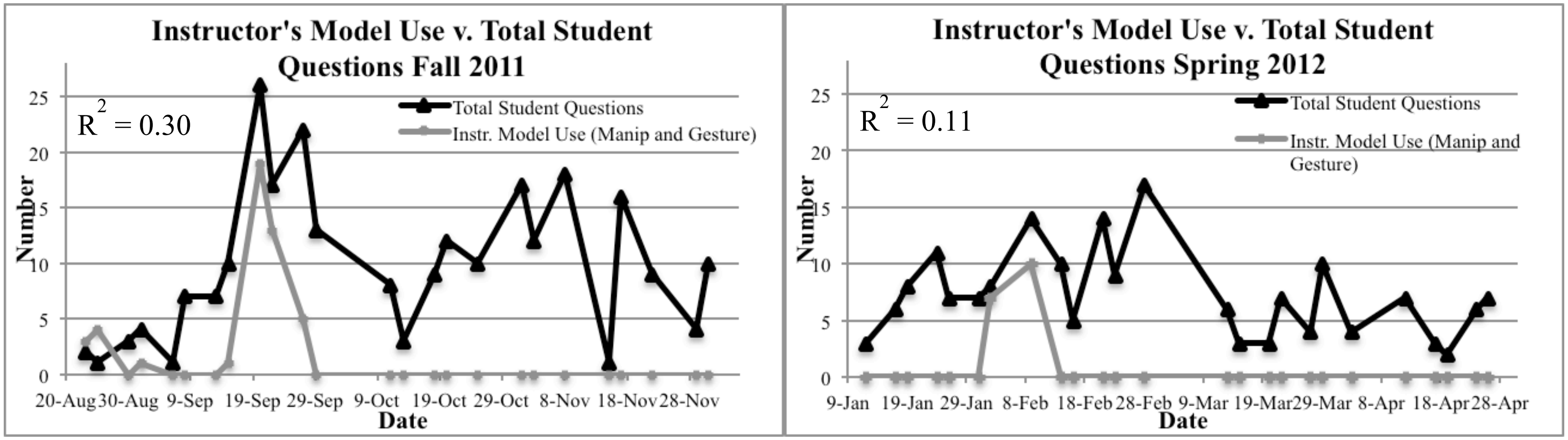


Figure D.7. Total student questions overlaid onto instructor's use of instructional models for fall (left) and spring (right).

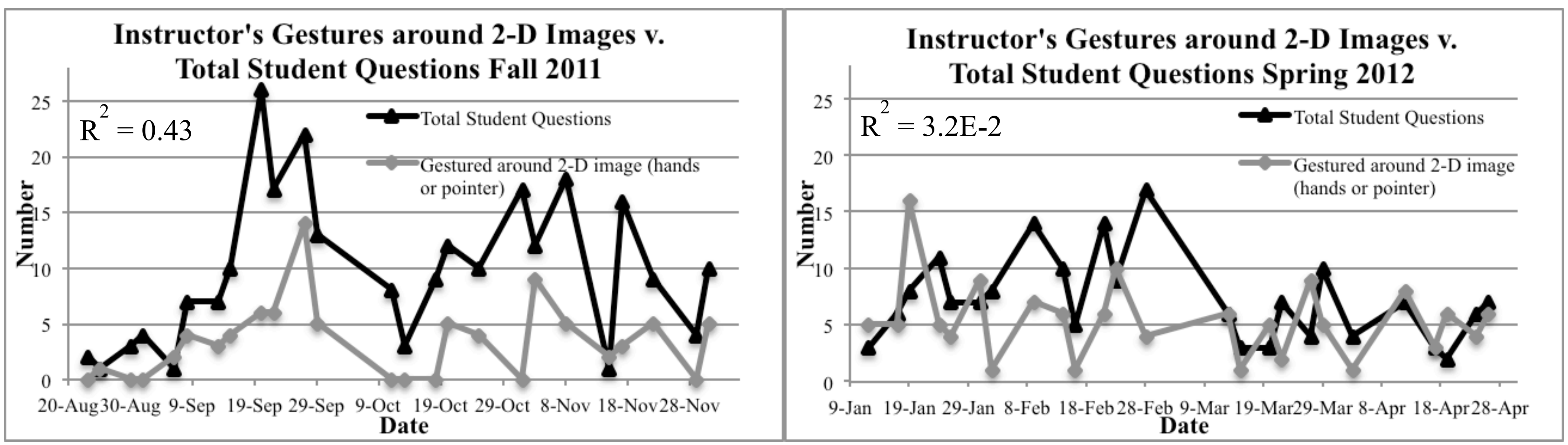


Figure D.8. Total student questions overlaid onto instructor's gestures around 2-D images (overhead screen, blackboard) for fall (left) and spring (right).

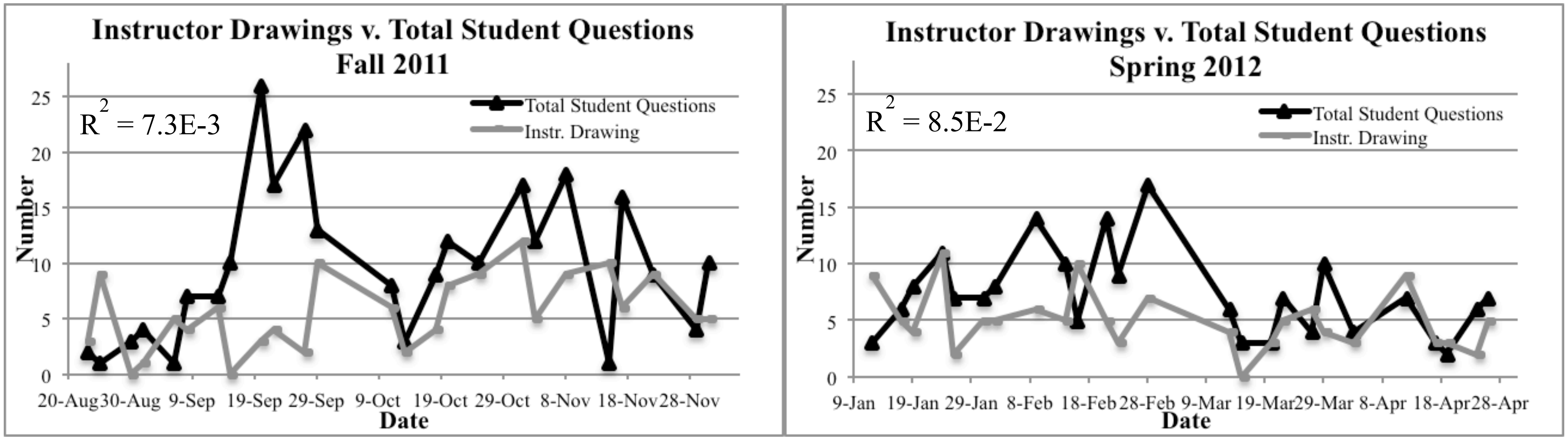


Figure D.9. Total student questions overlaid onto instructor's blackboard drawings for fall (left) and spring (right).

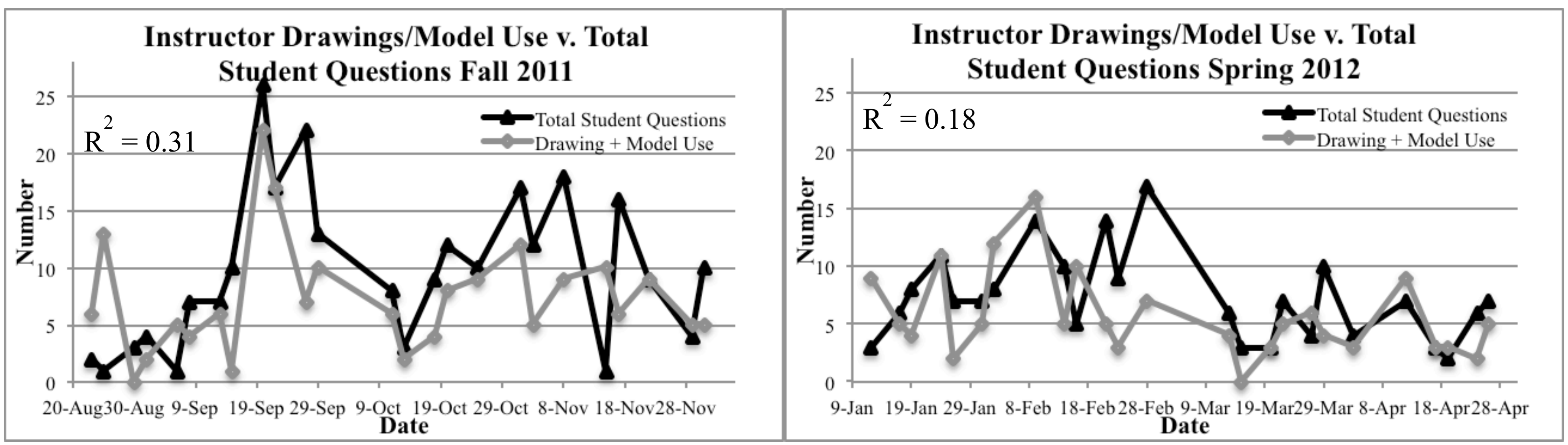


Figure D.10. Total student questions overlaid onto instructor's combined drawings and use of instructional models for fall (left) and spring (right).

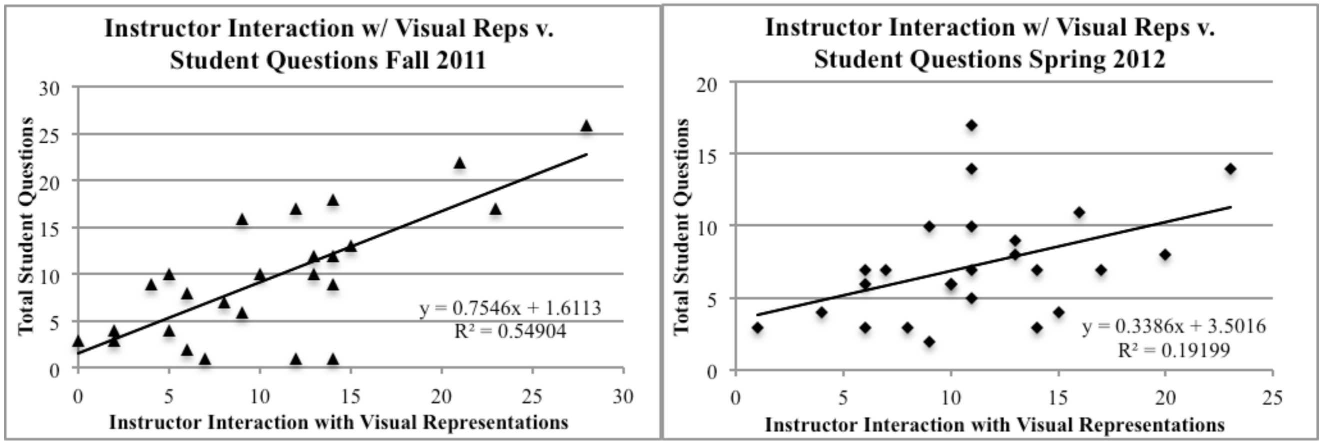


Figure D.11. The correlation plots resulting from plotting total student questions against the instructor's interaction with visual representations (drawings, model use, and gestures around 2-D images) for fall (left) and spring (right).

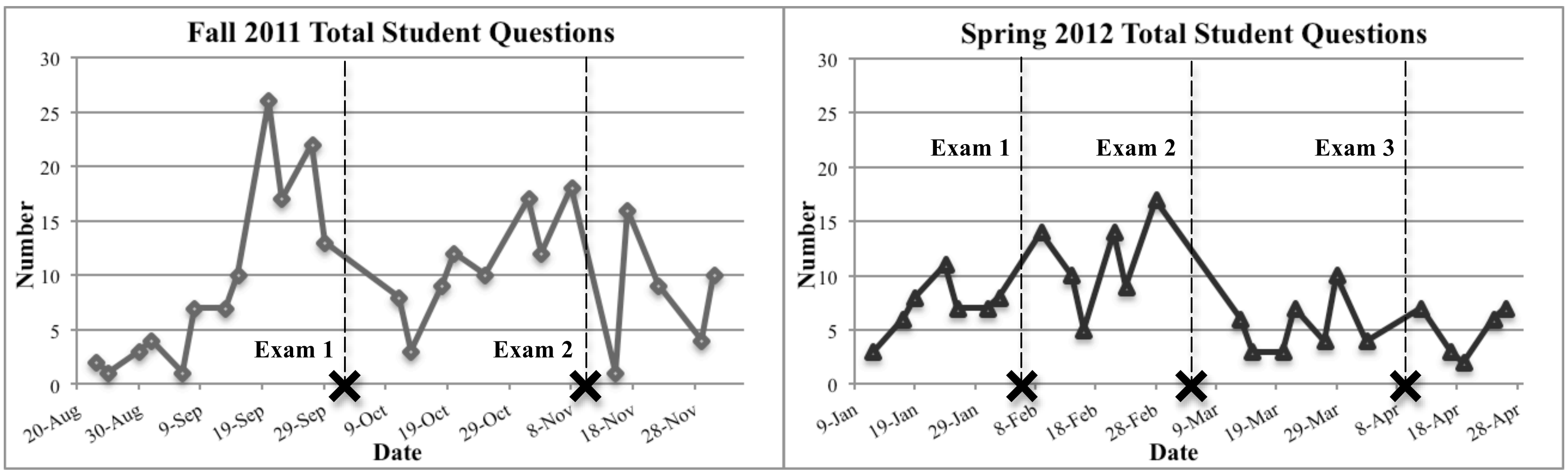


Figure D.12. Total student questions asked during lecture of Fall 2011 (left) and lecture of Spring 2012 (right).

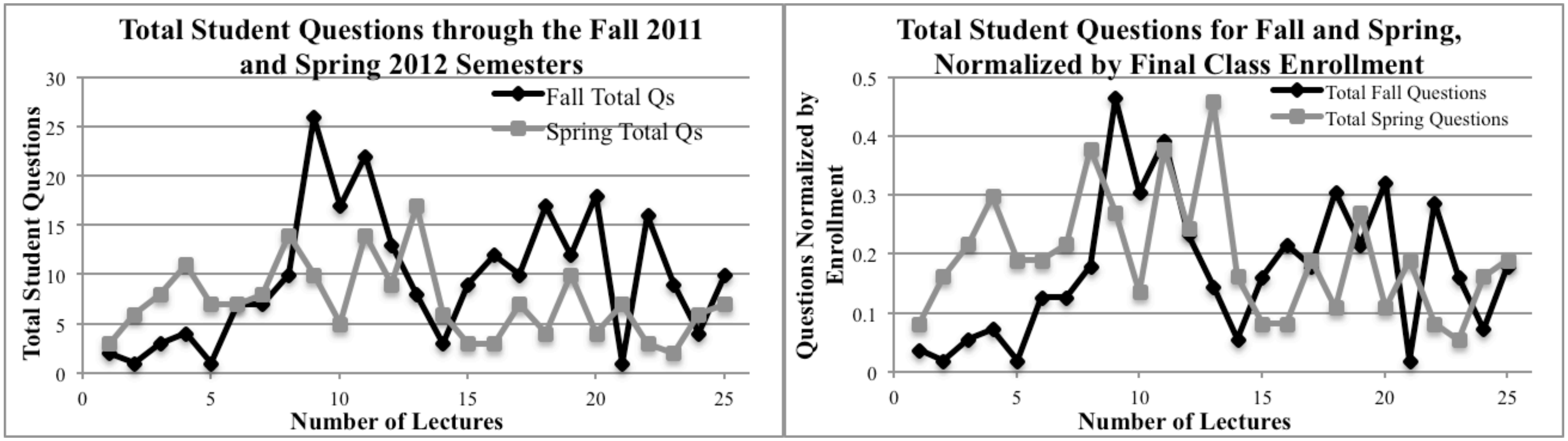


Figure D.13. Total student questions for each observed semester (right) and total student questions normalized by final class enrollment (left). Final enrollment was 56 for Fall 2011 and 37 for Spring 2012.

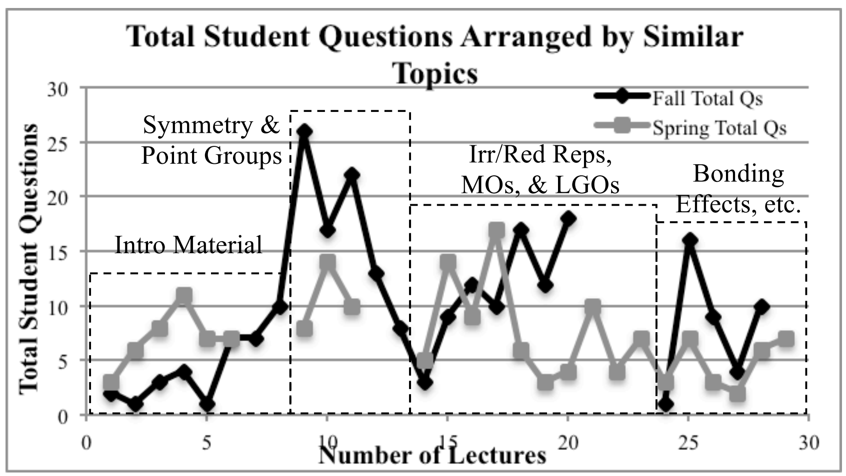


Figure D.14. Total student questions arranged by the primary topics discussed in each lecture for the Fall and Spring semesters.

