Michael Ford and Maria Varelas, Section Coeditors

When Is a Molecule Three Dimensional? A Task-Specific Role for Imagistic Reasoning in Advanced Chemistry

MIKE STIEFF
Department of Chemistry, Learning Sciences Research Institute, University of Illinois, Chicago, Chicago, IL 60607, USA

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ABSTRACT: Imagistic reasoning appears to be a critical strategy for learning and problem solving in the sciences, particularly chemistry; however, little is known about how students use imagistic reasoning on genuine assessment tasks in chemistry. The present study employed a think-aloud protocol to explore when and how students use imagistic reasoning for problem solving in organic chemistry. The analysis suggests that students employ imagistic reasoning preferentially for translating between various molecular representations. On more complex tasks typical of classroom assessments, the students' problem solving appears mostly dependent on the accuracy of self-generated inscriptions rather than the use of imagistic reasoning. The results indicate a variable interplay between imagistic reasoning and diagrammatic reasoning that suggests several pedagogical implications for teaching college chemistry. © 2010 Wiley Periodicals, Inc. *Sci Ed* **95:**310–336, 2011

Correspondence to: Mike Stieff; e-mail: mstieff@uic.edu
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INTRODUCTION

Spatial thinking is a fundamental component of learning and problem solving in science that involves a diverse set of cognitive skills that include imagistic reasoning, mental rotation, spatial perspective taking, and spatial visualization. Each of these skills specifically involves reasoning about spatial characteristics of scientific phenomena (e.g., magnitude, distance, and transformation over time) while problem solving. Among these cognitive skills, *imagistic reasoning* refers specifically to the process of generating and manipulating perceived analog image-like mental representations for thinking and problem solving (Hegarty, 2004a; West, 1991). For example, a biochemist may approach the design of a drug by imagining how well a molecule would fit into the active site of a specific protein. Across scientific domains (Clement, 2008; Kali & Orion, 1996; Kozhevnikov, Hegarty, & Mayer, 2002), analyses of problem solving with practicing scientists and students at all levels suggest that imagistic reasoning in particular is used to both understand problems and evaluate alternative solutions.

In the classroom, the role of imagistic reasoning is generally taken to be self-evident: The very nature of science suggests that imagistic reasoning is fundamental for student learning and problem solving. For example, imagistic reasoning may help students to consider the interactions between continental plates in geology, the organization of organelles within a cell in biology, and the structure of molecules in chemistry. Imagistic reasoning has been shown to play an important role in learning and practicing physics (Kozhevnikov et al., 2002), chemistry (Bodner & Guay, 1997), medicine (Keehner et al., 2004), and earth science (Kali & Orion, 1996). Indeed, such findings imply that supporting students' imagistic reasoning (as well as other forms of spatial thinking) in the classroom may be key to improving science learning for future generations (Gilbert, 2005; National Research Council, 2006).

Interestingly, laboratory and field studies have revealed that many problem solvers do not use imagistic reasoning in isolation during scientific problem solving. Rather, many individuals employ imagistic reasoning in tandem with alternative problem-solving strategies. Specifically in science and engineering, problem solvers frequently employ strategies that involve analytical reasoning from diagrams (e.g., Cooper, 1988; Schwartz & Black, 1996; Stieff, 2007). In this sense, *diagrammatic reasoning* refers specifically to the application of heuristics or algorithms to domain-specific diagrams to deduce complex spatial transformations without invoking mental images (Stieff, Hegarty, & Dixon, 2010). For example, a physicist might determine the direction of torque on the fulcrum of seesaw by assigning positive values to one direction and negative values to the opposite direction and calculating the cross product. Such work in physics and other domains has revealed a variety of strategies used by scientists and students that suggests spatial problem solving in science is often a hybrid reasoning process in which problem solvers choose among more diagrammatic and more imagistic solution strategies or use analog imagery in conjunction with algorithmic and heuristic reasoning processes (Hegarty, 2004b).

In chemistry, imagistic reasoning has been underscored as a fundamental cognitive activity, particularly at advanced study, that is overlooked by the teaching and learning research communities (Habraken, 1996). Such a role for imagistic reasoning seems obvious, as a central topic in chemistry concerns the relationship between three-dimensional spatial features of molecules and their chemical and physical properties. Indeed, historical reports from pioneers in chemistry, such as Kekulé, Watson, and Crick, indicate that spatial thinking is often the key strategy that leads to important discoveries about molecular structure (Rothenberg, 1995; Watson, 1968). Similarly, diagrammatic reasoning is central to the discipline. From early instruction, students must learn to use a wide range of chemical representations to represent the structure, composition, and spatial transformations of molecular objects. Students are exposed to increasing numbers of diagrams as they progress through chemistry instruction to illustrate molecules in both two and three dimensions and to depict structures from alternative perspectives or degrees of abstraction. Moreover, a major component of chemistry instruction centers on the use of analytical strategies for manipulating chemical representations without reference to internal mediating spatial representations (Stieff, 2004, 2007; Stieff & Raje, 2010). Without relying upon imagistic reasoning, these strategies allow experts (and presumably students) to preserve and transform the spatial information embedded in molecular diagrams using formal rules as they progress toward a solution.

Clearly, imagistic reasoning and diagrammatic reasoning are important for learning chemistry and nowhere is their interactive role more apparent than in the subdomain of organic chemistry. In this domain, taught at the college level, students are asked to reason about the spatial characteristics of molecular diagrams to determine molecular structure, functionality, and reactivity. Indeed, textbooks and teaching materials encourage students to "imagine molecules from different perspectives" or "see" the three-dimensional structure embedded in diagrams (Ege, 2003). It is in organic chemistry that researchers have invested the largest amount of time and effort to determine how a student's aptitude for imagistic reasoning predicts success on classroom assessments. A host of studies (Barnea & Dori, 1999; Brownlow, McPheron, & Acks, 2003; Keig & Rubba, 1993; Pribyl & Bodner, 1987; Small & Morton, 1983) have attempted to correlate standardized measures of spatial ability with classroom chemistry achievement to offer a variety of predictive models that explain the role of imagistic reasoning for problem solving about organic chemistry topics.

The independent and cooperative use of diagrammatic and imagistic reasoning by organic chemistry experts has been seen across a range of tasks found in typical organic chemistry curricula. Most recently, Stieff and Raje (2010) documented how expert chemistry instructors employ unique diagrammatic strategies to solve problems regarding stereochemistry, synthetic pathways, and reaction mechanisms without employing imagistic reasoning. In that study, experts were seen to rely heavily on imagistic reasoning only for completing tasks that involved translating molecular diagrams into new representations. Experts were also observed to employ imagistic reasoning and apply algorithms to diagrams in tandem to understand a problem or to evaluate the quality of a proposed molecular structure as they worked toward a solution. Among the diagrammatic strategies Stieff and Raje identified, experts applied several algorithms upon diagrams to make spatial information explicit as well as to predict the outcome of spatial transformations. Notably, experts were seen to frequently make use of diagram templates that illustrated a basic set of spatial features common to many molecular structures, such as bond connectivity or bond angles, which they then amended without invoking mental imagery. For example, as seen in Figure 1, experts were seen to systematically alter bonds in a given structure to generate families of molecules that contained structures with similar composition, but unique spatial relationships.

