Visualization and Diagrammatic Reasoning During Genuine Problem Solving in Science

Mike Stieff

University of California, Davis
School of Education, One Shields Avenue, Davis, Ca, 95818

Abstract

Mental visualization of diagrammatic representations is presumed to be a critical strategy for learning and problem solving, particularly in the sciences. However, little is known about how students employ visualization on genuine scientific tasks. The present study describes undergraduate chemistry students' use of visualization for problem solving using think-aloud protocols. The analysis suggests that students' reasoning is heavily guided by the form of the molecular diagrams given in the task and self-generated inscriptions. Visualization strategies appeared critical for task that required representation translations.

Exploring the Intersection of Visualization and Diagrammatic Reasoning in Chemistry

The affordances of diagrams to aid in reasoning has been underscored in several arenas. Computational models of diagrammatic reasoning have indicated how diagrams facilitate the organization of knowledge, scaffold problem solving, and invoke mental images (Larkin & Simon, 1987; Narayanan, Suwa, & Motoda, 1995; Olivier, 2001). Cognitive studies have indicated how problem solvers attempt to visualize diagrams and rely on them for spatial reasoning (Hegarty, 1992; Oxman, 1997). Similar to the efforts of Qin & Simon (1992), the present study attempts to apply some of the collective findings of these communities to investigate the extent to which diagrammatic reasoning and visualization intersect with domain knowledge in science. The results provide new insights on (1) how individuals learn to reason from diagrams in specific contexts and (2) the task-specific use of visualization in scientific problem solving.

Investigations of problem solving in science domains have hinted at a complex interplay between visualization and diagrammatic reasoning. By analyzing eye movement behaviors during problem solving, Hegarty (1992) inferred that students systematically and sequentially attempt to mentally animate diagrammatic representations for certain engineering tasks. Likewise, Qin and Simon (1992) identified a reciprocal relationship between visualization and inscription practices using qualitative investigations of problem solving among students of advanced physics. Such work supports computational models of diagrammatic reasoning that postulate a critical function of diagrams to preserve and coordinate spatial information during problem solving (Larkin & Simon, 1987).

The field of organic chemistry provides an excellent domain in which to extend studies of the interaction of visualization and diagrammatic reasoning during problem solving. Students of organic chemistry often reason about the spatial characteristics of molecular diagrams in order to determine molecular structure, functionality, and reactivity. Additionally, organic chemistry textbooks employ several unique diagrams of molecules in which spatial information is implicitly communicated; consequently, students must learn exclusive techniques to decode three-dimensional shape and structure from two-dimensional diagrams that lack the dimension of depth (Ege, 1999). Moreover, a major component of chemistry instruction centers on the use of non-imagistic strategies for manipulating molecular diagrams with little regard to the spatial information they contain. When teaching such strategies, instructors often encourage their students to use formalisms of molecular diagrams for making judgments about the three-dimensional features of a molecule. Although textbooks and instructors present these diagrammatic reasoning strategies as a more efficient and simpler strategy than the generation and manipulation of mental images of molecular structures, students often fail to correctly apprehend them (Taagepera & Noori, 2000).

Unfortunately, little is known about the interaction between visualization and reasoning from diagrams during genuine problem solving in this domain. Past studies have focused on the affordances of different molecular diagrams to represent the imperceptible molecular world (Johnstone, 1993), to communicate ideas and understanding between experts and novices (Kozma, et al., 2000), or to facilitate teaching (Wu, Krajick, & Soloway, 2001). Other work has explicated the manner in which molecular diagrams attempt to represent three-dimensional space in two-dimensions (Habraken, 1996; Keig & Rubba, 1993), but little has been said in these forums about how molecular diagrams and visualization strategies interact. Rather, they have focused mostly on the presumed difficulties with perceiving the embedded three-dimensionality of molecular diagrams and pursued correlations between achievement and visuo-spatial skills. Regardless, it is generally assumed that visualization is a key strategy for problem solving in chemistry (Habraken, 1996); however, the precise role of that strategy remains unclear.

Design of the Present Study

The present study attempted to characterize novice students' use of visualization and diagrammatic reasoning on traditional organic chemistry tasks. Thirteen students enrolled in introductory organic chemistry completed two 45-minute think-aloud interviews. During the interviews students performed a variety of organic chemistry tasks that included representative assessments on topics such as reaction mechanisms, product generation, stereochemistry, and the translation of molecular representations. Each interview was transcribed, and the transcripts were analyzed for instances in which students explicitly made use of visualization for problem solving.