APPENDIX E. Grading Rubric for Analytical Parameters within Complex Visualization Activities

The rubrics on the following pages provide information on how to classify student responses based on the four advanced deconstruction parameters discussed in Chapter 5:

- Analytical Deconstruction
- Valid Pattern Identification
- Personalized Strategy
- Extension of Symmetry

The complex visualization activities were formatted to outline the same types of questions each week—conforming to the Modeling Theory of Learning theoretical framework. The following list describes how students were instructed and guided to answer each question. Each describes what can be expected as a response in each question number.

1) Summary Question: Students answer the task in a variety of ways and may not necessarily volunteer analytical deconstruction or descriptions of patterns or strategies unless the task prompts them. If the task elicits any of these parameters, suitable responses should not be graded as such because students were following instructions.
2) Model Component Questions
    a. Elements: Students should list the simplest parts of the image. This is correct, but if they go beyond to describe relationships and patterns, look for signs of the indicated parameters.
    b. Relationships: Students should describe how the elements are related. Compound descriptions and extraneous detail to one kind of relationship indicate deconstruction. If a student's wording was suited to patterns or strategies, it would have been graded as either and indicated on the activity to guide students to address each question differently.
    c. Operations: Students should describe the dynamic relationships in the image. Grade the contents of this question the same as relationships.
    d. Patterns: Through wording and reference to key aspects of the image, students should describe relationships and operations in the form of a rule that the image adheres to.
3) Reality Comparison Question: Students should visualize an object/situation outside of the context of the worksheet and the course that reminds them of the image at hand.
4) Strategy Question: Students should describe the process they personally used to solve the task about the image or relay what they did to make sense of the image.

Analytical Deconstruction

Students' answers were categorized as valid deconstruction when they documented a break down of the image in a way that helped them understand the image.

Within valid questions, the response must conform to the detail description (necessary to consider). One point may be given per question containing analytical deconstruction. Additional fields listed may help to argue for/against difficult to categorize responses (optional, for reinforcement).

	Acceptable Indicators (1 pt)	Unacceptable Responses (0 pts)
Questions that may contain deconstruction **necessary*	• Within model component questions (2a-2d) • Within strategy question if student described the image without describing their process • All questions in Week 10	• Within summary question: students were asked to analyze through deconstruction—evidence in this question is only following directions
Detail description **necessary*	• Compound descriptions of relationships • Singular relationship supported by many adjectives/analogies (signs of effort to describe detail) • Statements that focus detail on a specific portion of the image	• Description of a singular relationship • General statements that don't relay information without the image to support the statement • Statements about given info that disregard the image • Use of language that misrepresents the image (not coherent with the image)
Symmetry **optional*	• Symmetry elements supported by a description/drawing of the location of the element • Comments on how the structure is laid out: repeating parts, what portions the sym element relates • Descriptions of which image parts result in a change from the sym element	• Lists of symmetry elements • Descriptions of general results of sym operations without referring to anything in the image

Valid Pattern Identification

The successful determination of a pattern helps students clarify the layout of the image. This is a compounded understanding of how relationships follow a pattern throughout the image and, ultimately, how students may comprehend what is presented in the image.

Within valid questions, the response must conform to the detail description (necessary to consider). One point may be given per question containing a valid pattern. Additional fields listed may help to argue for/against difficult to categorize responses (optional, for reinforcement).

	Acceptable Indicators (1 pt)	Unacceptable Responses (0 pts)
Questions that may contain patterns **necessary*	• Within pattern model component question (2d) • Within other questions that were graded as patterns to model the framework: shown by an arrow with credit given to that question • Any question in Week 10	• Any other questions within the activity • In Week 10, statements of Au atom groups—must describe an understanding of the pattern layout
Wording of the response **necessary*	• Statement signifies that the relationship happens throughout the image (a rule): Every time, each time, all the sides, etc • Singular or compound description that identifies the defining characteristics of the image and answers the task • Description of a pattern that clarifies the image	• Descriptions of relationships or patterns only applicable in one portion of the image—not a rule that may be applied to the image • Descriptions of patterns that do not match the image (incorrect) • Superficial description that is too vague to be correct
Example	• "Every yellow sphere connects to three blue molecules." • "The flat image has a C_6 rotation axis b/c it does not show orientation of rings in bond. The 3D has C_3 rotation axis b/c bonds are different. Flat image has 6 planes of reflection." • Week 9, want complete movement or detailed or directionalized rotation: "A total 90° rotation along the molecule and flip 180° along axis perpendicular to molecule."	• "three blue molecules connect to a yellow sphere" • Week 9: "a flip and a rotation"

Personalized Strategy

A valid strategy description is one that helped the student solve the task or understand the image. The ideal strategies are those that describe the process the student themselves used, including missteps, clarifiers, and what ultimately led students to the correct answer.

Within valid questions, the response must conform to the detail description (necessary to consider). One point may be given per question containing a valid strategy. Additional fields listed may help to argue for/against difficult to categorize responses (optional, for reinforcement).

	Acceptable Responses (1 pt)	Unacceptable Responses (0 pts)
Questions that may contain strategy **necessary*	• Within the strategy question (4) • Within other questions that were graded as strategies to modeling purposes: shown by an arrow with credit given to that question	• Any other questions within the activity
Wording of the response **necessary*	• Step(s) of a process that the student may have credibly used, useful or not	• General steps that do not refer to the specific image/task • Strategy so general that it would not be useful to solve the task • Answer to the task
Alternative wording **optional*	• Mistakes, repetitive, or unnecessary steps (shows what students tried) • Visual, vivid description (shows how students analyzed the image)	
Example	• "Look for parts which reduce the symmetry such as A starts as C6, but gets reduced to C3"	• Statements about looking at the differences and finding the symmetry

Extension of Symmetry

Extension of symmetry is students' documentation of visualizing or explaining motion with symmetry operations and movement practiced during the symmetry portion of the class. Students demonstrate this extension through constructive application of descriptive words and symmetry terminology. Besides Weeks 8 & 9 (where symmetry reference was not required), the other activities elicited symmetry terminology and visualization and may not be considered for symmetry extension.

Within valid questions, the response must conform to the detail description (necessary to consider). One point may be given per question containing the extension of symmetry. It's possible that extension of symmetry may overlap with the other parameters (deconstruction, pattern, strategy) if symmetry was used as a tool. Additional fields listed may help to argue for/against difficult to categorize responses (optional, for reinforcement).

	Acceptable Responses (1 pt)	Unacceptable Responses (0 pts)
Questions that may contain Sym Extension	• Within the Week 8 & 9 activities (all questions)	• Within activities 1-7, 10
Detail description **necessary*	• Use of symmetry operations and description in responses • Reference to symmetry operations in the description of manipulating the image • Reference to symmetry elements within the object/image	• Lists of symmetry elements • Descriptions of symmetry that don't make sense or disagree with either the image or the students drawings/coordinate axes •
Alternative Symmetry Use **optional*	• Use of symmetry operations as tools to move the image object • Descriptions using sym elements as adjectives or references • Descriptions of the result of sym operations (w/o stating the element) for Week 8: indicates use of symmetry	• Week 8, responses including only symbols or reducible reps (which were elicited) • Descriptions of the rotations, flips, and turns without mentioning planes or axes in Week 9
Example	• "flip over the axis", "C_2 turn", "vertical reflection down the middle" • "Rotate the entire molecule 180, making the 5-atom rings with both N and O switch in position."	• "Turn the outermost right ring [drawing] 45° towards the page, the benzene ring 75° towards the page, the five atom ring with the OH group 90° towards the page, and the final ring 90° with the ligand sticking outside of the page." (does not mention sym elements)

APPENDIX F. Complex Visualization Activities and Resulting Data

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Name: ________________________

Week 1: Caerlaverock

Read all the questions before you begin, but make sure you answer #1 last.
The image below displays an object with defining characteristics.[1] Use the questions to break the image down to very simple parts to describe if the image looks familiar to you. If you don't know what's displayed, describe what you can of the different parts of the image.

1. Describe how to get from point A to point B.

2. Describe the parts of the visual. Answer the following questions to help organize all the parts.
   a. *Elements*: What are the simplest parts of the image/problem/object/situation? (Sides, top, bottom, grass, water, materials, structures, materials)

b. *Relationships*: How are the simplest parts related to each other? (Surroundings, positions, numbers)

c. *Operations*: How do the parts interact? (Movement, intersections, changes)

d. *Patterns/Rules*: What overall patterns or rules do the parts, operations and relations follow (that you observe or infer)?

3. Connect the visual to reality. Name something that this visual looks like. Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Geograph Britain and Ireland. NY0265: Caerlaverock Castle. http://www.geograph.org.uk/photo/612761 (accessed January 22, 2012). Image Copyright Simon Ledingham.

Week 1 Activity Data:

Students' task was to describe how to get from point A to point B, which were both designated on a picture of castle ruins. Students reported the same kinds of processes throughout the activity. It was very common for them to mix up model components, relationships, operations, patterns, strategies, and the summary question. In general, students reported moving around the castle on the grass to the bridge, into the castle, finding some way to reach the tower, ascending the tower to point B.

Table F.1 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.1. Number of instances of observed deconstruction parameters demonstrated by students during the Week 1 complex visualization activity.

	Week 1: Castle						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp.**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	5	1	0	0	1	0	0
002	8	0	1	0	0	1	0
003	7	0	0	0	0	1	0
004	3	0	1	0	0	0	0
005	8	0	0	1	1	0	0
006	6	1	1	0	1	0	0
007	9	0	0	1	1	0	0
008	7	0	0	1	1	1	0
009	6	0	0	0	1	0	0
010	10	0	0	0	1	0	0
011							
012	8	0	0	1	1	0	0
013	6	0	0	0	0	0	0
014							
015							
016	4	0	0	1	1	0	0
017	6	0	0	0	1	0	0
018	2	1	1	1	0	0	0
019							
020	6	0	1	0	1	1	0
021	8	0	0	1	0	1	0
022	7	0	0	0	0	0	0
023	6	0	0	0	1	1	0
024	8	0	0	0	1	0	0

Table F.1 (continued)

025	4	0	0	0	0	0	0
026	1	1	0	0	1	0	0
027	1	1	0	1	1	0	0

Within the reality comparison question (Question 3 of the activity), 18 students made castle comparisons to the image. There were a few comparisons (Table F.2) that made additional comparisons that may relay a method of analysis students used when making their comparison.

Table F.2. Week 1 reality comparisons that were unrelated to the activity content.

ID #	Reality Comparison
002	"It honestly resembles a eukaryotic cell."
004	"The visual components to an amino acid attached to a protein structure."
006	"A blood vessel."
018	"The building and the lake look like a trapezoid."
020	"The general shape reminds me of an upside-down lamp shade."

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.3. Week 1 evidence of analytical deconstruction.

ID #	Documented Response
005	"Pt. B is not only across the water, but at a higher level; stairs are involved in getting to Pt. B"
007	"Outer layer first: grassy area→bridge→outside of castle→inside of castle→top of castle"
008	"To get to the castle, on foot, you must take the bridge, then to get to the upper level of the castle you must go up a staircase in the front or back right of the castle."
012	"Point B is higher than A. Once in the castle, you will have to find a way up stairs, rope, or elevator to it. Use the bridge to cross the water and enter the castle through the door."
016	"We are trying to get from point A to point B. There is a bridge, castle, water surrounding the castle. The castle has 4 sides, and one side is missing a wall. The top of the castle is open/uncovered. The castle is surrounded by forest and greenery."
018	"The building and the lake have the shape of a trapezoid. This picture was taken from the sky looking down to the building and surround. The building is in the middle of a lake and the bridge helps to get to the building from land/area around the lake. There's forest surrounding the land that contains the lake."
021	"Each platform is easily able to be separated from the others by cast of shadows, sloping fields, reflections in the water."
027	"Moat surrounds castle, is surrounded by brush/grass, which is surrounded by trees. Pathway cuts through grass, connects to bridge, which connects to castle. A is in grass, B is in castle."

Table F.4. Week 1 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
001	"For travel, it appears that the bridge is necessary to get from the land to the castle to bypass the moat."
005	"The water is not to be swam in so the bridge is unavoidable." "Pt. B is higher than Pt. A so a means of elevating is essential."
006	"The castle is inaccessible except for the bridge."
007	"You cannot go from one layer to the other unless they are connected."
008	"Assume that the ground (grass) is solid and that the bridge is safe to walk across and that the castle is open (open doorway) and that there are stairs either in the front or back of the castle."
009	"Can't walk on water; it serves as a barrier." "Building has multiple levels probably connected in some way (stairs)." "Bridge allows one to cross water barrier."
010	"water protects castle"
012	"You can't go through the walls, only doors or windows."
016	"We can assume that the castle is rock solid and that the front of the castle will [lead?] and provide access to the back of the castle."
017	"You must cross the bridge to get to the castle."
020	"hole in ground follows the general shape of the castle, all parts have 4 edges with two sides about the same size and a long and short end forming a trapezoid."
023	"bridges must be used to span water"
024	"It can be observed that we are moving to a higher elevation."
026	"gravity" "walls are stone, so thick and sturdy"
027	"Can't cross moat." "bridge is only way into castle" "castle is only way to tower"

Table F.5. Week 1 evidence of personalized strategies.

ID #	Documented Response
002	"I take into account possible movements that can be linked together to reach the destination."
003	"Take in surroundings and choose the easiest path that didn't involve getting wet."
008	"Imagine myself walking from point A to point B."
020	"I would consider the path you would follow by looking at the photo. I made sense of it by looking at the overall picture and then the constituent parts. I started at the outside when considering the parts b/c that is where pt. A is."
021	"Survey the different aspects of the area and make inferences based on elevation, reflections, structure, and shadows."
023	"Take an imaginary walk through the structure."

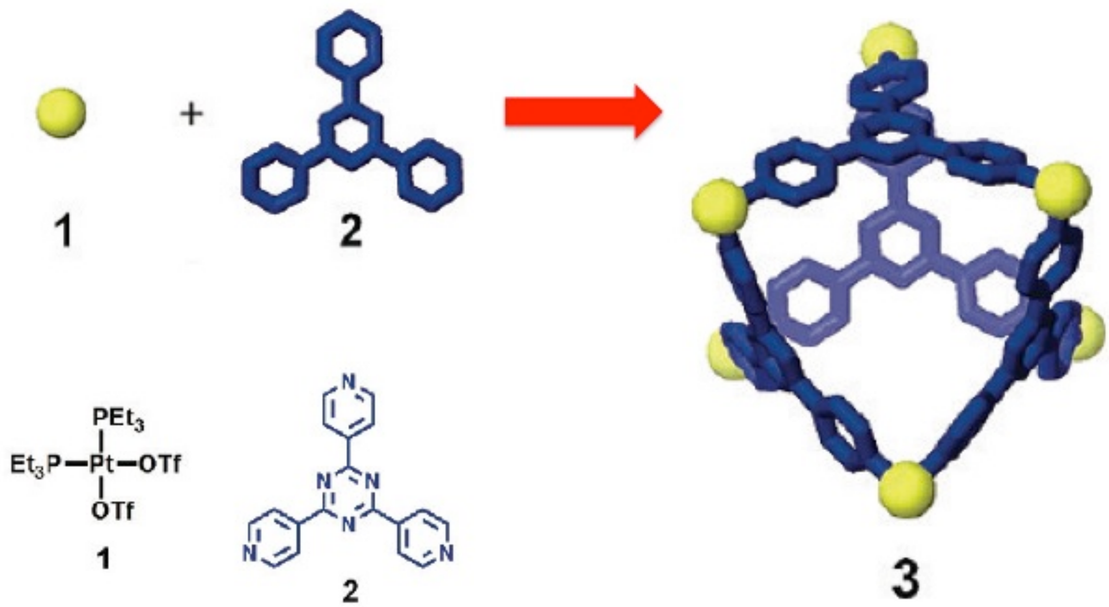
Table F.6. Instances of students using non-traditional means of travel.