Although the experts in that study advocated for the use of alternative strategies by students, it is unknown whether students learn to employ similar algorithms or rely on imagistic reasoning strategies seen among experts. Although experts may employ such algorithms in tandem with or alternative to imagistic reasoning on some tasks, they are not necessarily the easier or preferred strategy for students (Stieff, 2007), and students often fail to correctly apprehend their use (Taagepera & Noori, 2000). In an experimental analysis of mental rotation for solving stereochemistry problems, Stieff (2007) illustrated how undergraduate organic chemistry students relied on both imagistic reasoning and domain algorithms to solve canonical assessment items traditionally presumed to require imagistic reasoning. In that study, students were observed to perform equally well regardless of

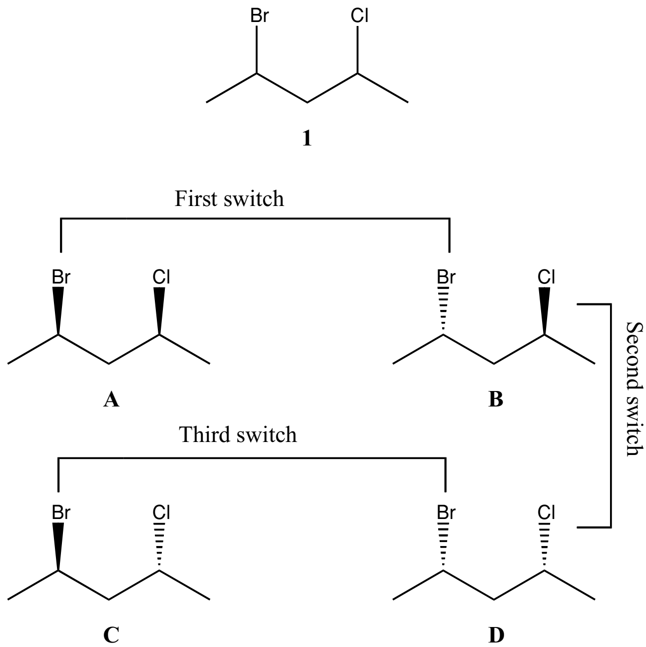


Figure 1. Experts generate families of molecules that have unique spatial structures by systematically drawing new bonds to indicate that relative spatial relationships between atoms. In the figure, dashes represent bonds projected below the plane of the page and dark wedges represent bonds projected above the plane of the page.

strategy used; however, a significant number of students were seen to rely exclusively on imagistic reasoning alone to solve the tasks despite exposure in the classroom to algorithms for determining spatial symmetry and comparing structures. Moreover, although some students in the experiment responded rapidly to direct instruction to use the taught algorithms and abandoned the imagistic strategy, others persisted in invoking and inspecting mental images despite the intervention.

There is no doubt that imagistic reasoning plays an important role in organic chemistry and that experts employ imagistic reasoning in tandem with analytical manipulation of diagrams while problem solving; however, it is unknown whether students use imagistic reasoning or diagrammatic strategies in ways similar to experts in the discipline. Although several studies have shown a moderate correlation between students' aptitude for imagistic reasoning and chemistry achievement, such studies offer little in the way of characterizing students' use of such strategies on genuine tasks. Whereas extensive analysis of problem solving in physics (Hegarty, 1992), engineering (Schwartz & Black, 1996), and geology (Kastens & Liben, 2007) has offered data to define a precise role for imagistic reasoning in each of these domains, such data remain outstanding for chemistry. Building on these previous efforts, this paper attempts to describe when and how students use imagistic reasoning in organic chemistry using in-depth analysis of student utterances and gestures during problem solving on assessment tasks. To this end, the present study asks the question, when do students employ imagistic reasoning for successful problem solving in organic chemistry?

DESIGN OF THE PRESENT STUDY

The study employed think-aloud, problem-solving interviews to identify when and how students use imagistic reasoning and algorithms in organic chemistry. The design utilized methods similar to studies in physics education that have explored students' conceptions and inscription practices. For example, Sherin (2001) used fine-grained analyses of student problem solving to deduce that students do not memorize and replicate physics equations and diagrams but instead generate them in the moment to reflect their understanding of the task, scientific principles, and intuitions. This method relies upon verbal reports, physical behaviors, and inscriptions to examine students' conceptions of phenomena and representations (cf. Ericcson & Simon, 1980; Siegler & Crowley, 1991). Such an approach is especially useful to an investigation of problem solving in chemistry: Analysis of think-aloud protocols can provide a more accurate glimpse of when, how, and why students apply alternative strategies.

Participants

Students who participated in the clinical interviews were solicited from the population of students enrolled in a two-semester organic chemistry course at a medium-sized research university in the United States. From the 31 students who volunteered to participate in the study, 14 students were randomly selected to complete the clinical interviews based on midterm progress reported by the instructor: seven of the participants were receiving a grade of B or higher in the course, and seven of the participants were receiving a grade of C or lower in the course. One participant withdrew from the study due to discomfort with the protocol and one participant failed to talk aloud during data collection activities; thus, 12 participants (3 male, 9 female) completed the study protocol. Each of these 12 participants completed one 30-minute interview (Interview 1) at the end of the first term of instruction and a second 60-minute interview (Interview 2) during the middle of the second term of instruction. Five of these participants were enrolled in a course designed for chemistry majors that had 25 enrolled students. The other seven students were enrolled in a survey course that had 114 enrolled students. The participating chemistry department had standardized its curriculum so each class progressed on approximately the same timeline. Instructors in each course used lecture-based methods that centered on extensive problem-solving examples and each regularly assigned problem-solving tasks outside of class.

Interview Design

Each interview employed concurrent verbal protocols to examine student problem solving. During each interview, students received a stapled packet of tasks and were instructed to complete each task in order and talk aloud while problem solving. Prior to beginning the first task, the students were asked to discuss how they solved an example problem from a recently completed in-class examination to practice speaking aloud. A camera was positioned to record students' inscriptions and gestures for later analysis. Students sat facing away from the interviewer, who remained behind the camera to observe and record their work. During each interview, the interviewer continuously prompted participants to talk aloud and asked clarifying questions as each problem was completed. Each participant received U.S. $40.