Transcription and review of the 25 clinical interviews established the data corpus, which comprised 19.5 hours of video. Students completed between 16 and 24 tasks as a function of the time each took to solve each task in the interviews. The combined total of all completed tasks resulted in 246 tasks in the corpus. Seventy of these tasks were *analyze* tasks, which required students to analyze the structure and reactivity of a compound. Twenty-eight were *translate* tasks, which required students to translate one molecular representation into a different one. Finally, 148 were *extended problem* tasks, which required students to draw reaction schemes, design syntheses, or propose reaction mechanisms.

The interviews were analyzed using accepted techniques of qualitative data analysis (Chi, 1997; Ericcson & Simon, 1980) with specific regard to utterances and gestures that indicated students were trying to visualize the three-dimensional structure of the molecular compounds in each task. For the purposes of this study, individual cases of student problem solving strategies were situated either *externally*, when students reasoned about spatial information using the diagrams, or *internally*, when students engaged in the visualization of imagined molecular structures. Examples of utterances that indicated the use of visualization included explicit references to attempts to "picturing or seeing a molecule" or "visualizing models from class". Physical behaviors that suggested the use of visualization included gestures to objects in empty space, grasping and rotating imagined objects, and physically moving diagrams with references to "visualizing it from different angles". A common example of reasoning from diagrams was an utterance in regard to spatial relationships within a particular diagram together with gestures to that diagram, such has "this line means the bond projects above the page." More important, were instances in which students duplicated particular spatial relationships from previous diagrams into new inscriptions without regard to whether the relationships were valid or references to engaging in visualization.

Two separate analyses of the data corpus illustrated a variety of interactions between diagrammatic reasoning and visualization strategies. First, a series of descriptive statistics on the coded data corpus revealed the frequency of visualization strategies across tasks for the entire participant group. Second, illustrative cases of the interviews indicated how students were able to selectively manipulate molecular diagrams to successfully complete a wide range of tasks.

Task-Specific Use of Visualization and Diagrammatic Reasoning

Analysis of participants' preferred strategies revealed that the interaction between visualization and diagrammatic reasoning is a function of the task demands. By parsing the data corpus into the three types of tasks enumerated above, the selectivity of student use of visualization was immediately apparent. Figure 1 illustrates how students used the embedded features and constraints of molecular diagrams on most tasks to scaffold their reasoning about spatial information. Notably, students engaged in behaviors that suggested they were trying to inspect a visualized mental image of a molecular diagram on *translate* tasks.

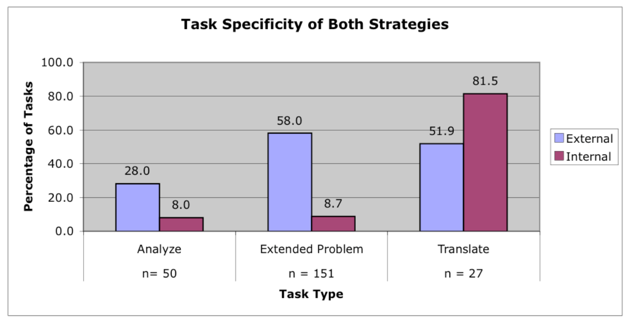

Figure 1. Student's use of visualization was specific to translation tasks in organic chemistry.

On *analyze* tasks, where students had to describe all relevant physical and chemical properties of a given molecular diagram, they appeared unlikely to engage in visualization of those diagrams. On the majority of these tasks, students did not make any utterances, behaviors, or inscriptions that suggested they had attended to spatial information embedded in the diagram. On 28% of these tasks, students did mention the spatial features of the molecule with specific reference to the diagram, but their utterances were of a unique sort. For the most part, utterances were in specific regard to the two tasks that included three-dimensionally rendered space-filling molecular representations. Upon viewing such representations, students mentioned that the representations helped them to "see how big it is" or "see how different groups interact". On 8% of these tasks did students mention trying to visualize the structures to discern additional information. Analyze tasks such as those used in the interviews corresponded to approximately 25 percent of the assessment items from students' coursework.