ID #	Method of Travel
004	Zipline
007	Call a friend with climbing gear
012	Elevator
024	Jet pack
025	Wormhole, castle is protected from the black knight

Name: ______________________________

Week 2: [6+4] Metal-Organic Supramolecule

Read all the questions before you begin, but make sure you answer #1 last.
The scheme below shows two molecular components (**1** and **2**) that self-assemble into molecule **3**, the starting material for further component substitution and structural modification.[1] Use questions 2-4 to break the image down in order to describe its symmetry elements. If you don't know how to interpret the molecule, describe what you can of the different parts of the image.



1. Describe (in words) the locations of all symmetry elements present in molecule **3**. Include all instances of a particular type of symmetry element. Use labels on the portions and parts of molecule **3** to help you put the locations into words.

2. Describe the parts of the visual. Answer the following questions to help organize all the parts.
   a. *Elements*: What are the simplest parts of the image/problem/object/situation? (Sides, top, bottom, atoms, bonds, shapes, structures)

b. *Relationships*: How are the simplest parts related to each other? (Surroundings, relative locations, positions, numbers)

c. *Operations*: How do the parts interact? (Intersections, connections, changes, motion of symmetry operations)

d. *Patterns/Rules*: What overall patterns or rules do the parts, operations, and relations follow (that dictate what assumptions you may make)?

3. Connect the visual to reality. Name something that this visual looks like. Does it resemble or remind you of anything you've seen before?

4. What *strategy* would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Zheng, Y.-R.; Lan, W.-J.; Wang, M.; Cook, T. R.; Stang, P. J., *J. Am. Chem. Soc.*, **2011**, 133, 17045–17055. Copyright 2011 American Chemical Society.

Week 2 Activity Data:

Students were given a scheme that showed platinum centers as spheres and trigonal planar ligands assembled into the shape of a truncated tetrahedron. In the summary question, students were asked to describe the locations of all symmetry elements in the assembled molecule and use labels to help put the locations into words.

Table F.7 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction or valid pattern determination. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.7. Number of instances of observed deconstruction parameters demonstrated by students during the Week 2 complex visualization activity.

	Week 2: [6+4] Metal-Organic Supramolecule						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp.**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	0	3	0	1	0	0	0
002	1	0	1	0	0	1	0
003	3	0	3	0	1	1	0
004	2	1	1	0	0	0	0
005							
006	0	0	1	2	0	0	0
007	2	0	1	1	1	1	0
008	4	1	1	1	1	0	0
009	6	0	1	0	1	1	0
010	1	3	0	0	1	0	0
011	5	3	1	0	1	0	0
012	2	0	0	1	0	0	0
013	2	0	1	2	2	0	0
014	6	6	0	0	0	0	0
015	2	0	2	0	0	0	0
016	0	0	0	0	1	1	0
017	1	0	0	0	1	1	0
018	2	0	0	0	0	1	0
019	6	1	1	0	0	0	0
020	0	0	1	1	1	1	0
021	1	0	2	0	2	1	0
022							
023	3	2	0	1	0	0	0
024							

Table F.7 (continued)

025	1	0	1	1	0	1	0
026							
027	4	1	0	1	1	0	0

Table F.8. Week 2 reality comparisons that were not symmetry related.

ID #	Reality Comparison
002	Human heart (metal complexes resemble heart valves, four faces for four chambers)
003	The pyramids, jacks, a firewall coding system
004	Six-sided die
006	3-sided crown
007	Diamond type structure
008	Box
009	A dice
011	Triangular prism
012	A group of triangles
013	A chain that links around itself
015	A can of something, a funky hat
019	Ball
020	Sort of 3-D diamond figure, parts of a beehive
021	Front end of a train, a model made out of kinex pieces
025	Jacks

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.9. Week 2 evidence of analytical deconstruction.

ID #	Documented Response
001	"There's one [molecular component] 2 on top and another located on the bottom. Three [molecular component] 2 make up the sides."
006	"Assuming the parts that overlap are the same as the visible parts," "Since there is no central object for the balls to bond to, they are connected by the 3 sided planar compound"
007	"Ligands also form triangular faces adjacent and opposite to the Pt faces"
008	"Axis of symmetry down the top "#1" atom through the bottom one."
012	"The 3 exterior rings of 2 are each attached to molecule 1. They form 2 3-D structures around [an] open space."
013	"Each group of six-membered rings is organized in an upside-down Y formation. The outside edges of these molecules are linked to a ball-shaped molecule, which links each formation together."
020	"The outer rings are then connected to the spheres at each edge."
023	"xy elements (1) equidistant from mid point. Elements (1) along z axis also equidistant. Molecules (2) are equal [angles] from center."
025	"The motion of the planes: spin clockwise, top and bottom don't move."
027	"Faces (part 2's) are connected to each other at extremities by part 1's."

Table F.10. Week 2 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
003	"Each side will always be triangular"
007	"each ligand must bond to 3 Pt"
008	"no #2 is ever directly connected to another #2"
009	"The (1) is always attached to 2 (2) molecules, connecting the (2). No (1) is connected to the same two (2) molecules"
010	"3 1's at each of the ends of 1 2 where each 1 connects an end of 1 2 to another"
011	"Each (structure 2) makes contact to a (1) and each (1) is connected to two (2)s"
012	"the 3 exterior rings of 2 are each attached to molecule 1"
013	"Each group of six-membered rings is organized in an upside-down Y formation. The outside edges of these molecules are linked to a ball-shaped molecule, which links each formation together." "Each face of the object somewhat resembles a trigonal plane."
016	"each yellow circle connects/holds together 2 blue molecules"
017	"The interactions with component 1 and 2 form triangular faces"
020	"These spheres are bonded to 1 other hexagonal ring which repeats the 4 ring formation"
021	"Each molecule 1 is connected to two molecule 2's"
025	"Each face has a rotation axis through its center"

Table F.11. Week 2 evidence of personalized strategies.

ID #	Documented Response
002	"Combine all visual elements to describe a way to orient (1) and (2) to make (3)."
003	"Break it apart into the sides and pieces. Then, find the symmetry of each piece and side."
007	"I would start by looking for planes of symmetry."
009	"I would look at the symmetry of the parts and use that to determine the symmetry of the whole. Also, it's mostly the symmetry of (2) that matters for this molecule."
016	"Structure one was a good reference for where each of the structure 2 molecules came together. They allowed me to see that this was a 3-D structure."
017	"Find symmetry in triangles first."
018	"Look for the same molecule/pattern to decide what operation to use to get the same image."
020	"Look at the constituent parts and describe how they make up the entire molecule."
021	"I would look at both molecules 1 and 2 separately, then look at molecule 3. I would then determine how molecule 1 and 2 are related to each other and why they are related to each other. Then I would see how molecule 3 is made up of molecules 1 and 2."
025	"Count the number of atoms that move when rotation about an axis."

The structure in the image has tetrahedral symmetry, so if students located all the operations, they'd end up with 24 (17 elements in unique locations in space). Of the 23 students in attendance, the following shows how many elements 18 different students reported. The remaining students wrote incorrect or made-up elements or did not attempt to answer.

Table F.12. Summary of the number of symmetry elements students identified in the Week 2 summary question.

Unique Elements	Student ID #
6 elements	009, 014, 019
4 elements	008, 027
3 elements	003, 023
2 elements	004, 007, 012, 013, 015, 018
1 element	002, 010, 017, 021, 025

The following shows students that successfully described a symmetry element along with its location as instructed in the activity.

Table F.13. Specific descriptions of symmetry element locations during Week 2.

ID #	Documented Response
001	"C_3 through the center of each [molecular component] 2"
007	"vertical planes of symmetry along both sides," "ligands also form triangular faces adjacent and opposite the Pt faces"
008	"2,3 and 4,5 are on a plane," "1,2,4; 2,3,6; 1,3,5; 4,5,6 are their own faces," "axis of symmetry down the top "#1" atom through the bottom one"
009	"connects to N atom on outer benzene rings"
010	"C_3 through center ring and spheres"
011	"There is a C_3 axis through each of the center of the (2)'s"
012	"Each face has E, C_3"
015	"a vertical line of symmetry right down the middle," "an S_3 around the sides," "a σ between the top and side"
017	"rotational axis A on the faces has C_3 symmetry"
018	"C_3 rotation around the y axis," "C_3 around the axis goes straight through the hole in 2"
019	"mirror through the middle," "rotate 1/3 through axis in the center of the group of hexagons, in the central hexagon"
020	"the outer rings are then connected to the spheres at each edge"
023	"each element (1) in the xy plane is equidistant to [the center]," "the elements (1) along the z axis…," "xy elements (1) equidistant from midpoint"
025	"4 atoms in horizontal plane"

Students were encouraged to use visual language in their descriptions. The following lists the descriptive language students incorporated.

Table F.14. Examples of descriptive, visual language during Week 2.

ID #	Descriptive Language
001	"triangle"
002	"triangle shape"
003	"triangle rings," "pyramidal structure"
006	"since there is no central object for the balls to bond to, they are connected by the 3-sided planar compound"

Table F.14 (continued)

009	"Here the symmetry of the (2) is much like that of a triangle"
010	"closed structure"
013	"ball-shaped molecule," "between any 2 adjacent ball-shaped molecules"
016	"rotating the molecule clockwise will look the same"
019	"rotate 1/3," "flip over by rotating ½"
020	"There are 4 #2 parts connected at each of their 3 corners to a #1 element which is attached to one other #2 element such that the combined 1 and 2 elements form a structure that looks like 2 pyramids connected at their bases"
021	"rotated and flipped"
025	"spin clockwise"
027	"triangle"

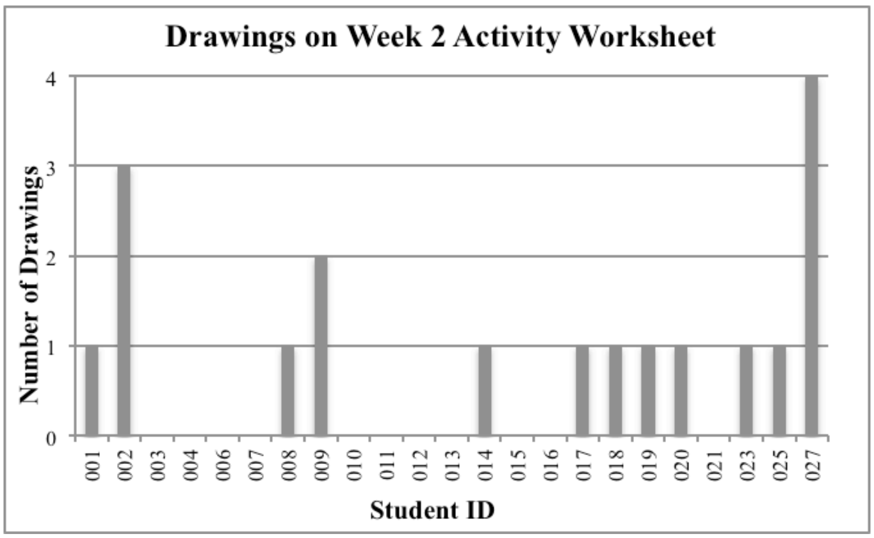


Figure F.1. Number of drawings, coordinate axes, arrows on the image documented by students.

Five students documented more advanced, yet incorrect answers than they supported in their descriptions. They demonstrated that they did not deconstruct and fully analyze the image.

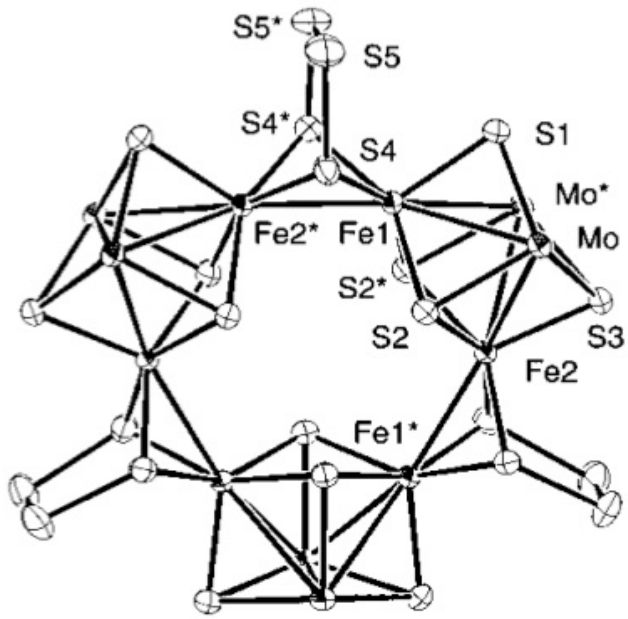
Table F.15. Evidence of advanced language and conclusions unsupported by observations during Week 2.

ID #	Documented Response
003	"24 parts" (*student multiplied '6 parts of symmetry' by 4 faces*)
004	"it is a tetrahedral structure" (*only listed E, C_n, and σ as symmetry elements w/o additional support*)
006	"octahedral shape"
023	"can be reflected or rotated 180 to return a similar looking structure," "octahedral structure," "octahedron"
025	"It's is a bipyramidal with a square base"

Name: ____________________________

Week 3: Cyclic Tricubane Cluster

Read all the questions before you begin, but make sure you answer #1 last.
The supramolecular structure below was synthesized by way of a deliberate, rational method instead of as a result of self-assembly.[1] Use questions 2-4 to break the image down in order to describe its symmetry elements. If you don't know how to interpret the molecule, describe what you can of the different parts of the image.



1. Describe (in words) the locations of all symmetry elements present in this molecule. Find all instances of a particular type of symmetry element. Use labels on specific parts and groups of parts to help you put the locations into words.

2. Describe the parts of the visual. Answer the following questions to help organize all the parts.
   a. *Elements*: What are the simplest parts of the image/problem/object/situation? (Sides, top, bottom, atoms, bonds, shapes, structures)

b. *Relationships*: How are the simplest parts related to each other? (Surroundings, relative **locations**, positions, numbers) How would you describe where a component is?

c. *Operations*: How do the parts interact? (Intersections, connections, changes, motion of symmetry operations) What function do the symmetry operations serve?

d. *Patterns/Rules*: What overall patterns or rules do the parts, operations and relations follow? What rules can you rely on to be true throughout the molecule?

3. Connect the visual to reality. Name something that this visual looks like. Does it resemble or remind you of anything you've seen before?

4. What *strategy* would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Kawaguchi, H.; Yamada, K.; Ohnishi, S.; Tatsumi, K. *J. Am. Chem. Soc.* **1997,** *119,* 10871-10872. Copyright 1997 American Chemical Society.

Week 3 Activity Data:

The structure for this week was a D_{3h} ORTEP structure of a self-assembled Fe-S-Mo molecule. As with Week 2, students were directed to describe the locations of all symmetry elements and all instances of each symmetry element to generate more detailed responses.

Table F.16 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.16. Number of instances of observed deconstruction parameters demonstrated by students during the Week 3 complex visualization activity.

	Week 3: Cyclic Tricubane Cluster						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	4	0	1	2	1	1	0
002							
003	6	1	2	0	0	1	0
004	6	0	1	0	0	1	0
005	8	2	0	1	1	0	0
006	3	0	2	0	0	0	0
007	5	0	1	0	0	1	0
008	0	1	2	1	0	1	0
009	8	0	0	3	0	1	0
010	8	1	0	2	0	1	0
011	8	4	0	0	0	0	0
012	8	0	0	3	0	0	0
013	3	0	1	2	1	1	0
014							
015	7	0	1	1	0	1	0
016	5	1	0	2	0	1	0
017							
018							
019	10	1	2	3	1	0	0
020	6	0	1	1	1	0	0
021	3	0	1	0	1	0	0
022							
023	6	4	0	0	0	0	0
024	2	1	0	0	0	0	0
025							

Table F.16 (continued)

026	4	0	0	3	0	1	0
027							

Table F.17. Week 3 reality comparisons that were not symmetry related.

ID #	Reality Comparison
001	Star of David, 6 pointed star
003	Rock, the ball dropping on New Year's Eve
004	Snowflakes
006	A triangle with symmetric tumors, benzene rings
007	EMT symbol
008	Legos, candy from Willy Wonka (everlasting Gobstopper)
013	"A pyramid with the edge protruding from equal areas"
015	Frisbee
019	A space ship, star (drawing of star of David)
020	Ring
021	"It looks like some kind of lunar module that lands on the moon, with the bottom triangular shapes as the landing gear and the rest of the figure as the bulk of the module."

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.18. Week 3 evidence of analytical deconstruction.