Interview Tasks

Eighteen interview tasks were constructed by the author in collaboration with the instructor of the major's course. Each task was a modified item from an in-class examination used by one or both course instructors. Item modification consisted of replacing the given molecule with a novel structure that was not presented on the examination. Each course

TABLE 1
Interview Tasks

Task Category	Task	Description
Analyze	1–5: *Analyze Structure (five examples)*[a]	Describe the important features of the given molecular representation
	6: *Reaction Feasibility*[b]	Discuss the feasibility of the ring opening of a pyrrazole compound
Translate	7: *Construct Newman*[a]	Re-represent the given Fischer projection (majors) or Chair (survey) as a Newman projection
	8: *Structural to Chair*[b]	Re-render the given structural diagram as a chair representation
	9:*Stereoisomers*[b]	Generate all four stereoisomers of the given structural diagram using Fischer projections
Extended problem	10: *Competing Reactions*[a]	Predict the product of the given $E1/S_N1$ reaction
	11: *Esterification*[a]	Predict the product of the given addition-elimination
	12: *Fused Rearrangement*[a]	Provide a mechanism that accounts for the given double ring expansion
	13: *Acid-catalyzed Cyclization*[b]	Generate the product of a cyclization
	14: *Monobromination*[b]	Generate all monobromination products of the reaction of $Br_2/h\nu$/2-methylpropane
	15: *Retrosynthesis*	Devise a synthesis for the given substituted α,β unsaturated ketone
	16: *Ring Expansion*[b]	Generate a mechanism that accounts for the given ring expansion
	17: *Styrene Dimer*[b]	Devise a synthesis for the given styrene dimer and the given reagents
	18: *$KMnO_4$ Oxidation*[b]	Deduce the starting material used in the given oxidation reactions

[a]Interview 1. [b]Interview 2.

instructor reviewed the tasks to ensure they were appropriate for students' chemistry ability and representative of in-class assessments. The 18 tasks from both interviews were grouped into three general categories. Tasks 1–6 (33% of interview tasks) asked students to *analyze* the reactivity, structure, functionality, or name of a molecule. Tasks 7–9 (17% of interview tasks) asked the students to *translate* a molecular diagram from one representation into another. Tasks 10–18 (50% of interview tasks) were *extended problems* that required students to generate a reaction mechanism, deduce the product of a chemical reaction, or propose a molecular synthesis.

Analysis of the 469 assessment items administered in each participating course indicated that the relative proportion of task types included in the interviews reflected the frequency of task occurrences on in-class examinations (25% analyze, 12% translate, 63% extended problem). A brief description of each task is given in Table 1, and the specific details of relevant tasks are discussed as they occur in illustrative cases below. Two of the tasks, as indicated in Table 1, administered in Interview 1 differed between majors and survey students due to minor differences in course progress at the time of the interview.

Analytical Techniques

The transcribed interviews were analyzed for verbal utterances using techniques described by Chi (1997) and Ericcson and Simon (1980) and for gestural behaviors using techniques described by Trafton, Trickett, and Mintz (2005). A constant-comparative methodology (Strauss & Corbin, 1994) was used to apply the coding scheme established for capturing chemistry problem-solving strategies reported previously by Stieff and Raje (2010). The analysis included two phases: generation of the data corpus and application of the framework to the data corpus.

Generation of the Data Corpus. The tapes were transcribed verbatim with annotation of all participant inscriptions and gestures, as detailed below. The transcripts for each task were analyzed as individual episodes of problem solving, and the video and worksheet inscriptions for all tasks constituted the data corpus. In total, the 24 clinical interviews (12 Interview 1, 12 Interview 2) included 18 hours of video and 216 student worksheets. Tasks 1–12 were presented in Interview 1 and Tasks 13–18 were presented in Interview 2. Each participant attempted all 18 tasks, but not all participants generated a solution for every task. Participants did not generate final solutions for two reasons: First, some participants abandoned a task out of frustration; second, the interviewer asked participants to abandon a task when they had worked without generating a solution for more than 10 minutes. This occurred on 11 tasks. In all cases, students were seen to apply a primary strategy regardless of success. Excluding tasks that were abandoned, a total of 205 completed tasks comprised the data corpus. Seventy-one of these tasks were *analyze tasks*, 28 were *translation tasks*, and 106 were *extended problem tasks*.

Application of the Framework to the Data Corpus. Using Stieff and Raje's (2010) analytical framework, each interview task was examined and coded according to verbal utterances, gestural behaviors, and inscriptions. Gestures were coded according to analytical frameworks employed Trafton and colleagues (Trafton et al., 2005, 2006): Three types of gestures (deictic, iconic, and noniconic) were identified in the videos. Deictic gestures included pointing to the worksheet or diagrams. Iconic gestures included hand gestures that involved grasping and rotating imagined objects over the workspace as well as body movements that reoriented the students' viewing angle to look at diagrams from different perspectives. Finally, personal gestures, such as scratching, and communicative gestures, such as a "thumbs-up" motion, were coded as noniconic gestures. Gestures were analyzed in two stages. First, each videotape was reviewed with the sound turned off and noting each gesture occurrence. Next, each videotape was reviewed again with the sound turned on, and each gesture was coded as deictic, iconic, or noniconic.

Following gestural coding, transcripts were then reviewed to code participants' concurrent verbal utterances as spatial-imagistic or algorithmic-diagrammatic. Verbal references to perceiving and inspecting mental images of molecules as well as dynamic spatial transformations during problem solving were coded as spatial-imagistic. These utterances were specific and included with such comments, such as "I'm imagining molecules" or "I'm trying to see it from the back." Verbal references to domain heuristics, using features of diagrams to predict solutions, or algorithms were coded as algorithmic-diagrammatic. Again, such utterances were direct (e.g., "You get the enantiomer if you just reverse these two groups.").

Participant artifacts were further analyzed for evidence that the student was engaged in imagistic reasoning while problem solving. Inscriptions of imagined spatial transformations or alternative viewing angles were coded as spatial-imagistic. Such inscriptions were varied. Participants used sketches of eyes or a face to indicate they were imagining a unique viewing angle or vector arrows to indicate rotational motion or spatial interactions between molecules. All other inscriptions were coded as nonimagistic. Such inscriptions ranged from the addition of numbering systems to compare the location of atoms in different inscriptions and basic template diagrams of generic structures related to the problem.

Finally, a participant's strategy type for a task was determined by establishing consistency between utterance, gesture, and inscription codes. Problem-solving episodes that contained an imagistic utterance code *and* either an iconic gesture or spatial-imagistic inscriptions were categorized as solved via a spatial-imagistic strategy (i.e., imagistic reasoning). Episodes that included algorithmic-diagrammatic utterances *and* either deictic gestures or nonspatial inscriptions were categorized as solved via an algorithmic-diagrammatic strategy. Episodes that were coded with both spatial-imagistic and algorithmic-diagrammatic codes were categorized as solved via a complex-mixed strategy. As in Stieff and Raje (2010), at least two of the three coded behaviors were observed on every task. An independent researcher reviewed and categorized a subset of 20 randomly selected tasks (~10% of tasks) from the data corpus. The two researchers' strategy categories for these tasks were identical.

TASK-SPECIFIC USE OF IMAGISTIC REASONING AND DIAGRAMMATIC REASONING FOR PROBLEM SOLVING

Application of the analytical framework revealed that students applied a range of strategies to solve tasks in the data corpus. Generally, students infrequently engaged in overt behaviors that indicated they used imagistic reasoning across tasks. Indeed, students rarely attended to the spatial information embedded in a given molecular diagram regardless of the nature of the task. Notably, students' behavior did suggest a preference for imagistic reasoning when tasks required a translation between molecular representations. On the majority of interview tasks, the participants did not translate between molecular diagrams, but instead engaged in lengthy problem-solving episodes on extended problem tasks. On such tasks, the students exhibited behaviors that suggested they engaged in the systematic generation and manipulation of molecular diagrams using specific algorithms that did not necessitate imagistic reasoning. Here, the relative frequency of strategy use across tasks and students are discussed, and five cases of unique strategies are illustrated. Although achievement is not a focus of the present analysis, students correctly solved 67% of the tasks.