This pattern of results persisted on *extended problem* tasks where students were asked to predict products, generate mechanisms, or propose syntheses in accordance with accepted concepts of organic chemistry. On 58% of these tasks, the participants referenced the diagram to note a spatial feature of a molecule. Evidence for this strategy was seen in instances of pattern matching and duplication mentioned above. On only 8.7% of these tasks did students appear to engage in the visualization of molecular diagrams. Frequently these behaviors took the form of students gesturing at an imagined molecule or mentioning that they were trying to visualize using their molecular modeling kits from class. Roughly 93 percent of the assessment items from the students' courses contained an extended problem component.

A dramatic reversal in strategy use was apparent on *translation* tasks. On 51.9% of the interview tasks, students referenced the diagram as a scaffold for visualization instead of merely mentioning spatial features such as size or shape. For instance, students would reference a spatial relationship in the initial representation that they then duplicated in the target molecule to which they were translating. On 81.5% of these tasks, the students engaged in clear behaviors that indicated they were attempting to manipulate an imagined three-dimensional visualized molecular structure. All students showed great difficulty in these tasks and many mentioned that they would be able to perform better if they had molecular modeling kits available. Approximately 12 percent of the assessments tasks from the students' courses contained a translation component.

Illustrative Cases of Visualization and Diagrammatic Reasoning

The overall trends within the data corpus revealed that students employed visualization strategies on approximately one-fourth of the tasks in the interviews. More specifically, the students appeared to use visualization strategies selectively to perform translations of molecular representations. Although students employed visualization for successful problem solving on the translation tasks, they rarely reported using visualization on extended problem solving tasks or on analyze tasks. Each student progressed through such tasks without explicitly addressing spatial information. Instead, the participants employed several heuristics for inscribing molecular diagrams that allowed them to generate successful solutions to the tasks. These heuristics appear to describe formal principles of diagrammatic reasoning in chemistry since they were ubiquitous among all the students and all the tasks. Below are three cases that illustrate the use of both visualization and diagrammatic reasoning for problem solving in organic chemistry.

Visualization for Translating Molecular Diagrams

Students engaged in overt behaviors that indicated they used visualization as a major component of their overall problem solving strategy on one or more translation tasks. The following excerpt from the interview with Carrie indicates how the students used visualization to translate given molecular diagrams into target diagrams that emphasized three-dimensional spatial features of the molecule. On this task (illustrated in Figure 2), Carrie attempted to translate the given two-dimensional line-angle diagram of a substituted cyclohexane into a chair diagram. Upon seeing the task, Carrie immediately noted she knew the basic chair diagram, which she inscribed. Subsequently, she engaged in behaviors that suggest she was trying to visualize a three-dimensional image of the molecular structure in question to complete the translation.

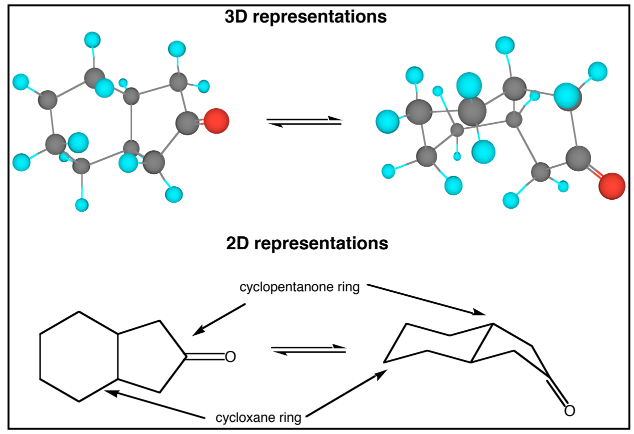

Figure 2. The bottom pathway indicates the diagrams typically used to represent the three-dimensional relationships in the top pathway.

Mike: Can you re-render this molecule as a chair?

Carrie: Uh...I'm so much more used to doing the chair as just the cyclohexane. I don't know how I would go about adding this whole thing to it. *Points to the cyclopentanone*. How would I do that...Well, this is just the old cyclohexane chair. *She draws out the cyclohexane chair*. Now I don't know if this bond-*points to one of the cyclohexane bonds she has drawn*-is supposed to represent this-*points to bridging bond between the rings*.

M: You can put it wherever you like. *She erases the cyclohexane and redraws it*. Why are you erasing?

C: It isn't pretty…How do I get the form of the pentane? I don't remember how you are supposed to draw the pentane.

M: Well, if you don't remember how to draw it, how would you figure it out?

C: Um...I'm trying to think of the molecular models.

M: The ones from class?

C: Yeah. I'm trying to see how it would be structured and I don't know if they go up and down all the time. *She stares at her hand while making alternating up and down gestures*.