ID #	Documented Response
001	"Si-Mo → Fe → S_5-S_4 → Fe → Si-Mo," "Each side of the figure alternates between S-S ligand and S-Mo ligand"
005	"Fe and Mo are bonded to themselves and S but multiple S atoms are bonded only to themselves"
008	"Fe on the innermost locations, S creates a fence between parts w/ Mo in it"
009	"Components A, B, C are surrounded on either side each by 2 of D, E, or F. The whole things is connected together in one continuous chain in a triangular-like chain," "A, B, C are connected through D, E, F. The symmetries involved allow the molecule to remain inherently the same through rotation, reflection, etc.," "There are three different C_2 elements with one center between the S_5 and S_5* of each section (A, B, C). There is also a σ_h element and 3 σ_v elements along the C_z [axes]."
010	"(Mo, Fe, S) structure connected to S structure through Iron (Mo, Fe, S) across from S (structure)," "C_3 rotation coming out of center; σ, σ', C_2→ cut in half vertically and rotate around"
012	"There are two main parts, the 8 atom structure A and the 4 atom structure B. The A and B structures alternate. B is on top, A is to the left and right of it. Bs are to the left and right of those and A is on the bottom. They alternate to form a ring containing 3 As and 3 Bs. B is made up of 4 sulfurs forming a rectangle that the viewer sees from the side. A is made up of 4 sulfurs, 2 irons and 2 Mo.", "The As and Bs alternate: B-top, bottom left, bottom right, A-top left, top right, bottom." "The As connect to each other by one iron molecule in each bottom corner. The Bs also connect to the As through these iron molecules to form triangles."

Table F.18 (continued)

013	"Made up of 3 triangular prisms linked by 3 groups of molecules," "S molecules are on the outer edges, linked to Mo molecules which are linked to the uppermost S molecules in the larger triangular prism structures and Fe molecules which link the larger triangular prism structures with each other"
015	"There is the main body with the linear attachments at every other spot"
016	There are 3 box-like structures separated by house shaped pentagons," "S_5's face outward away from the center of the molecule"
019	"Then there is a separate repeated group sort of like a prism with the two Mo atoms bisecting it." "Prisms are connected by iron groups to triangle boxes. Molecule can be approximated as planar hexagon with alternating prisms/triangle boxes at each vertex." "Due to alternating hexagonal location we can put an axis into, through the center and rotate 1/3 to get an identical molecular location. An axis from one group to the group opposite in location and character can be used to create 2 C_2 axes."
020	"2 sets of 3 identical shapes: one is made up of two triangular shapes connected to each other at the edges and the top points are connected to two other spheres to form a bridge."
026	"All Fe's are towards the inner cavity of molecule," "Fe serves as intersections between the different subunits or structures," (in strategy w/ coord axis): "C_3 through center out of page (z), σv up/down through yz axis, σ_h through yx axis, C_2 through y axis"

Table F.19. Week 3 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
001	"Each side of figure alternates between S-S ligand and S-Mo ligand."
005	"There is a reflection plane in the plane of the page and 3 reflection planes perpendicular to the page."
013	"Every atom forms a triangle with at least 2 other atoms which means every atom with the exception of the outer atoms have at least 3 bonds"
019	"Molecule can be approximated as planar hexagon with alternating prisms/triangle boxes at each vertex."
020	"They follow a 1, 2 pattern, bending to form a ring"
021	"Each of the boxes make a triangle from them. The triangular pieces form a triangle as well and connect the boxes."

Table F.20. Week 3 evidence of personalized strategies.

ID #	Documented Response
001	"Number of sides and note the pattern of ligands alternating between the 2 identified"
003	"Look at the individual shapes and then the overall shape and find common details/rotations/symmetries"
004	"look at molecule→ analyze its structure, possible planar structures, and focus on the groups and their location w/ respect to one another"
007	"Try to think of a similar object (simpler) and then look for symmetry"
008	"1-what's similar? → 3 box like things separated by 3 fence like things"
009	"To answer question one, I would first note the parts and any similarities between them. Then, I would find something in reality I could relate the visual to and use that to find symmetries."
010	"Try and rotate in mind, notice where shapes are the same (repeating elements)"

Table F.20 (continued)

012	"Look for repeating elements (parts A and B) and how they relate to each other"
013	"Look for operations to shift the molecule in turn first, then look for reflection areas"
015	"looking at the object practically and go through it piece by piece"
016	"I looked for molecules that were identical and then searched for ways to turn the molecule so that it looks the same"
026	"See what looks the same or similar and compare to the rest of molecule."

To answer the summary question, students had to describe or label where each symmetry element was. The D_{3h} point group has 12 operations, 10 distinct element locations, and 6 distinct elements. Out of 20 students, all but one attempted to answer the summary question.

Table F.21. Nature of students' drawings on the Week 3 activity.

Nature of Drawing	Student ID #
Symmetry Element Locations on Image	001, 003, 009, 010, 015, 019, 023, 024
Labeled the Image	012
Drew Coordinate Axis	001, 007, 024, 026
Drew Other Figures	004

In Table F.22, the number of unique elements, specific elements, and whether students used drawings or visual language is summarized. Some students supplemented their answers with a coordinate axis to indicate the location of a rotation axis or reflection plane. To allow the possibility that the axis was an analytical support rather than a visual support, the axis drawings are indicated in two cases that had no additional drawings.

Table F.22. Summary of symmetry elements and visualization artifacts used in Week 3.

ID #	# Unique Elements	Elements Named	Drawing	Visual Language
019	10	C_3, E, S_3, 3 C_2, 3 σ_v, σ_h	X	X
005	8	C_3, 3 C_2, σ_h, 3 σ_v		X
009	8	3 C_2, 3 σ_v, E, σ_h	X	
010	8	C_3, 3 C_2, 3 σ_v, Sh	X	
011	8	C_3, 3 C_2, σ_h, 3 σ_v		X
012	8	C_3, 3 C_2, σ_h, 3 σ_v	X	
015	7	C_3, σ_v, 3 C_2, σ_h, E	X	X
004	6	C_3, C_2, E, σ_v, σ_h, S_3	X	X
020	6	E, C_3, 3 σ_v, S_3		X
023	6	E, 2 σ_v, 3 C_2	X	
003	5	2 C_3, 3 C_2	X	X
007	5	C_3, C_2, σ_v, σ_h		X (with coord. axis)
016	5	E, 2 C_3, σ_v, σ_h		X
001	4	C_2, C_3, σ_v, E	X	X
026	4	C_3, C_2, σ_v, σ_h		X (with coord. axis)
006	3	C_3, σ_h, S_3		X
013	3	C_3, 2 σ_v		X

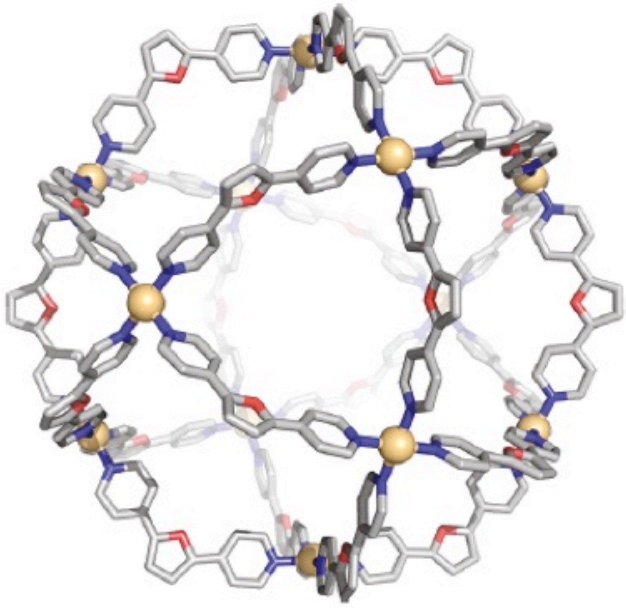
Table F.22 (continued)

021	2	C_3, E		X
024	2	σ_v, σ_h	X	X
008	Did not attempt			

Name: ________________________

Week 4: Self-Assembled $Pt(II)_{12}L_{24}$ Spheres

Read all the questions before you begin, but make sure you answer #1 last.
Below, two representations of the same self-assembled $Pt(II)_{12}L_{24}$ sphere are shown.[1] The second figure is a simplified representation of the first oriented in the same direction.



2

1. First, show (or describe the locations of) the symmetry operations you need in order to identify the point group. Then, tell me the point group of the structure.

2. a. What are the simplest parts of the image/problem/object? (**Atoms, bonds, edges, faces, shapes**)

b. How are the simplest parts related to each other? (**Surroundings, positions, locations**)

c. How do the parts interact/operate around each other? (**Movement, intersections, changes, what the sym operations do**)

d. What overall patterns or rules can you rely on the parts, operations, and relations to follow *each time* throughout the visual?

3. Name something that this visual looks like in reality. Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

Week 4 Activity Data

This week's image was two versions of a self-assembled sphere of 12 Pt(II) centers and 24 ligands. The left image was detailed enough that students could see what atoms made up the ligands while the right image was simplified. Students were instructed to show/describe the symmetry elements needed to find the point group. They didn't need to identify all the elements, but they needed to prioritize those they could identify and report which ones told them the structure belonged to the O_h point group.

Table F.23 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.23. Number of instances of observed deconstruction parameters demonstrated by students during the Week 4 complex visualization activity.

	Week 4: Self-Assembled $Pt(II)_{12}L24$ Sphere						
ID #	Summary Pts	Non-Attempts	Reality Comp	Decon-struction	Patterns	Personal Strategy	Sym Extension
001	15	0	1	1	0	1	0
002	2	0	1	0	0	0	0
003	0	0	4	1	1	1	0
004	41	1	1	1	1	0	0
005	4	0	1	0	0	1	0
006	8	0	0	1	1	0	0
007	5	0	1	1	1	0	0
008	2	3	0	0	0	0	0
009	4	0	1	2	2	1	0
010	6	0	1	1	1	0	0
011	7	0	1	2	0	1	0
012	11	0	1	0	1	2	0
013	3	0	1	1	0	1	0
014							
015							
016	4	0	1	0	0	1	0
017							
018	7	3	0	0	0	1	0
019	3	2	1	1	0	0	0
020	10	0	1	2	0	1	0
021							

Table F.23 (continued)

022	4	0	1	2	0	1	0
023	4	6	0	0	0	0	0
024	3	0	1	0	0	1	0
025	11	0	1	2	0	0	0
026	11	0	2	0	0	1	0
027	2	2	1	1	0	0	0

Table F.24. Week 4 reality comparisons that were not symmetry related.

ID #	Reality Comparison
001	"Expandable/retractable toy ball made of legos or kinex parts"
002	Stress ball
003	Jungle gym, flower, expandable ball, soccer ball
004	Soccer ball
005	Soccer ball
007	Soccer ball
009	Cube
010	Soccer ball
011	Old school rendering of a sphere in old video games
012	Sphere
013	Ball that's not completely round
016	Crystal-like structure/lattice
019	"Soccer ball with hexagon/octagon shapes instead of normal"
020	"One of those balls that fold in and expand"
022	Ball
024	A child's toy
025	A [die] with 12 sides
026	Soccer ball, buckyball
027	Jimmy Neutron Logo

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.25. Week 4 evidence of analytical deconstruction.

ID #	Documented Response
001	"Sides/faces-2 types, one with 3 edges and another with 4 edges"
003	"4 pentagon chains connected to sphere, 3 pentagons form a chain, spheres & chains form 6 pentagonal & triangular faces"
004	"the simplest parts (geometric figures) create a surface of triangles/squares that form an easy viewed surface"
006	"A symmetric molecule will have at least one plane of symmetry. Because the molecule has equivalent sides and no center, it will be equivalent when rotated. Because a line can be drawn from any side to any opposite side through the center, it has symmetry."
007	"Center atoms (Pt) in square planar conformation with molecular chains in between"

Table F.25 (continued)

009	"Circular atoms are corners that connect chains of rings. Each triangle-like section is surrounded by a square-like section at each side and triangle at each corner." "You can rotate on the corners and center of each plane and molecule will be unchanged. Circular atoms from intersections between chains of rings."
010	"Can spin 3 times going through center (and keep same) and 2 times, can spin 4 times when through center of octagonal things, reflections horizontal, vertical, dihedral"
011	"The three facing you form a triangle, and directly on the other side are the triangle 180° out of phase," "The triangles on each side are out of phase by 180°. So, they move together symmetrically by C_3 but also allow the possibility of S_6."
013	"There are the main hexagonal rings. The outer 2 rings are small and are only bonded by three atoms on each ring, while the innermost middle ring is bonded by 6 atoms on the edges of the hexagonal structure. The outer 2 rings are in staggered formation for the atoms."
019	"Each edge is an edge to the opposite shape, ie. 6 sided edges→ 3 main edges, each one making up one side of 8 sided shape"
020	"4 hexagonal rings connected together vertically and horizontally to form a 3-D structure, rings evenly spaced and connected together by the spheres," "The 4 rings are attached to the spheres that connect them to another ring directly between their edges"
022	"4 hexagonal shapes that cross w/ each other," "mirror plane through horizontal, [perpendicular] to C_6 axis and vertical C_6 rotation axis, every 16^{th} turn looks the same, [perpendicular] C_2's every 180° turn looks the same"
025	"It has 12 atoms, with each atom being bonded to its adjacent atoms by a chain of 3 cyclohexanes attached to one another. Between the atoms are edges from the middle cyclic hexane bridging outward. It also has 12 faces." "This 12 faced 'ball' is equally spaced atoms, no atoms in center of the ball."
027	"All atoms connected by ring system to make 3-D object with 14 faces (8 triangles, 6 squares)"

Table F.26. Week 4 evidence of valid patterns/rules documented in appropriate language.

003	"4 chains per sphere, 12 faces→ 2 different types of faces"
004	"All symmetry elements based on one principle axis are true for all principle axis in this molecule→ so it is 6x elements of principle axis to find symmetry operations→ then you have C_3 axis through emptiness"
006	"Each face is directly across the molecule from an identical face-mirror plane. Each atom is symmetrically positioned relative to the other atoms (evenly spaced)-center of inversion creates multiple planes of symmetry and rotation axes"
007	"Pt-chain-Pt-chain… 3-sided faces surrounded by 5-sided faces"
009	"Each triangle-like section is surrounded by a square-like section at each side and triangle at each corner." "You can always know that each of the 6 square faces are identical. You can rotate on each corner and the center of each plane."
010	"Can spin 3 times going through center (and keep same) and 2 times, can spin 4 times when through center of octagonal things, reflections horizontal, vertical, dihedral"
012	"When looking down on a single Pt, you can rotate 60° and have the equivalent molecule C_6, the axis of rotation is through 2 Pt"

Table F.27. Week 4 evidence of personalized strategies.

001	"1) Designate a set of axes, 2) Identify possible rotations [through] the center of each face, 3) Identify the highest order (C_n) and the number of C_n present, 4) Figure out if the structure can be inverted [through] its center."
003	"# the same faces, # the spheres, rotate molecule where there is sphere on bottom/top"
005	"First find principle axis, then any C_2 operations [perpendicular] to principle axis, then find reflection planes."
009	"I would relate the molecule to the representation of a cube and use that to help me find the elements of symmetry."
011	"Look for high symmetry and see if anything destroys it, and I see a triangle and a hexagon C_6 and C_3 are similar."
012	"Look for repeating elements and how they relate."
013	"Look at the main rotation axis then see if there are any other operations with a lower n."
016	"Look for parts that are similar in shape, find out how many are present and how you can move the [molecule] to do them"
018	"Look for the same molecule/pattern to decide what operations to use to get the same image"
020	"I began by looking at the smaller parts and then how they are related to each other"
022	"Go through the flow chart by finding the primary rotation axis and then checking for [perpendicular] C_2 axes, then investigate for mirror planes"
024	"Look for repeating patterns"
026	"σ through one of the atoms and the atom directly opposite of it→ 6 mirror planes, 4 C_3 [axes] through face of plane, C_4 through atoms directly across from each other, σ_h through central layer"

Five students described the point group patterns clearly with minimal mistakes in the summary question. Additional interpretation is added in italics. Seven students used inconsistent descriptions, were wrong, or left a lot blank.

Table F.28. Point group descriptions for the Week 4 activity containing minor mistakes.

ID #	Documented Response
001	"E-identity, i-inversion thru center, 6 C_4-axis is thru each side with 4 spherical atoms (3 on top and 3 underneath, 7 C_3-axis runs thru each side with 3 spherical atoms (6 on the sides and one that runs thru the top and bottom of sphere): Point group: O_h" "Sides/faces-2 types, one with 3 edges and another with 4 edges"
004	"Oh. These locations are the intersections of the main linkage centers (spheres)→draw a line between the opposite to get a principle axis. [All symmetry elements based on one principle axis are true for all principle axis in this molecule→so it is 6x planes if principle axis to find symmetry opposite→then you know C3 axis through emptiness."] ***Bracketed text graded as pattern.*
009	"4 C_2 axes at corners, 3 C_2 at center of each plane, σ_v plane. C_{2v}" ***She drew a cube into the structure and described the correct symmetry operations, but came to an incorrect conclusion.*
012	"4 C_3 through triangle space, 3 C_4 through square space, O_h. C_3, C_2, σ_v, σ_h, C_4, i"

Table F.28 (continued)

019	"Highest axis is $C_3 \rightarrow C_2$? Yes [therefore] D group; σ_h? No; σ_v? Yes [therefore] D_{3d}; But multiple C_3 axis, inversion? Yes; No C_5; Oh?" ***Referred to 8-/6-sided rings, but stated correct Pt vertices. Interpreted the bent ligands as two sides each.*
027	"C_3 rotation axis through each triangular face, C_2 rotation axis through each square face" ***Drew triangles and squares on the appropriate faces of the diagram. Also saw external rings.*

Table F.29. Inconsistent or incorrect point group descriptions for the Week 4 activity.