Frequency of Student Problem-Solving Strategies

Descriptive statistics for the data corpus indicate that the use of imagistic reasoning was highly dependent on the demands of a task. By parsing the data corpus into the three categories of tasks enumerated above, the selectivity of students' use of imagistic reasoning was immediately apparent. Participants' reported the use of algorithmic-diagrammatic strategies on a majority of *analyze* and *extended problem* tasks. On *translate* tasks, however, a large number of behaviors indicated participants attempted to employ imagistic reasoning to generate solutions.

TABLE 2
Percentage of Strategies Categorized as Algorithmic-Diagrammatic, Spatial-Imagistic, and Complex-Mixed for Each Task and Task Type

Task Type	Task No.	Algorithmic-Diagrammatic (%)	Spatial-Imagistic (%)	Complex-Mixed (%)
Analyze	1	100	0	0
	2	100	0	0
	3	100	0	0
	4	92	8	0
	5	100	0	0
	6	100	0	0
Translate	7	0	66	34
	8	14	86	0
	9	58	0	42
Extended	10	100	0	0
	11	100	0	0
	12	84	8	8
	13	100	0	0
	14	92	0	8
	15	100	0	0
	16	100	0	0
	17	100	0	0
	18	100	0	0

The details of the descriptive statistics highlight a task-dependent, interactive role for imagistic reasoning and diagrammatic reasoning in organic chemistry. The relative frequency of reported strategies is illustrated in Table 2 for each task and task type. On analyze tasks, which asked students to describe the relevant physical and chemical properties of a given molecule, participants were less likely to employ imagistic reasoning. Only one instance of an analyze task was categorized as solved via a spatial-imagistic strategy. Similarly, only three instances of extended problems tasks were categorized as solved via spatial-imagistic or complex-mixed strategies. Frequently, these behaviors included a student gesturing an imagined manipulation of a molecule and specifically mentioning an attempt to visualize the construction and transformation of a molecular model. A dramatic increase in the frequency of utterances and gestures pertaining to imagistic reasoning occurred on translate tasks. Forty percent of these tasks (11 instances) were categorized as solved via a spatial-imagistic strategy, and 29% (8 instances) were categorized as solved via a complex-mixed strategy.

Interestingly, all students reported great difficulty on *translate* tasks and many mentioned that they would be able to perform better if they had molecular-modeling kits available. Participants failed to complete 8 (29%) of the 28 *translate* tasks presented with statements reflecting an unwillingness to attempt problems of such type. When solving such tasks, frequent comments from students referenced the use of imagistic reasoning. For example, students stated, "Drawing helps me visualize it" and "I'm trying to think of molecular models," Five of the students explicitly stated that they had trouble solving the *translate* tasks because they lacked the necessary "spatial skills." Large individual differences in strategy preference were evident in the data set as well. As illustrated in Table 3, the majority of strategies identified in the data corpus were algorithmic-diagrammatic; however, students

TABLE 3
Frequency of Strategies Categories Identified in the Data Corpus by Participant

Student	Algorithmic-diagrammatic	Spatial-imagistic	Complex-mixed
M1	94% (15)	6% (1)	0 (0)
M2	94% (16)	0 (0)	6% (1)
M3	88% (15)	0 (0)	12% (2)
M4	82% (14)	12% (2)	6% (1)
M5	93% (14)	0 (0)	7% (1)
S1	83% (15)	11% (2)	6% (1)
S2	94% (17)	6% (1)	0 (0)
S3	83% (15)	11% (2)	6% (1)
S4	83% (15)	11% (2)	6% (1)
S5	94% (15)	6% (1)	0 (0)
S6	77% (10)	8% (1)	15% (2)
S7	83% (15)	11% (2)	6% (1)

Note: M1–M5 indicate students majors; S1–S7 indicate survey students. Observed frequency indicated parenthetically.

varied in their use of spatial-imagistic and complex-mixed strategies. Three students were not seen to employ spatial-imagistic strategies in isolation to solve a task, yet all students were seen to employ algorithmic-diagrammatic strategies on the majority of tasks.

This result is consistent with that of Stieff and Raje (2010) who reported that expert chemistry instructors also relied on imagistic reasoning primarily to translate between molecular representations. Like experts, students appeared to use molecular diagrams to scaffold their interpretation and manipulation of spatial information embedded in the task, if they attended to that spatial information at all. Although it should be noted that the problem-solving tasks in the present study are not identical to those used by Stieff and Raje, some interesting differences in strategy use can be seen when the results of each study are compared. Namely, students engaged in imagistic reasoning much more often than experts did on translate tasks; however, students engaged in imagistic reasoning less frequently than experts across all tasks. The paucity of behaviors suggestive of imagistic reasoning and the frequent references to the molecular diagrams did not suggest that students avoided spatial thinking altogether during problem solving. Rather, it indicates that the study participants infrequently engaged in the generation and manipulation of mental images of molecular structures on tasks that did not require representation translations. On other tasks, however, students frequently engaged in spatial thinking by applying domain algorithms and heuristics to diagrams. In contrast to experts, students rarely engaged in complex-mixed strategies, which were observed among the majority of experts: Students in the present work tended to employ either a spatial-imagistic strategy or an analytic-diagrammatic strategy exclusively to problem solve.

Illustrative Cases of Student Problem-Solving Strategies in Organic Chemistry

The overall trends within the data corpus indicate that students employed imagistic reasoning strategies, independently or concurrently with diagrammatic reasoning strategies, on relatively few tasks. Specifically, the students appeared to use imagistic reasoning preferentially to translate between molecular representations. Two tasks from Interview 1 and one task from Interview 2 required a representational translation as the primary goal of the task. Although translations were unnecessary in the other tasks, some participants occasionally chose to translate the representations given on these tasks. The use of imagistic reasoning for the translation tasks is perhaps not surprising: Such tasks often require the student to perceive three-dimensional features of a molecule that are implicit in the given molecular representation. Consequently, the preferred strategy appeared to include visualization of these spatial relationships before inscribing them into the target representation.

Each participant appeared to visualize the molecular structures in translation tasks using one of two frames of reference commonly employed on spatial reasoning tasks (Bryant & Tversky, 1992; McNamara, 2003). First, participants sometimes used imagistic reasoning in a fairly basic sense using an exocentric frame of reference. That is, the student would look at a molecular diagram and explicitly state that they were attempting to visualize a mental image of the molecule with concurrent iconic gestures that represented the visualized molecule. Following this, the student appeared to inspect and manipulate the generated mental image to gain insight into the task and to formulate a solution. Second, other students approached the mental imaging of molecular structures from an egocentric reference frame. Here, students would study the given diagram from different perspectives by rotating the task packet or repositioning their bodies with respect to the diagram and stating that they were imagining the structure from another angle. For example, one student moved his head to the level of the workspace, looked at the diagram from an oblique angle and stated that he was "trying to see what it looks like."