Carrie's utterances and gestures suggest she was trying to make use of a visualization strategy to deduce the correct structure for the target representation. Her behavior also suggests that the diagram helped to scaffold the visualization strategy in specific ways. First, she noted that she was familiar with the accepted procedures for drawing a basic chair structure, which she inscribed. From this point, she attempted to imagine how the additional features of the novel molecule in the task would be added onto the base inscription. During this process, Carrie explicitly stated that she attempted to visualize her molecular modeling kit from class to perceive the spatial relationships within the given molecule. Her ostensible visualization behaviors included staring at the diagram, looking away from the diagram, and using gestures to indicate the alternating directions of each bond in the molecule.

All of the participants completed the majority of translation tasks in this manner. Each student would systematically study the given molecular diagram from different angles by rotating the task packet and then report (both through utterances and gestures) manipulating a mental image from different viewing angles. After the initial inspection, the student would then attempt to inscribe the representation that reflected their imagined molecular diagram. In effect, students' use of visualization for these translation tasks appeared critical for their success.

Students Use Diagrams to Duplicate Spatial Relationships

The primary problem solving behaviors that suggested students relied heavily on reasoning from diagrams on the majority of tasks were students' frequent duplication of given molecular diagrams and their attempts to match shapes between a given molecular diagram and a target molecular diagram. All students exhibited these behaviors on approximately 49% of the tasks in the entire corpus. The pattern matching strategy proved vital to students' problem solving strategies. Typically, students used a pattern matching strategy as the overall frame of reference for driving their solution strategies through means-ends analysis. Indeed, the strategy seemed requisite for many extended problems involving the generation of a synthesis or a reaction mechanism. Tasks that required the student only to predict a product were characterized by these strategies less frequently.

For the former tasks, the pattern matching strategy had the following character. First, the student would look at the given diagrams and the target molecular diagram(s) and then count the atoms represented in each of the diagrams to determine if additional reagents were necessary for the task. Following this, the student would state that the immediate goal was to decide how to change the given molecular diagram into the target molecular diagram by moving bonds or atoms. As participants generated each new diagram in their solution, they would compare that diagram to the target molecule and decide if the overall shape and structure of the last inscription brought them closer to or further away from the shape and structure of the target molecule. Progress continued as long as the shapes became more congruent; however, if they became more disparate the students either halted or generated a new strategy. Students rarely attended to the fact that the inscriptions generated by this strategy often violated spatial relationships predicated by accepted chemistry concepts.

The duplication strategy was of a different sort and reflected students' use of their previously inscribed diagrams to generate new diagrams in conjunction with matching the pattern of the target molecule. Students were inaccurate at depicting the correct structure or shape of a molecule when the shape of individual structures within the molecule had changed because of one or more steps in their strategy. Instead, the students were inclined to duplicate structures or shapes from a previous inscription into their new inscription without attending to requisite transformations in shape and structure. Students' duplication strategies were of two distinct, but highly related, kinds. First, students chose to duplicate the overall shape and internal structure of a molecule when making a new inscription that they would later change as their solution evolved. Second, students altered the overall shape or structure of a new inscription to which they then added the spatial features of previous inscriptions by directly duplicating them.

Figure 3 illustrates a sequence of molecular diagrams inscribed by David on one extended problem task. The task, *competing reactions*, asked the students to predict the five products that resulted from an internal rearrangement of atoms within a molecule. While problem solving, David generated a diagram that contained the correct intermediate structure that later rearranges (the molecular diagram on the left). He then indicated the bond movements that explain the rearrangement and inscribed the second molecular diagram from the left. Here, the duplication practice is evident. Despite the fact that David altered the internal spatial structure of one particular atom (indicated with the bolded, dashed circles) from a tetrahedral shape to a planar shape, he duplicated the tetrahedral spatial relationships in his new diagram and the two subsequent diagrams that serve as his final answer. David's duplication practice suggests that he did not attempt to visualize the molecular structures related to the problem, but instead copied the shapes and structures from one inscription to the next. This practice is further supported by the fact that both of David's chosen answers (the two diagrams furthest to the right) are identical to one another, but rotated in different directions, which he did not realize.

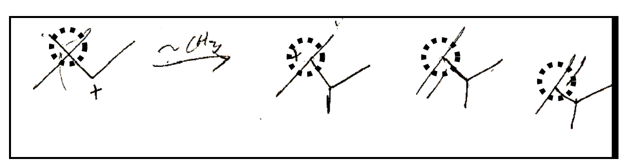

Figure 3. David maintained the original structure, despite performing several operations that mandate changes in internal spatial relationships of the circled atom.