ID #	Documented Response
002	"T_d" (*in summary question),* "Pt bonds to 4 hexagons, whereas hexagons may be bonded to other hexagons."
007	"E, C_{3xy}, C_{2xy}, C_{2xz}, C_{2yz}: D_3 point group"
008	"6 σ, C_6, σ', C_2: C_{6h}" ***No drawings*
016	"T," "each sphere & 4 bonds are symmetric & connect to one another," "Can assume each sphere is symmetrical and the bond, from the sphere are symmetrical/same length/same bonds. Each tetrahedral shape is symmetrical and connects to the next."
023	"Inversion center, C_2, $2\sigma_v$; C_{2v}"
024	"I have marked the planes of symmetry. It can be rotated about the primary axis to give 3: O_h" ***No other mention of rotation axes or indications of element locations. Unsure how he got the answer.*
025	"4 C_3 principle [axes], 6 C_2, σ_h: D_{3h}" ***Referred to the ligands as chains of cyclohexanes*

Eight students described alternate interpretations of the image that sometimes led to incorrect point group determination. This misleading visualization could be identified and corrected.

Table F.30. Documented evidence of students' misleading visual interpretation of the image.

Interpretation	ID #	Documented Evidence
Identified large outer rings instead of faces	011	"I see 12 faces/sides. All of it is inside a hexagon. " ***Reported correct answer.*
	013	"There are three main hexagonal rings. The outer 2 rings are small and are only bonded by three atoms on each ring, while the innermost middle ring is bonded by 6 atoms on the edges of the hexagonal structure. The outer 2 rings are in staggered formation for the atoms." ***Reported a T_d point group b/c he saw C_3, C_2 and I elements.*
	020	"12 spheres, 4 hexagonal rings," "4 hexagonal rings connected together vertically and horizontally to form a 3-D structure. Rings evenly spaced and connected together by the spheres." ***Reported D_{6h}*
	022	"12 Pt atoms, 24 L atoms, 3 per bond, 4 hexagonal shapes that corss w/ each other." ***Reported D_{6h}*
Identified all faces as identical	006	"The atoms are located in the center of each face, each face is identical, each face is attached to 4 other faces."
	026	"Pattern of each face repeated (same face on every side)" ***Reported D_{3h} but had written 'octahedral symmetry'*

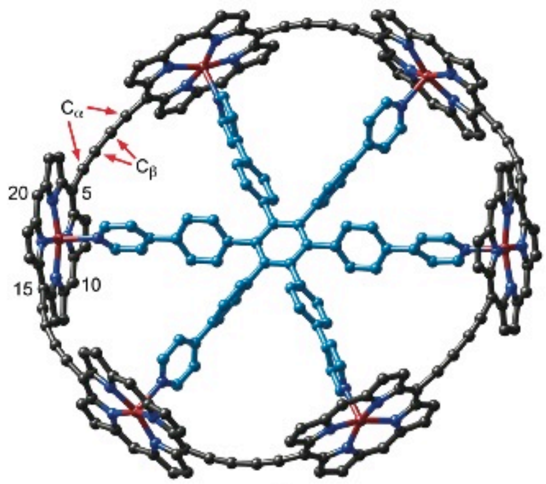
Table F.30 (continued)

Reported incorrectly numbered faces	003	"4 pentagon chains connected to sphere, 3 pentagons form a chain, spheres & chains for 6 pentagonal & triangular faces."
	010	*7 hexagons, 7 octagons listed in elements*

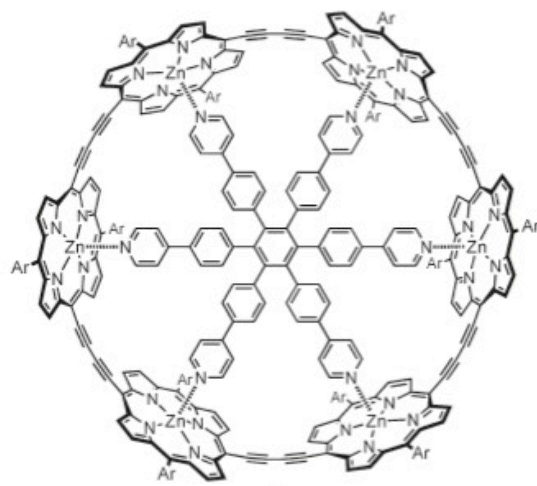
Name: ________________________

Week 5: Templated Cyclic Porphyrin Hexamer

Read all the questions before you begin, but make sure you answer #1 last.
Below, two representations of the **same** cyclic porphyrin hexamer that was templated with a hexadentate ligand.[1] Figure **A** represents the actual conformation and buckling of the porphyrin belt while figure **B** displays basic geometries and multiple bonds.



A



B

1. a. Give the point group of each figure as it is shown.
   b. These represent the same structure. What symmetry elements (if any) does the simplified structure (**B**)
   have that are not present in the actual structure (**A**)?

2. a. What are the simplest parts of the images/problems/objects? (**Atoms, bonds, edges, faces, shapes**)

b. What are the differences between how the simplest parts are related to each other? (**Surroundings, positions, locations**)

c. What are the differences between the way the parts interact/operate around each other in each image? (**Movement, intersections, changes, what the sym operations do**)

d. How do the overall patterns or rules differ between the two images? *Remember—you can rely on the parts, operations, and relations to follow a **pattern/rule** each time they appear throughout the image.*

3. Name something that this visual looks like in reality. Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

Week 5 Activity Data:

The image in this activity introduced visual comparison into the intervention. Students were provided with two images of the same structure: a 2-D structure and a ball-and-stick structure with true bond angles represented. Symmetry is removed when the lowest-energy bond angles are considered in the ball-and-stick structure. Students were instructed to give the point group of each structure and state the elements differed between the two. The point group of the structure on the left was D_{3d} and the structure on the right was D_{6h}. Many students documented that they differentiated between the C_3 and C_6 rotation axes in the images.

Table F.31 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.31. Number of instances of observed deconstruction parameters demonstrated by students during the Week 5 complex visualization activity.

	Week 5: Templated Cyclic Porphyrin Hexamer						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	10	3	2	0	0	1	0
002							
003	5	2	4	1	0	0	0
004	2	0	1	2	1	1	0
005	3	1	1	1	0	0	0
006	7	0	3	0	1	0	0
007	7	2	0	1	0	0	0
008	0	3	1	0	0	0	0
009	7	0	1	2	1	0	0
010	4	0	2	2	0	0	0
011	4	3	1	0	0	1	0
012	3	0	1	2	0	0	0
013	3	0	1	2	0	1	0
014							
015	2	0	1	2	1	0	0
016	2	0	1	1	0	1	0
017	3	0	1	2	1	1	0
018							
019							

020	5	0	1	1	1	1	0
021	4	0	1	1	0	0	0
022	9	1	1	0	0	0	0
023	5	5	0	0	0	0	0
024	2	0	1	1	0	0	0
025	4	0	1	1	0	0	0
026	2	0	1	2	1	0	0
027	3	2	1	2	0	0	0

Table F.32. Week 5 reality comparisons that were not symmetry related.

ID #	Reality Comparison
001	Spokes on a bicycle, hubcaps on a wheel
003	Snowflake, ferris wheel, bear trap, merry-go-round
004	Wagon wheel
005	Snowflake
006	Bike wheel, snowflake, frisbee
008	Orange cut in half
009	Wheel
010	Wheel, snowflake
011	Bicycle wheel w/ 6 spokes
012	Wheel and spokes
013	Ferris wheel
015	Frisbee
016	A car rim
017	Donut ring
020	Ferris wheel
021	Bicycle wheel
022	Bracelet with a center
024	Ferris wheel
025	Buckyball
026	Wheel with spokes
027	6-spoked wheel

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.33. Week 5 evidence of analytical deconstruction.

ID #	Documented Response
003	"A forms 3 unique [axes] with the rings, B forms 6 [axes] C_6"
004	"The different components connect together like the spokes of a wheel," "The spokes undergo a 90° shift from one spoke to the other→ the parts work together as a rotating circle"
005	"The long C chains 'inside' the molecule consist of benzene rings that are rotated at different angles"

Table F.33 (continued)

007	"alkyne linkages of porphyrin rings to each other, 5 benzene chains link porphyrin rings to opposite porphyrin ring"
009	"central cyclohexane attached to other cyclohexane at each corner which are then attached to another cyclohexane at the opposite corner, those are then attached to bigger sections labeled as D that are all connected," "In A, the cyclohexanes are all tilted at different angles. This will affect the symmetry operations of that diagram."
010	"Spreads out from center benzene, outer ring is (Zn complexes) connected with c_α and c_β's," "C_6 in B, not so much in A, lots of C_2's [perpendicular] in B, reflective planes in B, not so much A"
012	"A benzene ring in the center with 6 benzene/pyridine connected (coming out of the center one), there are 6 porphyrin rings in a circle around the outside edges, the porphyrin rings are connected by 4 carbons with alternating single/triple bonds," "B has C_6 and a mirror plane in the plane of the paper and a vertical mirror plane, A does not because the benzene-pyridines are not in the same plane"
013	"The outer 8-rings structures are organized in a circle, the inner hexane rings are tilted to each other," "Less symmetry operations due to the tilting on the inner six-membered rings in the actual confirmation"
015	"One is in 3-D and the other is Lewis structure, the 3 lines can be split into 6—all connected by a central cyclic structure," "a) the three central lines rotate as you change lines, all things are connected, b) all things are in the same plane, looks like a dish"
016	"The 6 branched groups from the center benzene ring are all connected by carbons via the Zn structures."
017	"Benzene rings connect to center ring. Then each chain of benzene rings connects to a ligand. Figure A has tilted rings, so B is much easier to think about." "Figure A has restricted symmetry operations because it has tilted rings. Figure B is easier to rotate since it's planar."
020	"The aromatic rings are connected to one in the center, connected to another, then to the Zn by a N on the ring, the porphyrin rings are connected around the edges by 2 alkyls"
021	"Each side is tilted in a different direction from the previous one"
025	"In A, we notice that there are 3 C_2's, corresponding benzenes buckle in the same direction as the ones in the same axes."
026	"From center there are six chains to outer ring, at end of chain is Zn structure, opposing chains are on axis with each other (same angles)," "A is less planar→ benzene rings twist, B: each 1/6 of the circle is the same, A: parts of circle have different angles"
027	"In B, all the benzenes look flat, but in A, the benzenes are at angles to one another," "In A, you don't see that the porphyrin rings are connected with conjugated triple bonding chains"

Table F.34. Week 5 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
004	"The real image is more complex than the simple→ the simple has much more symmetry based around the plane of the molecule σ_h, the real one does not have symmetry based around principle axis→ therefore $\sigma_{v/d}$"
006	"The flat image has a C_6 rotation axis because it does not show orientation of rings in bend, the 3-D has C_3 rotation axis because bonds are different, flat image has 6 planes of σ_v, 3-D has 3 planes of σ_v"
009	"A→ tilts in cyclohexanes, no C_6 symmetry, B→ C_6 rotational axis, [perpendicular] C_2 axis"
015	"The patterns are pretty similar. There is a C_6 axis down middle on both, there is an I, 3 C_2 axis, E, the A image has more complications seeing this, for A there is no C_2 since the atoms have particular orientations"
017	"Figure A has an alternating pattern of the angle of the arms. Figure B is uniform throughout."
020	"B is flat in the center, A has alternating benzene rings that are not flat"
021	"Each side is tilted in a different direction from the previous one"
024	"B is a flat image giving it an extra symmetry operation when considering the plane of the paper."
026	"A is less planar→ benzene rings twist, B: each 1/6 of the circle is the same, A: parts of circle have different angles"

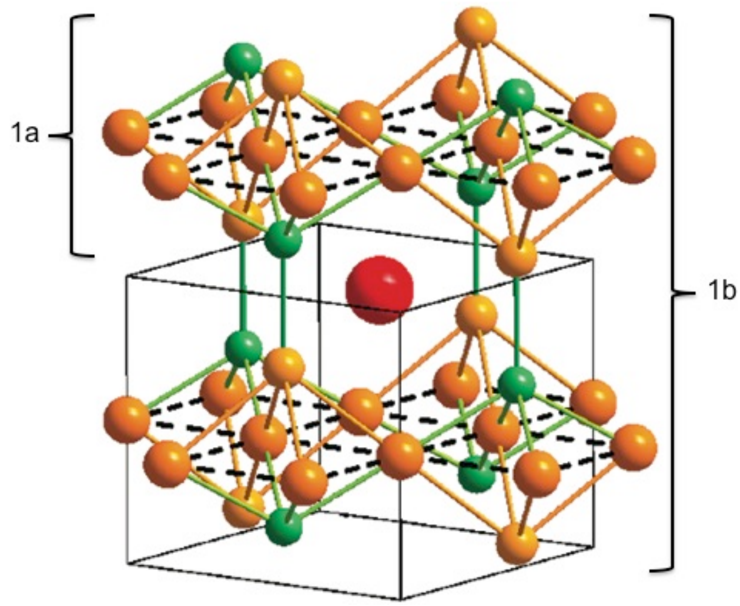
Table F.35. Week 5 evidence of personalized strategies.

ID #	Documented Response
001	"1) Identify set of axes, 2) Identify highest order via maximum C_n (rotations), 3) Identify [perpendicular] C_2 to C_n, 4) Search for σ planes, 5) inverse?"
004	"I would imagine the wheel rotating around the central axis"
011	"Start at center (high symmetry), look for parts which reduce it, such as 'a' starts a C_6 then gets reduced to C_3"
013	"Get the symmetry operations and find point group for structure B, the representation, first. Afterwards, see whether the operations can apply to the actual structure."
016	"Look for similar/symmetrical shapes, look for rotation and mirror planes"
017	"Use the center ring to put my primary rotation axis. Use ligands as the outer points for the axis. Watch how the angle of the benzene rings change as the structure is rotated."
020	"Began by looking at the smaller parts then how they relate to one another"

Name: ________________________

Week 6: $SrAu_3Ge$ Nets

Read all the questions before you begin, but make sure you answer #1 last.
Below is an image that describes the structure resulting from fusing Sr, Au, and Ge at very high temperatures.[1] The gold spheres represent Au, the green represent Ge, and the red sphere represents Sr.



1. a. What is the point group of the top-most net in the figure?
   b. How, if at all, does the point group change when you consider both nets and the strontium atom? Answer by describing/showing symmetry elements that are gained or lost.

2. a. What are the simplest parts of the image/object? (**Atoms, bonds, edges, faces, shapes**)

b. How do the atoms relate to one another in one net and how do the two nets relate to one another? (**Surroundings, positions, locations**)

c. What operations would you enact on each net to identify any symmetrical, *indistinguishable* positions? (**Movement, changes, what do the symmetry operations do**)

d. What patterns or rules do you see in each net? *Remember—you can rely on the parts, operations, and relations to follow a* ***pattern/rule*** *each time they appear throughout the image.*

3. Name something that this visual looks like in reality. Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Lin, Q.; Corbett, J. D. *J. Am. Chem. Soc.*, **2012**, *34*, 10, 4877–4884.

Week 6 Activity Data:

This week's activity changed the focus of the comparison from two separate structures to the comparison of an internal portion of a structure to the whole structure. Students were instructed to find the point group of half of the image as presented and adjust their analysis to include the whole structure as presented. Students had to justify a different point group or retaining the same point group. As it appears in this image, the point group of both the half and the whole structures is D_{2d}.

Table F.36 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.36. Number of instances of observed deconstruction parameters demonstrated by students during the Week 6 complex visualization activity.

	Week 6: $SrAu_3Ge$ Nets						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	0	4	0	0	1	0	0
002							
003	1	0	3	2	0	1	0
004							
005							
006	1	0	2	1	0	1	0
007	0	5	0	0	0	0	0
008							
009							
010							
011	2	1	0	1	1	1	0
012	1	1	2	0	0	0	0
013	1	1	0	1	1	1	0
014							
015							
016	0	1	0	1	1	1	0
017	2	0	1	1	1	1	0
018	0	2	1	0	0	1	0
019							
020							
021	0	0	1	0	1	1	0

Table F.36 (continued)

022	1	0	0	1	1	0	0
023	0	1	1	1	1	0	0
024							
025							
026							
027	1	0	1	2	0	0	0

Table F.37. Week 6 reality comparisons that were not symmetry related.