Behaviors suggestive of imagistic reasoning occurred rarely on extended problem-solving and analyze tasks. When they did occur on extended problem tasks, students appeared to use imagistic reasoning for ad hoc representational translations. On analyze tasks, students appeared to use imagistic reasoning to distinguish three-dimensional connectivity implied by molecular representations that obscured such information. On the majority of these two types of tasks, however, it appeared that students did not employ spatial-imagistic strategies to problem solve. Instead, the students seemed to generate solutions by manipulating molecular diagrams in unique ways that allowed them to avoid consideration of the embedded spatial information. The students' strategies appeared to rely on the assumption that the formalisms of chemistry diagrams would preserve and predict any spatial transformations necessary for a solution; thus, they frequently ignored important spatial features of molecules in analyze and extended problem tasks.

Two common heuristics that maintained or manipulated spatial information represented by diagrams were observed on extended problems. First, some students made use of a heuristic that included duplication of the overall shape and structure of a molecule when making a new inscription that was then modified as the solution emerged. Second, some students applied a heuristic that involved altering the basic shape and structure of a given diagram to which they later added spatial information directly from previous diagrams. In addition to these two heuristics, a minority of students employed an innovative algorithm that involved translating between diagrams without imagistic reasoning that allowed them to complete translate tasks that the majority of students completed via imagistic reasoning. Below representative cases of one imagistic-reasoning strategy, the two diagramming heuristics, and the algorithm are discussed. One example of the concurrent use of imagistic reasoning with a heuristic is also illustrated. Although the focus of this study is to identify the use of imagistic reasoning for problem solving, the greater frequency of diagrammatic strategies used by the participants warrants detailing unique examples of such strategies as well. These latter cases are particularly interesting in that they illustrate how students

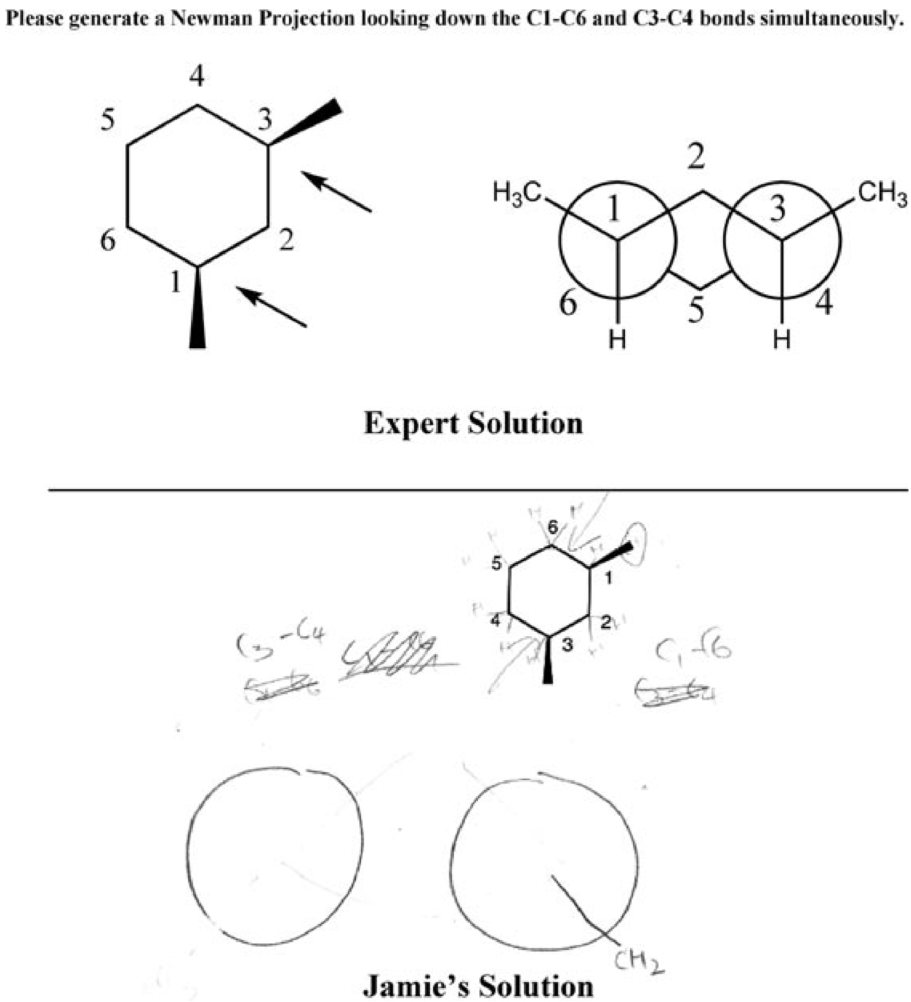


Figure 2. The Construct Newman task requires the rendering of two Newman projections, as in the expert solution (top). Jamie's inscriptions for the task are illustrated at the bottom.

can engage in spatial thinking without using imagistic reasoning. In each case, participant gestures and physical behaviors are indicated with italics and behaviors used as evidence of specific strategy use are indicated in bold when transcripts are presented.

Case 1: Mental Transformation of a Visualized Structure (Spatial-Imagistic). The first case presents an example of how some students employed imagistic reasoning to solve translation tasks. Using such strategies students would often report attempts to mentally visualize molecular models or two-dimensional diagrams to understand the task or to generate a solution. Statements such as, "I'm trying to visualize it" or "I'm imagining models" were common in these cases in tandem with grasping and rotating hand gestures. We observed this strategy 14 times in the data corpus. In the present case, Jamie attempts to solve the *Construct Newman* task translation using a mental rotation strategy from an exocentric frame of reference. Briefly, the task requires students to consider the internal spatial relationships within a cyclic structure and render the molecule using an orthographic projection (depicted in the upper right of Figure 2). To solve the problem, Jamie engaged in several behaviors that suggested she was viewing an imagined molecular structure that she mentally manipulated to problem solve.

Jamie immediately recognized that the task required her to produce a Newman projection with a simultaneous display of two carbon-carbon bonds in the given diagram. She begins by immediately drawing two circles (indicated in the bottom of Figure 2), one for each carbon-carbon bond, but then she stops abruptly. Next, she appears to generate and inspect a mental image of the chair structure to determine how to render the substituents on the ring from the correct perspective. She rotates the task packet so that the relevant face of the ring is toward her and then begins to grasp at an imagined molecular structure. As if she is holding the molecule, Jamie rotates her hands into alignment with the two circles she originally inscribed. At this point, she indicates she knows the solution and begins to inscribe all of the additional bonds in the Newman projection. Yet again, she pauses, before deciding that what she has drawn is incorrect, which leads her to erase all depicted bonds. She stares silently at the task for an extended period of time and rotates her left hand above the table intermittently. When asked whether she was visualizing molecular structures before she abandons the task, she states clearly that she is trying to remember the structure of her molecular models.