Figure 4 illustrates how Cassie duplicated the internal spatial relationships of one atom from a previous inscription into a new diagram after first altering the overall shape of the molecule in question. When asked to determine the product for the *acid-catalyzed cyclization* task, Cassie was one of the few students to realize that a cyclization would occur in the molecule. In her first inscription at the top of Figure 3, she indicated the reactive sites that would result in the alternative five- and seven-member rings that she believed were possible given the conditions of the reaction. She then proceeded to discuss the conceptual underpinnings of the problem and likelihood that the reaction would occur at one site or the other. Ultimately, she determined both products were likely.

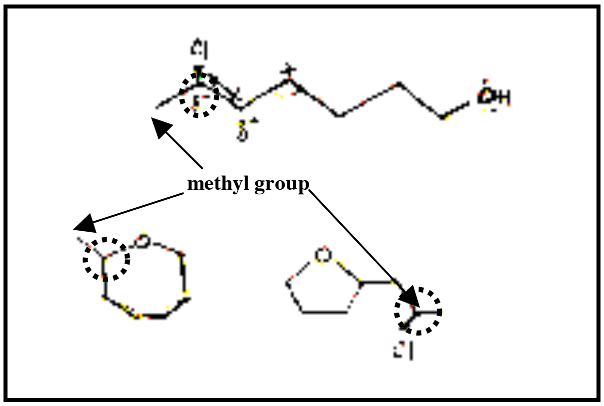

Figure 4. Cassie duplicated the internal spatial relationships of the circled atom from her first inscription into subsequent inscriptions. Cl=chlorine, O=oxygen, H=hydrogen.

The bolded, dashed circles in Figure 4 indicate Cassie's duplication of stereochemistry, or intramolecular spatial relationships. When inscribing the seven-member ring on the bottom-left, Cassie first drew the ring, then pointed to the initial diagram and noted that the methyl group (indicated in each diagram with an arrow) would be one atom away, which she duplicated in the six-member ring as her answer. Although Cassie indicated that her choice of a solution strategy would result in an inversion of the spatial relationships between atoms attached to the methyl group, she did not indicate this in her answer; she simply drew a line to indicate the methyl group. The process was similar for the second structure. After first drawing the five-member structure on the bottom right, she then added the additional bonds that connect the methyl group. Although her final structure is correct, she did not appear to engage in a visualization strategy to determine whether the spatial relationships were altered. She simply counted that the chlorine was two atoms away from the ring and then duplicated the stereochemistry from the original structure.

Both of these examples from Cassie and David suggest that students neither attend to the spatial information embedded in molecular representations nor do they rely on visualization during extended problem solving. Instead, the students appear to duplicate spatial relationships from earlier inscriptions. At this point, it is unclear precisely why they chose this strategy. One possible explanation is that they chose not to attend to spatial relationships because they instead were occupied with the chemical principles necessary to explain the formation of a product or a reaction mechanism. This explanation is in accordance with those reported in physics problem solving that have suggested conceptual reasoning and visualization occur serially during extended problem solving (Qin & Simon, 1992).

Summary

The results of the analysis provide evidence for a task-specific use of visualization in chemistry that is highly dependent on inscription practices. Students were predisposed to visualize three-dimensional mental images of molecular structures when they needed to translate or re-render a given molecular representation. On 81.5% of these tasks, students explicitly stated that they were attempting to visualize a molecular structure or gesture in such a way that indicated they were doing so. Conversely, students did not engage in visualization strategies on extended problem solving tasks that did not require representation translation. On fewer than 9% of such tasks did students engage in behaviors that suggested the use of visualization as a problem solving strategy. Instead, the students relied on their inscriptions to preserve spatial information during problem solving.

Not only did students eschew visualization strategies on the majority of tasks in the interviews, they rarely made reference to the spatial features of individual molecules. Indeed, when asked to analyze the important features of particular molecular structures, the students noted spatial features on less than 18% of the tasks. Moreover, the students themselves commented on the limited applicability of spatial information. Thus, visualization appears to be the preferred problem-solving strategy used by students primarily when translating one molecular representation into another, but not a mandatory strategy for interpreting and manipulating molecular diagrams during problem solving.