ID #	Documented Comparison
003	Beehive in the middle, egg with red dot embryo, "quadrapod (like a tripod but 4)"
006	Square, cube
012	Box, grid
017	Diamonds
018	Cube
021	"It looks like the structure could be something from a playground"
023	Spinning tops
027	"Sullivan pyramids"

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.38. Week 6 evidence of analytical deconstruction.

ID #	Documented Response
003	"One: opposite orientation of colors, forms a cross pattern, Two: green is opposite at connection, surround red sphere, square," "diamond staggered/no eclipse"
006	"They are identical, they have 2 C_2 [axes], both have 4 green molecules, bonded together by identical bonds"
011	"Since squarish shape can have C_2 and a σ_v. Because opposite corners are the same and adjacent are different so no C_4."
013	"Atoms are arranged in a cube like formation with an atom at the face. The Au atoms are the most numerous and the Ge atoms alternate up and down along the structure. The Sr atom is in the middle of the structure."
016	"The atoms are connected by single bonds. The 2 nets are connected by longer single bonds. The center sphere is surrounded by the smaller spheres which form a net above and below it."
017	"2 Au atoms connect the two sides of the net. The Ge atoms are staggered. The two nets are the same. They're connected by Ge and Au atoms."
022	"No mirror planes on top net. But there is a C_2 axis w/ [perpendicular] C_2's. C_2 as a whole w/ [perpendicular] C_2's again, only dihedral mirror planes."
023	"C_2 about x on each net yields symmetrical positions" *(coordinate axis drawn)*
027	"Atoms are arranged into 4 diamond like structures, 2 nets are the same, connected at top vertices of diamonds," "squares of diamond [drawing] are gold atoms, tops are either gold or Ge (tips in one diamond are opposite, and opposite diamond are opposite"

Table F.39. Week 6 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
001	"Ge atoms alternate→top atom in one bipyramidal and bottom atom in the other bipyramidal for one section"
011	"[The] tops and bottoms of the square prisms alternate between Au and Ge, each has one corner in the center so the center is surrounded by a square"
013	"The green atoms alternate up and down positions in the net"
016	"For every green-orange-green sphere line, there's one next to it and one above or below it"
017	"Each diamond on the net has two Ge atoms. Both diamonds have a different position of the Ge atoms."
021	"The image on one side of a net is displayed as a mirror image on the other side."
022	"Ge bonded to Au in each net and then bonded to the other net in the same way. For every one Ge, there are 4 bonds to Au's."
023	"Each net has 4 Ge atoms and 16 Au atoms. Each Ge is bonded to 4 Au atoms."

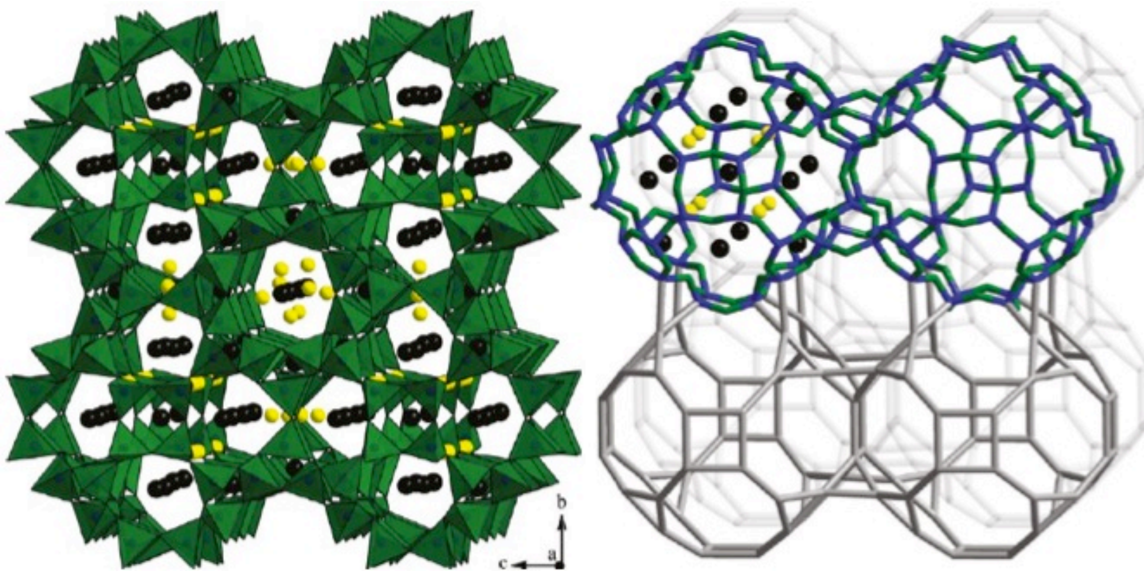
Table F.40. Week 6 evidence of personalized strategies.

ID #	Documented Response
003	"Cut it in half, maybe into 4ths"
006	"Rotate it along every possible axis, find symmetry operations, compare top and bottom, use flowchart to determine point group"
011	"Start from center, work my way out."
013	"Find the symmetry operations, then assign the point group. The operations mostly deal with the green Ge atom."
016	"Look for similar parts and figure out where rotations can occur, followed by reflections, followed by inversions if applicable"
017	"Set the C_2 operation axis down the structure. Then check for 2 more perpendicular C_2 [axes]. If they work, then I would look for a horizontal plane to reflect. These C_2 [axes] have to go through the center Sr atom though."
018	"Look for the same molecule/pattern to decide what operation to use to get the same image."
021	"First, identify the atoms or molecules and how they are related to one another. Then determine what operations were necessary to make them appear that way."

Name: ________________________

Week 7: Microporous Oxonitridophosphate

The oxonitridophosphate structure below {$Ba_{19}P_{36}O_{6+x}N_{66-x}Cl_{8+x}$ ($x \approx 4.54$)} resembles aluminosilicate zeolites.[1] The Ba^{2+} (black) and Cl^{-} (yellow) ions are caged within the oxonitridophospate cages (green tetrahedra). The crystal structure (left) and the progressively simplified collection of cage structures (right) represent the SAME STRUCTURE.



1. a. What is the point group of a single cage?
   b. What is the point group of all cages combined?
   c. List/describe the symmetry elements gained or lost when moving from a single cage to all cages combined. If there's no change, list the elements that you need in order to identify the point group.

2. a. What are the simplest parts of the image? (**Atoms, bonds, edges, faces, shapes**)

b. How do the parts relate to one another in one cage and how do the collection of cages relate to one another? (**Surroundings, positions, locations**)

c. How would you move the individual cage/collection of cages to find any *indistinguishable* positions? (**Movement, changes, what can you do to transform cages into each other**)

d. What patterns do you see in the individual cage/collection of cages? *Remember—you can rely on the parts, operations, and relations to follow a **pattern/rule** each time they appear throughout the image.*

3. Name something that this visual looks like in reality. Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Sedlmaier, S. J.; Döblinger, M.; Oeckler, O.; Weber, J.; auf der Günne, J. S.; Schnick, W. *J. Am. Chem. Soc.*, **2011**, *133*, 31, 12069–12078. Copyright 2011 American Chemical Society.

Week 7 Activity Data:

The image for this activity required students to, like Week 6, compare a portion of the structure to the whole. This structure was much more complicated than the previous week and students compared a single ‘cage’ to the collection of eight, though many only analyzed the front four cages. The point group of a discrete cage is O_h (due to the presence of C_4 and C_3 rotation axes and reflection planes). The collection of 8 cages, as represented in the image, would also belong to the O_h point group. If students interpreted the back four cages as shadows, the collection of four cages belongs to the D_{4h} point group.

Table F.41 displays the assigned points under several parameters for each of the students attending that week’s recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.41. Number of instances of observed deconstruction parameters demonstrated by students during the Week 7 complex visualization activity.

	Week 7: Microporous Oxonitridophosphate						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	0	4	0	1	0	0	0
002	3	0	1	1	0	0	0
003	4	0	3	1	1	1	0
004							
005							
006	0	0	2	0	0	1	0
007	2	1	1	0	0	0	0
008							
009	1	1	0	2	1	1	0
010	1	0	0	2	0	0	0
011	2	3	0	1	1	0	0
012	3	0	1	1	2	1	0
013	2	0	2	0	0	1	0
014							
015	1	0	1	2	1	1	0
016	2	0	1	1	0	1	0
017	3	0	0	1	1	1	0
018							
019							
020							

Table F.41 (continued)

021	3	0	1	1	1	0	0
022							
023	0	2	1	0	0	0	0
024	0	2	0	0	0	0	0
025	3	0	1	0	0	1	0
026	1	2	0	1	0	0	0
027							

Table F.42. Week 7 reality comparisons that were not symmetry related.

ID #	Reality Comparison
002	Rubik's cube
003	Saw blade, jungle gym, round/square cactus
006	Rows of apartment buildings, building blocks
007	"Design on a stained glass window (non 3D)"
012	4 blocks
013	"Microscope structures of polymer spherulites, clover (entire structure)"
015	Flotation device
016	Snowflake
021	"This looks like two dumbbells connected to each other"
023	Green hobgoblin
025	4 soccer balls

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.43. Week 7 evidence of analytical deconstruction.

ID #	Documented Response
001	"1) Each single cage makes up one of the 4 corners of the structure, 2) 8 yellow Cl^- ions visually make up a cube in the center of each cage, 3) The other cage is centered between the 4 corner cages, 4) Between each cage there is a cluster of 4 Cl^- ions."
002	"Rotate by 90° or 36° with respect to x, y, or z [axes]"
003	"Dark green spheres/balls are in straight lines through all openings, yellow spheres connect triangles together and connect to form an octagon in the middle of cages"
009	"They are all the same basic cage, C_4 rotations on x, y, and z axis, C_3 rotation through middle of each triangle, reflection planes," "Individual cage patterns in c. Collection of cages has C_2 on x & z axes and C_4 on y axis. Plus reflection planes through z & y axes."
010	"4 cages around center cagey thing, ions inside sections of cage, separated alt. Cl^- and Ba^{2+}," *in answering how to move the individual/collection of cages:* "turn 90° through center into page, flip 180° diagonal, horizontal, vertical, reflection in plane of page and vertical and horizontal"
011	"There are four cages, they are all the same, they are bound in a square plane each with two adjacent sides bound to another, (If you look through a triangle, the one opposite it through the center, the opposite triangle is out of phase by 180°)"

Table F.43 (continued)

012	"There are four cages, 2 on the top and 2 on bottom, they each touch 2 other cages, 1 cage: 6 identical faces, but a 'face' is not flat"
015	"They all interact holding the structure of the cage together. With the collection of cages, they all mesh together supporting one another. One shape surrounded by 4 cages and the same with each individual cage." "Move on top of one another, they are all identical in shape so if placed in a row, you will not be able to distinguish."
016	"Each cage looks the same. There are 4 cages connected with center gap in the middle. Shapes within cages include square, octagon, triangles."
017	"The square faces are connected by the octagonal faces in the corner cages. These cages have two different types of atoms. Each corner cage is connected to each other by the center cage."
021	"The black and yellow atoms form a shape in the middle of one sphere. The black atoms form the middle and exterior while the yellow atoms for in between."
026	"Bottom two are the same, top two are the same, both seem to have same general structure but the bonds are bent on top"

Table F.44. Week 7 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
003	"Each contain same # of spheres of both colors, each has a square through the middle"
009	"Individual cage patterns in c. Collection of cages has C_2 on x & z axes and C_4 on y axis. Plus reflection planes through z & y axes."
011	"If you look through a triangle, the one opposite it through the center, the opposite triangle is out of phase by 180°"
012	"They each touch 2 other cages, 1 cage: 6 identical faces, but a 'face' is not flat," "The sides of the cages are identical, the way the cages connect is the same for all 'joints'"
015	"The same shapes and order for shapes are all around the cage. Small cage with 4 cages around it. With the collection, it has a lot of the same patterns: has one shape with 4 identical shapes surrounding it."
017	"All 4 cages are the same. All the atoms in them are in the same position. A C_4 operation through the center of structure should be able to repeat the pattern."
021	"I see six squares and 12 octagons making up each cage. Connecting each cage is a rectangular-shape prism."

Table F.45. Week 7 evidence of personalized strategies.

ID #	Documented Response
003	"Flatten it out, cut in half, split into 4ths, work from the middle out"
006	"Identify symmetry operations, choose a central axis, choose # of cages to use, use flow chart to determine point group"
009	"Use the point groups of the parts to help me characterize the whole."
012	"Look for symmetry elements of one cage, then consider symmetry of the entire structure"
013	"Find the symmetry elements as it relates to the atoms first, then the individual cages, then the whole structure"
015	"I looked at the shape, found the highest order rotational axis, then looked for other symmetry elements as well"

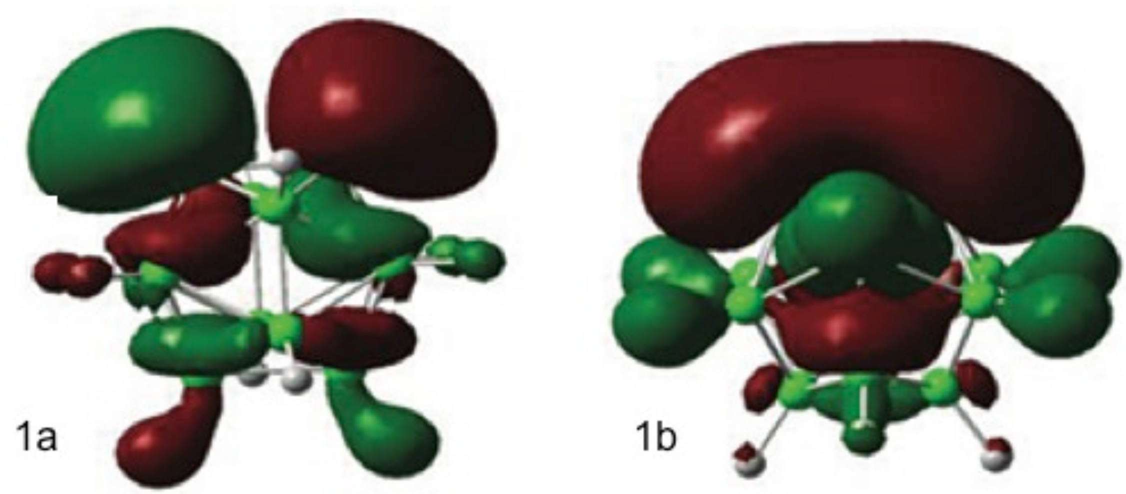
Table F.45 (continued)

016	"Looked for symmetrical shapes in each cage, tried different rotations and concentrated on where the yellow and black atoms went and if their angles changed"
017	"Put my principal axis through the cube face. Check for # C_2 [perpendicular] axis, then check for σ_h and σ_v. I would look for the point group of a square planar molecule. This simplifies the process."
025	"Find symmetry of 1 of the cages"

Name: ________________________

Week 8: $B_{12}H_{10}^{2-}$ Frontier Orbitals

The frontier orbitals that result from removing two hydrogens from $B_{12}H_{12}^{2-}$ were calculated to understand the reactivity of the compound.[1] $B_{12}H_{12}^{2-}$ is icosahedral (I_h point group), but when hydrogens are removed from adjacent boron atoms, the molecule is reduced down to C_{2v} symmetry. Below, the HOMO (1a) and LUMO (1b) are shown.



1) Identify the symmetries of the two frontier orbitals. Justify your answer and *write the reducible representation* for each.
   a. Give the reducible representation and the symmetry for the MO on the left.

   b. Give the reducible representation and the symmetry for the MO on the right.

2) a. What are the simplest parts of the image? (**Atoms, bonds, edges, faces, shapes**)

b. Choose one of the images. How are the simplest parts in that image related to one another? (**Surroundings, positions, locations**)

c. Using the same image, how would you move the parts to find indistinguishable positions? (**do not just list symmetry operations—describe what the symmetry operations do**)

d. Describe the patterns you see in the orbitals of the images.

3) Name something that this visual looks like in reality. Does it resemble or remind you of anything you've seen before?

4) What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Pancharatna, P. D.; Balakrishnarajan, M. M.; Jemmis, E. D.; Hoffmann, R. *J. Am. Chem. Soc.*, **2012**, *134*, 13, 5916–5920. Copyright 2012 American Chemical Society.

Week 8 Activity Data:

The images for this week were the LUMO and HOMO of $B_{12}H_{10}^{2-}$ superimposed onto the ball-and-stick structure. Students were told that the point group was C_{2v} and were instructed to identify the symmetries of the two orbitals and support their answer with reducible representations for each. Students were given the C_{2v} character table next to the images on the projector for the duration of the activity. The correct answers for these were B1 with a reducible rep of 1, -1, 1, -1 for 1a and A1 with a reducible rep of 1, 1, 1, 1 for 1b. Mentally enacting the operations onto the structures would help students see if the operations yielded symmetrical or anti-symmetrical results.

Table F.46 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, a reducible or irreducible representation was not considered analytical deconstruction unless accompanied by description.