Jamie: She reads the question aloud then begins to draw two circles. She labels one circle C1-C6 and the other C3-C4, then stops drawing. Wait. **If I'm looking . . .** ***Jamie rotates the task packet 30 degrees counterclockwise, then places both hands above the table as if grasping the molecule and rotates her hands clockwise ~30 degrees.*** Uh . . . what would come in the middle? If it's C1 then I'm looking at it this way. ***She draws an arrow toward C3, then raises her right hand and flips it upside down***. Then that means . . . *She pauses a moment and draws in Hs around the given diagram.* ***She again raises both hands over the table, grasps and rotates them clockwise.*** So whatever is going out over here—*She taps the right side of her C1-C6 circle*—will have to just come over here and that's an H. *She draws an H on the left side of the circle.* No, then everything would be Hs. *She draws a CH_3 then a CH_2 and an H on the C1-C6 circle. She stops, then erases all of the bonds she has drawn . . .* ***She looks away from the diagram and rotates her left hand clockwise and counterclockwise intermittently without verbalizing for two minutes.*** *She draws an arrow toward the C1-C6 bond in the original diagram and then circles one of the dark wedges at the top of the task.* Hmmm . . . .

Interviewer: Are you trying to picture it in you head?

Jamie: **Yeah. I'm trying to remember the molecular model again**. I know that if I look at it from one side and then the other, behind it would come up . . . but I don't know how I would do that. *She pauses and then moves to another problem.*

The bold text in the above excerpt highlights Jamie's overt behaviors that indicate that she approached the task using an imagistic reasoning strategy. Her behavior on this task also suggests that the diagram helped to scaffold the visualization strategy in specific ways. She first rotated the given diagram so that she could view the diagram from a perspective directly down the bonds indicated in the task instructions. At this point in the interview, it becomes evident that Jamie engages in the visualization of a mental image of the molecular structure as she imagines rotating it into alignment with her partially constructed Newman projection. These behaviors persist with and without concurrent utterances as she struggles to determine the spatial relationships in the ring.

This strategy has been documented among experts (Stieff & Raje, 2010), and many of the students completed translation tasks in much the same manner. To do so, each student would systematically study the given molecular diagram from different angles by rotating the task packet, repositioning their bodies with respect to a diagram, or stating that they were manipulating a mental image. After the initial inspection, the student would then attempt to inscribe the representation that reflected the imagined molecular diagram. As seen in Table 2, some students used another strategy in tandem with imagistic reasoning on a few translation tasks. In most of these instances, the students attempted to generate the target representation by directly copying information from the given diagram to the target. Students were mostly unsuccessful when attempting to visualize a given structure because they failed to attend to some embedded three-dimensional feature that was hidden by the formalism of the given diagram. For example, tasks that ask students to generate Newman projections require depiction of spatial relationships from the terminal end of a molecule that are not explicitly represented in the dash–wedge formula given in the problem statement. Similarly, tasks that ask students to generate Fischer projections require the student to redraw the given dash–wedge formula as it would appear after rotating several bonds as well as two 90-degree rotations of the entire molecule depicted in the given diagram. Instead of attending to these requirements, students assumed each representation depicted spatial relationships in the same way, which led to erroneous diagrams. Regardless, spatial-imagistic strategies, such as Jamie's, were the primary strategies used by students on the translate tasks.

Case 2: Holistic Duplication of Spatial Information (Algorithmic-Diagrammatic). The first algorithmic-diagrammatic strategy observed in the interviews suggests that students often relied on heuristics to modify diagrams to preserve and predict spatial relationships on extended problem-solving tasks regardless of whether these relationships transformed. The general affordance of diagrams to preserve spatial relationships in this manner has been noted elsewhere (e.g., Larkin & Simon, 1987), but the present study revealed a unique instantiation of the affordance during genuine problem solving in organic chemistry. The "holistic duplication heuristic" was a strategy that involved the duplication of entire diagrams at each step in a solution. Using holistic duplication, a student would first inscribe a complete duplication of any diagram initially given in a task. Following the initial duplication, the student would then remove a particular part of the duplicated diagram and replace it with a new inscription that resulted from a decision about the reactivity of the depicted molecule. In turn, this new inscription was duplicated and again modified as the student progressed. This strategy was observed 28 times in the data corpus. Notably, this strategy was not reported among experts in Stieff and Raje (2010).

An examination of "David's" inscriptions for the *Competing Reactions* task in Interview 1 illustrates how students used the heuristic. The Competing Reactions task asked students to predict at least five molecular compounds produced by a chemical reaction in which the internal bonds of the starting compound rearrange spatially. The task is complex and requires consideration of two alternative reaction pathways that precede the internal three-dimensional rearrangement of bonds. The top scheme in Figure 3 illustrates an idealized expert solution, which highlights the intermediate products from the two pathways and the resultant products in the solution. Although additional products can be generated from the reaction, students were instructed to provide only five structures.

David's approach to the task exemplifies the use of the holistic duplication heuristic to construct a sequence of diagrams without attending to transformations of spatial

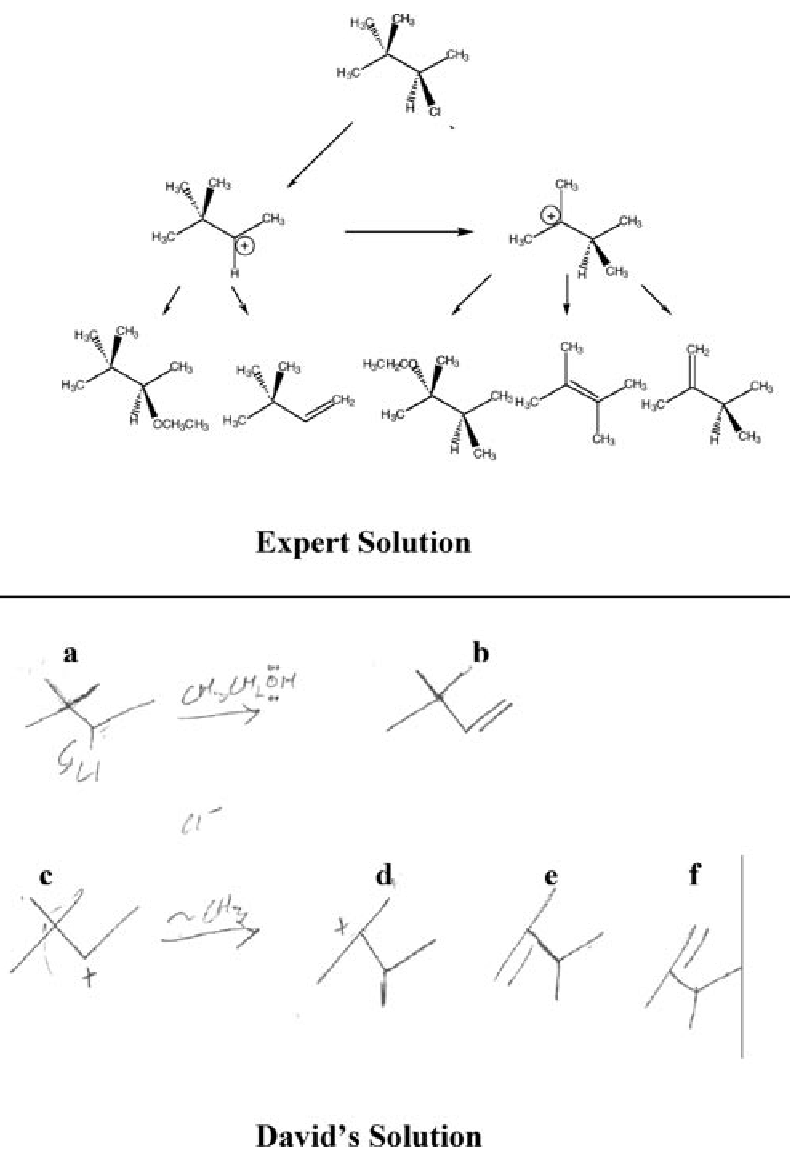


Figure 3. David's solution to the Competing Reactions task rendered below an idealized expert solution.