Instead, students appear to employ specific heuristics of manipulating molecular representations when solving extended problems that are typical of organic chemistry assessments. On the majority of such tasks, study participants tended to engage in specific practices of diagrammatic reasoning that precluded visualization. First, the students engaged in processes of pattern matching in which they identified structural relationships between target molecules and given molecules, which drove their problem solving through a means-end analysis. Second, they used duplication processes with which they copied overall shapes, structures, and internal spatial relationships from one diagram to another. In doing so, the students did not display any behaviors that pointed to visualization strategies. Indeed, the students seemed wholly dependent on their inscriptions as they progressed through a solution: Any errors that they inadvertently made when generating an inscription completely hindered their progress. This practice occurred even when the students were completely correct with regard to the underlying concepts of a task. Surprisingly, students were more likely to distort accepted chemistry concepts to agree with a faulty diagram than they were to search for and correct diagram errors. Each of these practices suggests that the students relied more on the direct perception of given or generated inscriptions than they did on visualized mental images of three-dimensional structure for solving genuine tasks in organic chemistry.

Acknowledgements

This work was supported, in part, by a Spencer Foundation Dissertation Fellowship and a Northwestern University Dissertation Year Fellowship. I would like to acknowledge the insight and criticism on this work by Bruce Sherin, David Uttal, Brian Reiser, and Richard Silverman.

References

American Association for the Advancement of Science. 1990. *Science For All Americans*. New York: Oxford University Press.

Chi, M. T. H. 1997. Quantifying Qualitative Analysis Of Verbal Data: A Practical Guide. *Journal of the Learning Sciences* 6(3): 271-315.

Ege, S. N. 1999. *Organic Chemistry: Structure and Reactivity* (4th ed.). Boston: Houghton Mifflin.

Ericcson, K. A.; and Simon, H. A. 1980. Verbal Reports As Data. *Psychological Review* 87: 215-251.

Habraken, C. L. 1996. Perceptions Of Chemistry: Why Is The Common Perception Of Chemistry, The Most Visual Of Sciences, So Distorted? *Journal of Science Education and Technology* 5(3): 193-201.

Hegarty, M. 1992. Mental Animation: Inferring Motion From Static Diagrams Of Mechanical Systems. *Journal of Experimental Psychology: Learning, Memory & Cognition* 18(5): 1084-1102.

Johnstone, A. H. 1993. The Development Of Chemistry Teaching. *Journal of Chemical Education* 70(9): 701-705.

Keig, P. F.; and Rubba, P. A. 1993. Translation of Representations of the Structure of Matter and Its Relationship to Reasoning, Gender, Spatial Reasoning, and Specific Prior Knowledge. *Journal of Research in Science Teaching* 30(8): 883-903.

Kozma, R.; Chin, E.; Russell, J.; and Marx, N. 2000. The Role Of Representations And Tools In The Chemistry Laboratory And Their Implications For Chemistry Learning. *Journal of the Learning Sciences* 9(2): 105-143.

Larkin, J. H.; and Simon, H. A. 1987. Why A Diagram Is (Sometimes) Worth Ten Thousand Words. *Cognitive Science* 11: 65-99.

Narayanan, N. H.; Suwa, M.; and Motoda, H. 1995. Behavior Hypothesis From Schematic Diagrams. In *Diagrammatic Reasoning: Cognitive and Computational Perspectives*, J. Glasgow, N. H. Narayanan, and B. Chandrasekaran, eds., 501-534. Menlo Park, CA: The AAAI Press.

Oxman, R. 1997. Design By Re-Representation: A Model Of Visual Reasoning In Design. *Design Studies* 18:329-347.

Olivier, P. 2001. Diagrammatic Reasoning: An Artificial Intelligence Perspective. In *Thinking with Diagrams*, A. Blackwell, ed., 63-78. Dordrecht: Kluwer.

Qin, Y.; and Simon, H. A. 1992. Imagery As Process Representation In Problem Solving. *Proceedings of the Annual Conference of the Cognitive Science Society* 14: 1050-1055.

Taagepera, M.; and Noori, S. 2000. Mapping Students' Thinking Patterns In Learning Organic Chemistry By The Use Of Knowledge Space Theory. *Journal of Chemical Education* 77(9): 1224-1229.

Wu, H.-k.; Krajcik, J. S.; and Soloway, E. 2001. Promoting Conceptual Understanding Of Chemical Representations: Students' Use Of A Visualization Tool In The Classroom. *Journal of Research in Science Teaching* 38: 821-842.