Table F.46. Number of instances of observed deconstruction parameters demonstrated by students during the Week 8 complex visualization activity.

	Week 8: $B_{12}H_{10}$ Frontier Orbitals						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001	0	6	0	0	0	0	0
002							
003	0	4	6	0	0	0	0
004	1	0	1	2	0	1	1
005	0	1	1	0	1	0	0
006							
007	0	1	1	1	0	1	1
008							
009							
010							
011	10	2	2	2	0	1	0
012	10	0	1	1	1	1	1
013	0	0	1	1	0	1	1
014							
015	1	0	2	0	0	1	1
016	0	2	1	1	0	0	1
017	0	6	0	0	0	0	0
018	8	4	0	1	0	0	1
019	0	0	1	0	1	1	0
020							

Table F.46 (continued)

021	1	0	1	1	0	1	1
022							
023	0	4	2	0	1	0	1
024	0	0					
025	0	2	1	0	0	0	0
026	0	2	1	1	0	0	1
027	0	5	0	0	0	0	0

Table F.47. Week 8 reality comparisons that were not symmetry related.

ID #	Reality Comparison
003	Gnome, boxing gloves, turtle, sleds/skis, fly, goggles on a face
004	Turtle
005	Turtle
007	Jelly beans
011	Turtle, clover
012	Kidney bean
013	Hot air balloon
015	Hot dogs, dog chew toy
016	Alien
019	Robot
021	Turtle
023	Turtle, alien
025	Miniature robot

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.48. Week 8 evidence of analytical deconstruction.

ID #	Documented Response
004	"The 1B image has a symmetrical by rotating but no horizontal symmetry element. The large green nodes surrounding the molecule have sets of two directly opposite from the other." "I would rotate the molecule based upon an axis that extends through the "top" and "bottom" of the molecule rotate along that axis→ as well as reflect the front to back along the plane of the paper and the anti-plane to the paper." "→green lobes two down, one up [drawing of the shape of the lobe patterns with labeled]"
007	"1B) 180° rotation is possible to maintain symmetry"
012	"The one on the right is symmetric. The one of the left has a mirror plane along the axis of rotation."
013	"A C_2 would be able to rotate the 1b structure on its y-axis, but the different charge makes C_2 an unusable operation in the 1a structure. σ_v is present in both structures, and the 1b structure can be reflected on the xy and yz plane while the 1a structure can only be reflected on the xy plane."
016	"A C_2 about the center of the big red glob orbital through molecule [drawing of rotation around a vertical axis]"

Table F.48 (continued)

018	"If you split them into ½ (through the plane coming out of the board) you get the same pattern on both sides: 1a) but they are in different colors, 1b) they have the same color"
021	"Rotate by C_2 which flips sides, reflect by $\sigma_{v(yz)}$"
023	"In 1A the orbitals are anti-symmetric with respect to the primary axis. In 1B the orbitals are symmetric with respect to the x-axis."
026	"Put a z axis and rotate around for atoms to switch positions, mirror axis on same plane"

Table F.49. Week 8 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
005	"There only seems to be a mirror image pattern, indicative of C_{2v}"
012	"The one on the right is symmetric. The one of the left has a mirror plane along the axis of rotation."
019	"1a)→yz plane sign change reflection plan, 1b)→ yz plane sign consistency across yz reflection plane"
023	"In 1A the orbitals are anti-symmetric with respect to the primary axis. In 1B the orbitals are symmetric with respect to the x-axis."

Table F.50. Week 8 evidence of personalized strategies.

ID #	Documented Response
004	"I would visualize axis of rotation first"
005	"Find which parts of the character table correspond to each orbital"
011	"Ignored everything but the largest lobe"
012	"I'm not entirely sure what it's asking but if I did it right, try the symmetry elements, see what happens, develop the reducible representation"
013	"See if the C_{2v} point group matches either structure, if not, then find another point group to find the reducible for the structure"
015	"I simply assigned a main rotational axis and discovered all the symmetry elements."
019	"Count orbitals. Perform operations and see how they move or if sign changes."
021	"Rotate symmetry operations to a point group. Write down operations for that point group to help write down the reducible representations."

Table F.51. Week 8 evidence of extension of symmetry.

ID #	Documented Response
004	"I would rotate the molecule based upon an axis that extends through the "top" and "bottom" of the molecule rotate along that axis→ as well as reflect the front to back along the plane of the paper and the anti-plane to the paper."
005	"1B) 180° rotation is possible to maintain symmetry"
012	[coord axis drawing] "C_2 rotates around z axis, $\sigma_{v(xz)}$ mirror plane xz, $\sigma_{v(yz)}$ mirror plane yz"
013	"A C_2 would be able to rotate the 1b structure on its y-axis, but the different charge makes C_2 an unusable operation in the 1a structure. σ_v is present in both structures, and the 1b structure can be reflected on the xy and yz plane while the 1a structure can only be reflected on the xy plane."
015	"I simply assigned a main rotational axis and discovered all the symmetry elements."
016	"A C_2 about the center of the big red glob orbital through molecule [drawing of rotation around a vertical axis]"

Table F.51 (continued)

018	"If you split them into ½ (through the plane coming out of the board) you get the same pattern on both sides: 1a) but they are in different colors, 1b) they have the same color"
019	"1a)→yz plane sign change reflection plan, 1b)→ yz plane sign consistency across yz reflection plane"
021	"Rotate by C_2 which flips sides, reflect by $\sigma_{v(yz)}$"
023	"In 1A the orbitals are anti-symmetric with respect to the primary axis. In 1B the orbitals are symmetric with respect to the x-axis."
026	"Put a z axis and rotate around for atoms to switch positions, mirror axis on same plane"

Given that the structure belonged to the C_{2v} point group, students could determine that only one C_2 was present and were able to align the z-axis with the principal rotation axis.

Table F.52. Summary of coordinate axis use for Week 8.

Coordinate Axis Use	**Student ID #**
Correct orientation	001, 005, 012, 019, 023, 026
Incorrect/incomplete orientation	013, 016

Some students correctly considered the whole molecular orbital as a single pattern to represent. Others attempted to write a reducible representation of the parts of the image which was indicated by the value of the character of E being greater than 1. Table F.53 summarizes students' varied answers to the summary question and reports whether students attempted to reduce their representations, if they provided symmetry labels, and whether or not they were correct.

Table F.53. Summary of students' answers to the summary question of Week 8.

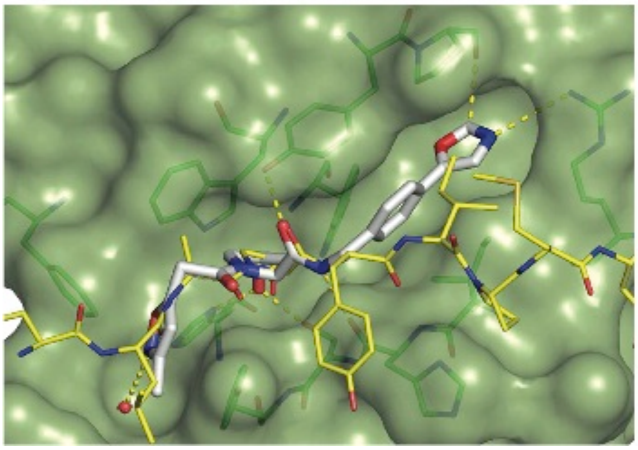
Reducible Representation	**ID #**	**Reduced?**	**Symmetry Labels?**
Wrote correct reducible representation of single orbital pattern	011	Yes	Yes *(correct)*
	012	Yes	Yes *(correct)*
	018	Yes	Yes *(half correct)*
Constructed reducible representation of various parts of the image *(character of E >1)*	001	No	No
	003	No	Yes *(incorrect)*
	005	No	No
	013	No	No
	015	No	No
	019	No	No
	021	No	No
	023	No	No
	025	No	No
	026	No	No
None written	004	No	Yes *(half correct)*
Symmetry labels set up only	007	No	No
	017	No	No
No attempt	016		
	027		

Name: ________________________

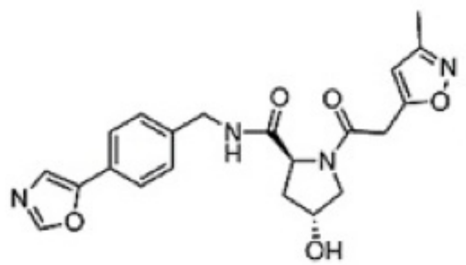
Week 9: Binding the VHL Enzyme

Enzymes are catalysts that speed up the reaction of the substrate into a product. Enzymes and substrates follow the “lock-and-key” model where a enzyme (lock) targets a specific substrate (key). In the figure below, the 2-D molecule was synthesized to model the natural substrate that binds to the VHL enzyme.[1] Both the synthetic molecule and natural substrate are illustrated binding to the enzyme in the image.

Enzyme with superimposed
Synthetic Molecule and Natural Substrate



Synthetic Molecule



1) **Describe the steps** of how the *synthetic molecule* must be manipulated to match its orientation indicated in the enzyme picture. When describing motions of the synthetic molecule, use the rings in the structure as a reference to specifically explain each of your actions (rather than specific atoms). Use either degrees (i.e. 180°) or rotation axis (i.e. C_2) notation in your descriptions.

2) a. What are the simplest parts of the image? (**Atoms, bonds, edges, faces, shapes**)

b. How do the parts of the synthetic molecule relate to the green enzyme? (**Surroundings, positions, locations**)

c. How do you move the individual rings of the synthetic molecule to fit the enzyme pocket? (**turns, flips, motions**)

d. *Overall*, what general motion makes the synthetic molecule fit into the enzyme pocket.

3) Name something this visual or the process you've described is similar to in reality. Does it resemble or remind you of anything you've seen before?

4) What strategy would you use to answer question 1? If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

Week 9 Activity Data:

This was the second application-based activity where students could compare the 2-D structure of a synthetic molecule to the line image of the reoriented molecule in an enzyme environment. The general motion students needed to communicate was to turn the molecule ~180° around an axis going into the paper and tilt the molecule (so the bottom of the molecule as shown points into the enzyme) around 90°. Students were instructed to describe motion of the rings with degrees (180°) or symmetry terminology (C_2).

Table F.54 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). Due to the nature of the summary question, responses to this question were not considered for analytical deconstruction. An overall motion, with specified direction, of the synthetic molecule was sought for the determination of a valid pattern.

Table F.54. Number of instances of observed deconstruction parameters demonstrated by students during the Week 9 complex visualization activity.

	Week 9: Binding the VHL Enzyme						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001							
002	1	0	1	1	0	0	0
003	2	1	4	1	0	0	0
004	3	1	1	2	0	0	2
005	2	1	1	1	1	1	1
006	5	0	2	0	0	1	1
007							
008	0	4	0	0	0	0	0
009	9	0	1	2	1	0	1
010							
011	1	2	0	1	0	0	0
012	2	2	0	2	0	0	0
013	9	1	0	2	0	1	0
014							
015							
016	1	2	0	1	1	1	1
017							
018							
019	3	3	0	0	0	1	1
020							
021							

Table F.54 (continued)

022	2	0	0	1	0	1	1
023	1	5	0	0	0	0	1
024							
025	1	0	1	0	0	0	0
026	0	2	0	2	0	1	1
027							

Table F.55. Week 9 reality comparisons that were unrelated to the activity content.

ID #	Reality Comparison
002	[Bicycle]
003	Soda cap, screws, laying pipe, puzzle
004	Flattening origami
005	"Fitting shapes into holes as a child"
006	"Catching putty-putty molds to hand, car parallel parking"
009	"Puzzle pieces and rotating them to fit in certain empty spaces"
025	"Resembles glycolysis and the multiple enzymes associated with it"

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow.

Table F.56. Week 9 evidence of analytical deconstruction.

ID #	Documented Response
002	"Rings should be moved a 1/8 turn counterclockwise and a 1/8 turn along the traditional x-axis."
003	"The molecule is a puzzle piece and the enzyme is the frame showing the position."
004	"The corners of the pentagonal ends bond to the enzyme (the nitrogen groups) and the two hetero groups interact," "Move the far right around central axis (1) and then rotate down clockwise 160°; Left end→ flip molecule and turn counterclockwise into plane 60°"
005	"The 5-membered rings w/ O and N need to rotate 90° as well as the phenyl group."
009	"The synthetic molecule is the molecule represented in gray on the colored picture. The green and yellow parts are the enzyme." "Rotation around the cyclohexane between the two oxygen double bonds."
011	"The [drawing of left-most ring] is standing up, slight twist"
012	"The synthetic molecule is surrounded by the green enzyme. It binds to the green enzyme at 5 locations." "The entire molecule must be flipped. The [drawing of right-most ring] with the methyl must be rotated 90° and the [drawing of 2nd ring from left] must also."
013	"Rotate the entire molecule 180°, making the five-atom rings with both N and O switch in position, and making the benzene the second ring from the right. Turn the outermost right ring [drawing] 45° towards the page, the benzene ring 75° towards the page, the five atom ring with the OH group 90° towards the page, and the final ring 90° with the ligand sticking outside of the page." "Turn the rings with the N and O groups 90° towards the page, the benzene ring 45° towards the page, and the ring with the N and OH ligand 90° towards the page."

Table F.56 (continued)

016	"A 180° rotation ([perpendicular] to the plane of the molecule) so that methyl of synthetic points down"
022	"180° rotation [drawing of rotation around a vertical axis], then 180° rotation [drawing of rotation around a horizontal axis]"
026	"laid out in opposite directions (must flip one), green enzyme is not planar as synthetic molecule may be," "turn synthetic 180° on x and 90° on y [drawn coordinate axis], bend bond between ring 1 and carbonyl, put ring 2 in boat conformation, turn ring 4 60° from ring 3 along bond"

Table F.57. Week 9 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
005	"A total 90° rotation along the molecule and flip 180° along axis perpendicular to molecule."
009	"Rotation around the cyclohexane between the two oxygen double bonds"
016	"A 180° rotation ([perpendicular] to the plane of the molecule) so that methyl of synthetic points down"

Table F.58. Week 9 evidence of personalized strategies.

ID #	Documented Response
005	"Look at either ends of the chain to determine orientation"
006	"Compare 2-D structure to structure in picture, list differences, determine how those differences occur, use a model to determine possible movements"
009	"Pick out which part of the first picture has the synthetic molecule and then manipulate the synthetic molecule in the second picture to possess the same orientation."
013	"Fit the overall structure together, then match some of the colored edges of the ring to atoms in the structure and rotate."
016	"Looked at end part of the molecule and matched them with the "virtual" image in enzyme."
019	"Look at one ring and figure out how to move whole molecule to match its orientation."
022	"Pick an end and determine where it is in the picture with the enzyme, then determine what you must do to the molecule so that end will be in a new position."
026	"Turn molecule so your looking at the side and flip 180° so ring 1 is to the left, bend bond to 45° angle between ring 1 and carbonyl, put ring 2 in boat conformation."

Table F.59. Week 9 evidence of extension of symmetry.