relationships. David's sequence of inscriptions is illustrated in the bottom of Figure 3. David produces diagram 3b by first duplicating his previous diagram (3a), removing the "Cl," and then adding a double bond to generate an answer. From this point, he reasons that his proposed answer can generate additional solutions; thus he duplicates structure 3b, removes one bond, and replaces it with the positive charge (+) to create 3c. He correctly deduces that to produce a solution, structure 3c would rearrange again, which he notes with the "$\sim CH_3$" symbol. For his solution, he ultimately generates two diagrams (3e, 3f). To do this, he again applies the duplication heuristic to create each structure. First, he duplicates 3c, then erases and rearranges the locations of a single bond and the positive charge to generate 3d. Next, he generates the precursors to 3e and 3f by duplicating 3d twice. Finally, he completes his solution by erasing the (+) in each diagram and adding the double bonds to give 3e and 3f.

David: *David draws the first structure (3a) in the top left of Figure 3.* ***He draws an arrow with ethanol on top of it and then an arrow to indicate that the Cl dissociates. He then duplicates 3a, erases the Cl group, and draws a double bond to leave 3b.*** Okay, there's an elimination product.

Interviewer: Okay.

David: I've got some more elimination products in there. ***He duplicates 3b underneath 3a.*** So . . . Well, we've got a plus charge there. ***He erases the double bond from the duplication and draws a + symbol to indicate a positive charge leaving 3c***. It has access to this—but that's carbon, carbon, carbon—*he identifies each of the groups to the left of the + by pointing at them*. So, it's not going to happen. Alright! Possibly, um . . . you need . . . . there's going to be a shift probably. Whether it is a hydrogen shift or a methyl group shift, I am not exactly sure. You've got a plus charge here. The problem is, if anything, it will probably be a methyl shift here, *He circles the carbon to the left of the +.*

Interviewer: Okay.

David: So, it will be a methyl shift here and we will be left with this. ***He draws a*** $\sim CH_3$ ***over and arrow to indicate the methyl shift and then duplicates 3c to the right of the arrow, he then erases one of the methyl groups and the + and then reverses their respective positions to leave 3d***. So then . . . ethanol is going to rip off a hydrogen from either here or here I think—*He points to the two methyl groups to the either side of the + in 3d*. And, let's see the possible products. ***He duplicates 3d twice to the right of the last structure. In the first duplication, he erases the + and draws a double bond toward the bottom to leave 3e. Then, in the second duplication, he erases the + and draws a double bond toward the top to leave 3f.*** There!

The use of the holistic duplication heuristic in this way allowed students to preserve spatial relationships between inscriptions without considering spatial transformations or spatial relationships between or within structures. For example, David's strategy (as well as the expert strategy) predicates an alteration of the spatial configuration of the bonds indicated with the dashed circles from three to two dimensions. By inscribing a holistic duplication at each step, David preserves the original shape in subsequent diagrams after (3a) and neglects these transformations. Contrast this with the diagrams indicated in the expert solution that highlight the transformation of spatial relationships with dash–wedge formulas. Like David, other participants repeatedly applied the heuristic to line–angle diagrams such as those in Figure 3 that did not highlight three-dimensional relationships. As a problem-solving heuristic, the holistic duplication practice used by organic chemistry students often led to correct solutions. However, the failure to attend to dynamic spatial relationships in many tasks often generated unexpected errors. For example, by duplicating each structure from (3d) and making post hoc modifications, David failed to realize that 3e and 3f are identical molecular structures that are merely rotated.

Case 3: Local Transformation of Spatial Relationships (Algorithmic-Diagrammatic). The second algorithmic-diagrammatic strategy involved the execution of a specific spatial transformation followed by the duplication of all other spatial relationships between

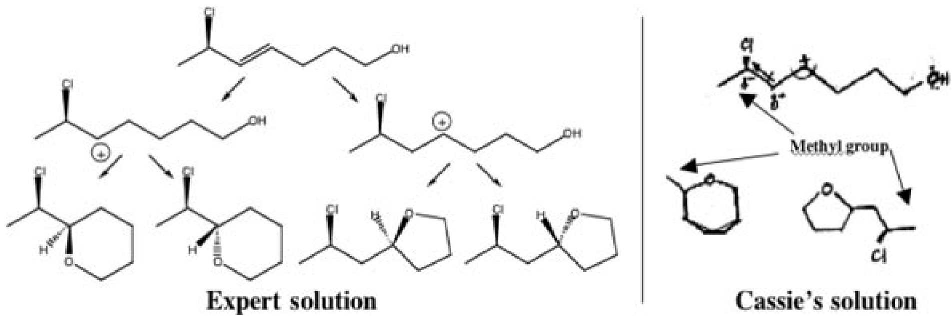


Figure 4. Cassie's solution to the Acid-catalyzed Cyclization compared to an idealized expert solution.

inscriptions. As opposed to the holistic duplication heuristic, students used the "local transformation heuristic" to first decide how the shape or structure of a portion of a given molecular diagram changed before generating a new inscription. Although the students attended to the spatial transformations in a local region of the diagram, they would duplicate all other spatial relationships outside of that region. In practice, students would often generate new diagrams by inscribing one diagram that reflected a unique spatial transformation to which they then added other spatial information from one or more previous diagrams. This strategy was observed 19 times in the data corpus. As with the previous strategy, Stieff and Raje (2010) did not report observing this strategy among experts.

Figure 4 illustrates how Cassie used the localized transformation heuristic on the *Acid-catalyzed Cyclization* task. Briefly, the task asked students to predict the possible product from the addition of a generic acid to a linear organic compound that contained both halogen and alkene (i.e., double-bond) functional groups. To solve the problem, students must consider the relatively likelihood that the reaction will produce one of two potential intramolecular cyclizations that result in pairs of either a five- or six-atom ring (illustrated in the expert solution of Figure 4). When asked to determine the outcome of the reaction, Cassie quickly realized that a cyclization would occur. In her first inscription (Figure 4, top-right), she correctly indicates the reaction could result in two structures with rings of different size. After discussing the conceptual underpinnings of the problem, Cassie determines that two products were equally likely, which she ultimately inscribes as her answer. Notably, Cassie generated a solution that included both a five- and a seven-atom ring; however, her final structures did not attend to the relevant spatial transformations that resulted from the proposed cyclizations.

Cassie: Acid, okay. Since there is acid that means there is going to be H . . . protons. *She draws hydrogen ions at the top of the page.* So, you would end up with. *She redraws the given diagram and underlines the OH.* Oh, this one is interesting!