ID #	Documented Response
004	"Rotate structure 180° with a vertical axis on the plane of the paper. Rotate whole molecule around axis similar to molecule along plane of paper." "Move the far right around central axis (1) and then rotate down clockwise 160°; Left end→ flip molecule and turn counterclockwise into plane 60°"
005	"Rotate molecule 90° along axis that follows the chain. Then flip it 180° along axis into the page."
006	"Whole molecule rotates about a C_2 axis, [left-most ring] and benzene ring rotate 90° from plane of the page"
016	"Rotate 90° (in the plane of the molecule across longer end of the molecule)… and then rotate 180° along axis [perpendicular] to the molecule (out of the bond)"

Table F.59 (continued)

019	"Rotate synthetic on axis approximately through all nitrogens just less than 90° rotation (top towards me). Then do 180° rotation on axis [perpendicular] to paper through center of synthetic molecule"
022	"2 C_2's must be performed, one on the z axis and one on the x as drawn above. This will turn the molecule so it is oriented correctly into the binding pocket."
023	"The synthetic molecule must be rotated 180° about the y-axis [drawn on image into the page]"
026	"Turn synthetic 180° on x and 90° on y [drawn coordinate axis], bend bond between ring 1 and carbonyl, put ring 2 in boat conformation, turn ring 4 60° from ring 3 along bond"

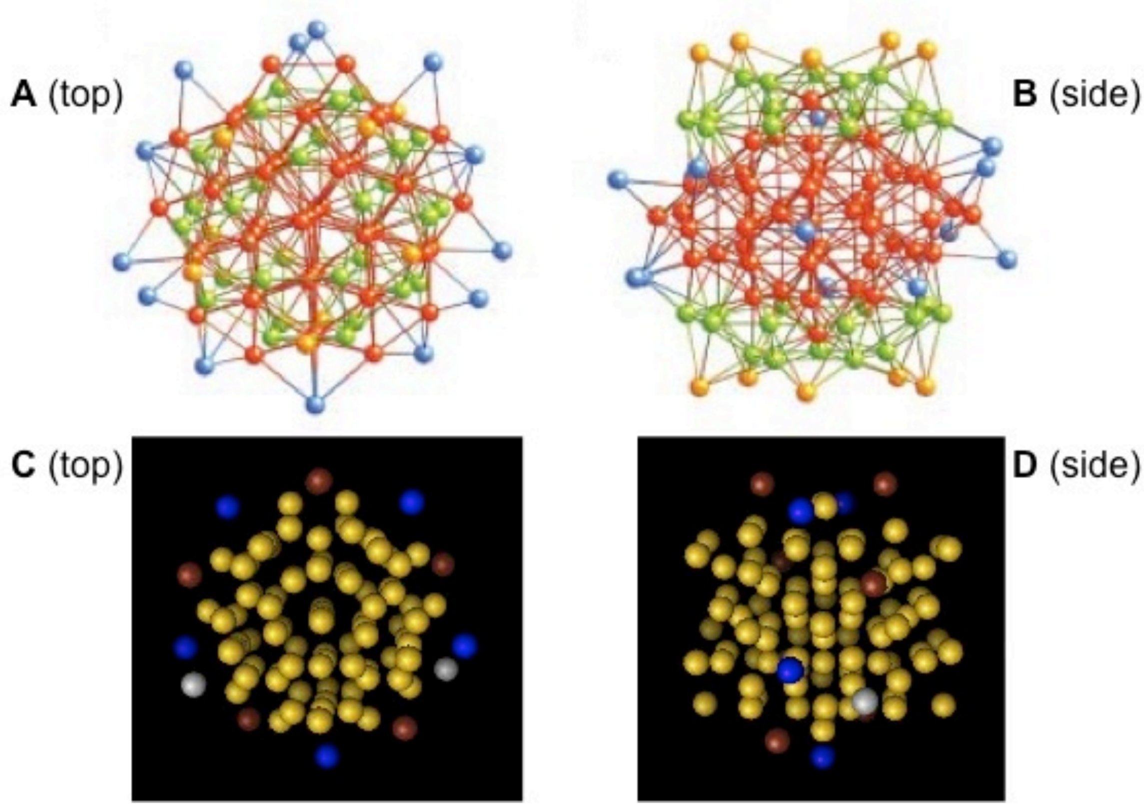
Table F.60 Summary of students' answers to the summary question of Week 9.

Character of Summary Question Response	**Student ID #**
Extent and direction of both the 180°/C_2 rotation and specific motion of all of the rings	009, 013
Extent and direction of the 180°/C_2 rotation and extent of ~90°/C_4 motion of one ring	002, 003, 004, 005, 012, 016, 026
Extent of both the 180°/C_2 rotation and the ~90°/C_4 motion of one ring	006
Extent and direction of the 180°/C_2 rotation	011, 019, 022, 023
Irrelevant response	025
No attempt	008

Name: ____________________________

Week 10: Mark's Decahedron

Below, the core of a gold nanoparticle is shown (Au_{102}(p-MBA)$_{44}$) in different views from two different sources.[1, 2] The ligands (p-MBA) have been excluded from the images for clarity. Out of the 102 gold atoms inside the structure, 89 adhere to a specific point group—the dominating point group of the nanoparticle. **The authors have color-coded groups of Au atoms in terms of similar bonding patterns.**



1. a. List the symmetry elements required to identify this point group and list the images (A, B, C, D) that helped you determine that specific element.

   b. What is the dominating point group of the nanoparticle?

2. a. What are the simplest parts of the image *in terms of different groups of gold atoms*?

b. How are the Au atom groups related to each other? (Surroundings, positions, numbers)

c. How would you move image A to get image B? How would you move C to get D? Specify what action you're taking and the extent to how much you're moving the image.

d. Which Au atom groups contribute to the same dominating symmetry pattern?

3. Name something that this visual or any of its parts looks like.Does it resemble or remind you of anything you've seen before?

4. What strategy would you use to answer question 1?If you cannot answer the question, describe the steps you took to make sense of the visuals given, then answer question 1.

[1]Reprinted (adapted) with permission from Mednikov, E. G.; Dahl, L. F. *Small*, **2008**, 4, 5, 534-537. Copyright © 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
[2]From Jadzinsky, P. D.; Calero, G.; Ackerson, C. J.; Bushnell, D. A.; Kornberg, R. D. *Science*, **2007**, 318, 430-433. Reprinted with permission from AAAS.

Week 10 Activity Data:

The final activity featured four images: the top and side orientations of a 102-atom gold nanoparticle from two different sources. All but 13 of the atoms adhered to a dominating point group and students were tasked in identifying the point group and which groups of atoms belonged to that symmetry. To correctly answer the task, students had to omit the blue spheres from the A/B images and omit the red, white, and blue spheres from the C/D images. Consideration of both images (top and side) was required to see that the belts reduced symmetry rather than gave cues for a C_5 rotation axis.

Table F.61 displays the assigned points under several parameters for each of the students attending that week's recitation. Shaded rows indicate that the student was not present during the activity. Summary points were graded by the researcher and the undergraduate assistant. Non-attempts were either blank or an irrelevant comment was offered instead of an answer to the question (maximum non-attempts is 7). The summary question asked only for the dominating point group and a list of symmetry elements and used images required to determine it. All questions could be examined for analytical deconstruction. Symmetry extension was not a valid parameter to identify on this activity because students had not yet learned symmetry.

Table F.61. Number of instances of observed deconstruction parameters demonstrated by students during the Week 10 complex visualization activity.

	Week 10: Mark's Decahedron						
ID #	**Summary Pts**	**Non-Attempts**	**Reality Comp**	**Decon-struction**	**Patterns**	**Personal Strategy**	**Sym Extension**
001							
002							
003	2	2	4	1	0	0	0
004							
005	5	0	1	2	0	1	0
006	4	0	2	1	0	1	0
007	0	2	1	1	0	0	0
008	1	1	1	3	0	0	0
009	2	0	1	2	0	1	0
010	4	1	0	1	0	1	0
011	3	2	0	2	1	1	0
012	3	0	1	1	1	0	0
013	2	1	0	2	0	1	0
014							
015	2	0	1	3	1	0	0
016	3	0	1	2	1	1	0
017							
018							
019	2	1	0	1	1	1	0

Table F.61 (continued)

020							
021							
022							
023	2	5	0	1	1	0	0
024	0	4	0	0	0	0	0
025	4	1	0	2	0	0	0
026							
027	4	2	0	0	0	0	0

Table F.62. Week 10 reality comparisons that were not symmetry related.

ID #	Reality comparison
003	Cat's cradle, an animated monster's face (transformer), collapsing/expanding sphere, a target
005	Star
006	"Ball with patterns drawn on it, cut diamond"
007	Spider web
008	Jungle gym
009	Fireworks
012	Star design
015	Star
016	Snowflake

Records of student documentation that was rated as a successful deconstruction parameter are listed under the corresponding categories that follow. The operation question (2c) asked students how they would move image A to get B and C to get D.

Table F.63. Week 10 evidence of analytical deconstruction.

ID #	Documented Response
003	*In response to 2c:* "For both, perform half of a C_2 rotation from top bottom or bottom to top"
005	"There seems to be 3 main layers from the top view," *in response to 2c:* "Rotate 90 upwards; Rotate 90 left or right"
006	*In response to 2c:* "C→D = rotate 90° vertically, ~45° spin along new vertical axis"
007	[Drawing of a C_4 going vertically from the left side to the top a 'C' in a square], [drawing of a C_4 coming horizontally out of the paper from the left to the front around an 'A' in a square]
008	"Blue fence around everything, orange box in the middle, green caps on top and bottom, yellow crown on top and bottom of the green," "orange> green> blue> yellow," *in response to 2c:* "rotate 90° towards us, for axis [drawing of labeled coordinate axis, rotating CCW around vertical z], rotate 90° about z"
009	"Small group in center, star-like shape of gold atoms, U-shape, 5 blue points, 5 red points, 2 white points, a lot of confusion on the side view," *in response to 2c*: "Turn it 90° around z-axis"

Table F.63 (continued)

010	"Without the white, D_{5d}; from [image] C, C_5 from center in, C_2's from 1 brown or blue straight across to between other two, C_{2v} with white"
011	"Red at points of pentagon and yellow is in shape of pentagon and blue are points of a pentagon out of phase by 180°, white ones destroy C_5 & C_2 [perpendicular]," "*in response to 2c:* A→B [drawing of left-pointed arrow with arrow rotating upward] C2 (180°), C→D [drawing of downward-pointed arrow with arrow rotating to the right] C2 (180°)"
012	"Rotate 90°, A-B [drawing of arrow rotating down around horizontal line] 90° forward, C-D [drawing of left-right rotation around vertical line] 90° sideways"
013	"The gold atoms are bunched up in A, C, and D structures. The yellow atoms are spread out between the orange gold atoms in structure B." *In response to 2c:* "I'd move image A 90° towards the front of the page to get image B, and image C 90° to the right of the page to get image D."
015	"There are five points in the molecule, the molecules are arranged in a bulls eye pattern," "[They gold atoms] are replications, have the exact same patterns at 5 different points," *in response to 2c*: "You would perform a C_4^1 movement, basically rotating it to its side"
016	"Each 'layer' has a different number of atoms but make the same shape. Depending on how you look at it, the C view looks like 2 'snowflake' 5 point layers," *in response to 2c:* "C_4 through side, C_4 through top/bottom"
019	*In response to 2c:* "Rotate 90° through axis from top of page to bottom of page"
023	"A central column of Au atoms, an inner pentagonal shaped structure consisting of 10 columns of gold atoms"
025	"The 5 individual atoms in blue that stand out so we can determine the molecule's primary axis." "The molecule seems to only have vertical reflection planes. Looking from the top view is the best way to determine the primary axis of symmetry."

The pattern question was changed in this activity to have students explicitly state which groups of Au atoms contributed to the overall symmetry rather than detracted. Instead of looking only to the pattern model component question, a description of the overall symmetry/point group signified a pattern since the descriptions were not requested in this activity.

Table F.64. Week 10 evidence of valid patterns/rules documented in appropriate language.

ID #	Documented Response
011	"Red at points of pentagon and yellow is in shape of pentagon and blue are points of a pentagon out of phase by 180°, white ones destroy C_5 & C_2 [perpendicular]"
012	"From image C-central 2 surrounding groups of yellow, red, blue, not white"
015	"There [is] a group of 5x(?) atoms composing the main symmetry points"
016	"When looking at it through (C view) the top, 2 layers of 'gold' spheres"
019	"Looked like a [drawing of a pentagon] C_5 at first, then look at rotation to D and realize that atoms are not all in same horizontal plane"
023	"A central column of Au atoms, an inner pentagonal shaped structure consisting of 10 columns of gold atoms"

Table F.65. Week 10 evidence of personalized strategies.

ID #	Documented Response
005	"Consider symmetry elements of a star with 5 points"
006	"Consider molecule from all angles, choose either A & B or C& D to use, identify symmetry elements, use flow chart to identify point group"
009	"Use blue & red points to find dominating pattern. Then use white points to narrow down the pattern & [exclude] certain symmetries."
010	"Take out the white Au atoms"
011	"Determine dominant point group and then see what destroys it"
013	"Try to find a MAIN rotation axis, because if it works for the most part, it can be used as the primary axis. Small parts that might prove the point group wrong could be used to identify other possible symmetries or find a different point group."
016	"I used the 5 red and 5 blue atoms as a reference for the C_5 symmetry"
019	"Looked like a [drawing of a pentagon] C_5 at first, then look at rotation to D and realize that atoms are not all in same horizontal plane"

Table F.66. Summary of students' performance on the Week 10 summary question.

Reported Dominating Point Group	Student ID #
Correct point group identification (D_{5h})	005, 011, 027
Correct rotation axis (D_{5d}, C_{5v}, C_{5h}, C_5)	003, 009, 010, 012, 013, 015, 016, 023, 025
Incorrect answers	019, 024
No answer	006, 007, 008

The modified operation question in this activity (*How would you move image A to get image B? How would you move C to get D? Specify what action you're taking and the extent to how much you're moving the image.)* aimed to prompt students to connect the two views of the nanoparticles and observe which images they analyzed.

Table F.67. Week 10 responses to the modified operation question.

Motion	ID #	Documented Response
Correct motions	003	"For both perform half of a C_2 rotation from top to bottom or bottom to top." **Moved images A/B only*
	005	"Rotate 90° upwards. Rotate 90° left or right." **Moved images C/D only*
	006	"A→B = rotate 90° vertically" (incorrect) "C→D = rotate 90° vertically ~45° spin along new vertical axis" **Moved images C/D only*
	007	[drawings of a C_4 on A moving from the bottom to the middle and a C_4 on C moving from the left to the middle] **Moved both sets of images*
	008	"Rotate 90° towards us." "For axis [drawing], rotate 90° about z."
	009	[drawn axis] "Turn it 90° around z axis." **Moved images C/D only*
	011	"A→B [horizontal rotation drawing] C2 (180°)" "C→D [vertical rotation drawing] C_2 (180°)"
	012	"Rotate 90° A—B [horizontal rotation drawing] 90° forward. C—D [vertical rotation drawing] 90° sideways"

Table F.67 (continued)

	013	"I'd move image A towards the front of the page to get image B, and image C 90° to the right of the page to get image D."
	015	"You would perform a C_4^1 movement. Basically rotation it to its side." **Moved images C/D only*
	016	"C_4 through side. C_4 through top/bottom."
	019	"Rotate 90° through axis from top of page to bottom of page." **Moved images C/D only*
Incorrect/unrelated motions	010	"rotate 90° toward us"
	024	"A→B => C_2 axis in the plane of the page"
	025	"I would turn the molecule 90° degrees and do the same for C→D"
	027	[drawing of a point with 90° rotation in the plane of the paper and a line with an arrow rotating upward and 90°]

The modified pattern question asked which atom groups contributed to the dominating symmetry pattern. The documented responses to this question demonstrated that many students used the non-symmetrical belt atoms to cue symmetry. The inclusion and omission of appropriate groups is indicated in bold formatting.

Table F.68. Summary of the student responses to the modified pattern question of Week 10.

Images Referenced	**ID #**	**Documented Response**
A/B and C/D	003	"**Yellow** and blue (C & D), **green** and blue (A & B)"
	006	"Blue atoms in image A, red atoms in image A, **yellow atoms** in image B, **green atoms** in image B, **yellow**/blue/red atoms in image C, **yellow atoms** in image D"
A/B	008	"Blue" **Referred to images A/B for the rest of the worksheet*
C/D	005	"The **yellow atoms** mostly do so as well as blue (**not white or red**)"
	009	"White, blue, red" **Refers to images C/D for the rest of the worksheet*
	010	"**Yellow**, brown & blue"
	011	"**Yellow** & red & blue, **not white**"
	012	"From image C—**central 2 surrounding groups of yellow**, red, blue. **Not white.**"
	013	"The blue Au atom groups contribute to the dominant symmetry pattern, there are 5 around the big cluster."
	016	"Blue, red and **gold**"
	019	"Blue/red in C, D"
	027	"The **yellow**, blue, & white"

Students' responses to the deconstruction questions help lend insight on the variety of summary question responses. When stating the dominating point group or describing the atom groups that contribute to the point group in the Week 10 activity, many students misinterpreted the visual cues that led them to an incorrect interpretation of the image. This could mean that students use the simplest cues they can find to indicate symmetry. Bold formatting indicates the portion of the answer that directed observed interpretation.

Table F.69. Documented responses describing image C/D atom groups used to answer the summary question of Week 10.

Observed Interpretation	**ID #**	**Documented Response**
Correct omission of belt atoms	019	"Looked like a C_5 at first, then look at rotation to D and **realize that atoms are not all in same horizontal plane**."
	023	"A central column of Au atoms, an inner pentagonal shaped structure **consisting of 10 columns of gold atoms**."
Incorrect inclusion of blue atoms	025	"The 5 individual **atoms in blue** that stand out so we can determine the molecule's primary axis."
Incorrect inclusion of blue and red atoms	009	"Use **blue and red points** to find dominating pattern. Then use white points to narrow down the pattern and [exclude] certain symmetries."
	010	"Without the white, D_{5d}. From 'C', C_5 from center in, C_2's **from 1 brown or blue** straight across to between other two."
	011	"**Red at points of pentagon** and yellow is in shape of a pentagon **and blue are points of a pentagon out of phase** by 180°"
	012	"From image C-central 2 surrounding groups of yellow and **red, blue**."
	013	"**Blue atoms and red atoms in C are in a C_5 rotation axis**, and is used to find the main rotation axis."
	016	"I **used the 5 red and 5 blue atoms as a reference for the C_5** symmetry."
	027	"**2 pentagons (blue, red)** from the top"