Interviewer: Why?

Cassie: Because of the fact that there is the OH . . . because it also has a lone pair, which has the possibility of picking up a hydrogen. I think we are going to end up with a cyclic ring of some sort.

Interviewer: Why?

Cassie: Because, from what I can tell, this—*she points to the double bond*—is going to abstract a hydrogen, leaving a positive charge on one of these two. *She points to the two carbons in the double bond.* This one is more electronegative, most likely this one. *She points to the left carbon in the* *alkene, closest to Cl group*. The Cl won't hyperconjugate and will try to steal electron density from this carbon. *She draws in a dipole arrow pointing from the indicated carbon toward the Cl and places a symbol indicating a partial charge.* So you end up with a positive charge here—*She draws in a + to indicate the positive charge on the right carbon in the alkene.* So, 1, 2, 3, 4 carbons away—*She counts the carbons between the O and the positive charge she has inscribed and then draws the five-member ring below her initial diagram without drawing any groups external to the ring.*

Interviewer: Okay.

Cassie: That will give you a cyclic ether. But, I'm trying to decide exactly where the positive charge goes because that's a bit too small for a ring even with 5. I think the result is that—*She begins counting carbons from the carbon next to the Cl group*. Now, I'm thinking that it's going to be something like that. ***She draws the seven-member ring next to the five-member ring, again without any external groups***. And we put a methyl right there. ***She draws in the external methyl group on the seven-member ring*. And, 1, 2, 3—*She returns the original diagram and counts the number of carbons to the left of the positive charge, then adds the same number of carbons to the five-member ring before drawing in the Cl group on a dark wedge.*** That's my gut reaction. I'm not sure it's right. I think it is the safest answer.

Cassie's partial solution resulted from her use of the localized transformation heuristic. To solve the task, Cassie first noted that the given structure would cyclize. She began by debating whether the chloride would "spontaneously dissociate" or whether she should add the acid across the alkene. After debating the reactivity of each functional group for several minutes, she ultimately decides to consider both in her solution. She then draws arrows indicating the potential formation of each ring, which she erases before inscribing the base five-and seven-atom rings. What is notable about Cassie's use of the heuristic is that she inscribed each ring without including the extracyclic groups. Once the rings were depicted, she then returned to her original diagram to decide what additional structures she needed to add to each ring. For the seven-atom ring, Cassie pointed to her initial diagram and noted that the methyl group would be "one atom away" from the oxygen, and then drew a methyl group to the left of the oxygen (as in Figure 4). Although Cassie's choice of a solution strategy would generate a unique spatial relationship between the methyl group and the ring, she did not indicate this in her answer. The addition of the external group appeared trivial to Cassie once she had completed the local spatial transformation to generate the ring. Likewise, Cassie's process was similar for creating the five-atom ring. After first inscribing the ring, she then determined the additional atom needed to connect the methyl group to the ring by counting aloud how many atoms were between the methyl group and the positive charge in the first diagram; she then drew a methyl group to the right of the oxygen in the ring to which she added an ethyl group and the chloride on a bold wedge. As with her first answer, at no point did Cassie consider potential stereo-specific outcomes of the five-atom cyclization: she merely duplicated structures from the first diagram into her final solution.

Case 4: Algorithmic Translation of Diagrams (Algorithmic-Diagrammatic). The third algorithmic-diagrammatic strategy used once by two students revealed the availability of an algorithm that allowed for the translation of molecular representations without imagistic

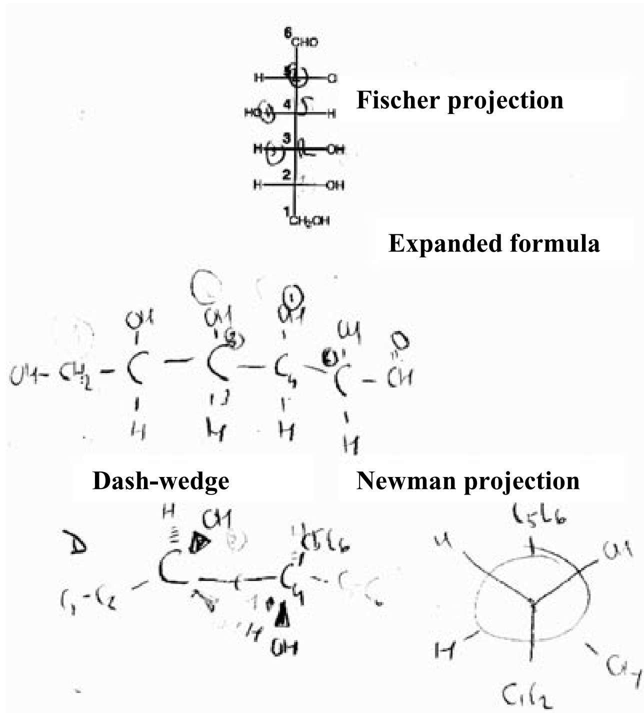


Figure 5. Multiple representations depicted by Malayna on the Fischer to Newman task.

reasoning. This strategy is remarkable given the frequency of imagistic reasoning for solving such tasks seen among students in the present study as well as by chemistry experts (Stieff & Raje, 2010). Using a "multiple representational mediator" algorithm, the students manipulated molecular diagrams without any observable behaviors indicative of imagistic reasoning. Briefly, the algorithm involved four distinct steps: translate the given diagram into a new representation, assign Cahn–Ingold–Prelog R/S designations to asymmetric centers in each representation, draw the target representation using the dash–wedge formula as a template, and assign R/S designations in the target representation to ensure consistency.

Malayna illustrates the use of this algorithm on the *Fischer to Newman* translate task in the following excerpt. As the transcript illustrates, Malayna first explicitly states that she must translate the Fischer projection into an expanded formula to "see what's attached to what," as in Figure 5. With the intermediate representation inscribed, she then applies a learned algorithm to define the relevant spatial relationships in both representations (i.e., R/S labels). From the expanded formula, she then generates another intermediate representation, a dash–wedge perspective formula, to highlight the spatial relationships that she must preserve in the target Newman projection. Rather than generate a mental image of each representation to compare them, she instead applies the R/S algorithm to ensure the dash–wedge formula contains the same spatial relationships indicated in the expanded formula. After inscribing the base structure of the Newman projection (i.e., the interior circle and six radiating bonds), Malayna accomplishes the final translation by duplicating the bonds from the dash–wedge to the Newman. First, she copies the H, OH, and C_1-C_2 atoms on C3 to the proximal bonds (Υ) in the Newman projection; she then duplicates the H, OH, and C_4-C_5 atoms on C4 to the distal bonds (⅄). In effect, the algorithm allowed Malayna to use the formalisms of each individual molecular representation to complete the translation by creating a sequence of inscriptions that more closely approximated the target representation when she perceived the direct translation to be too difficult.

Malayna: I just want to draw what is attached to what. *She hesitates and then begins to draw out an expanded formula while verbalizing components*. C, OH, C . . .

Interviewer: So, you are redrawing the Fischer?

Malayna: Yeah, but not with lines, just to see what's attached to what.

Interviewer: Ok.

Malayna: **So this is—I guess assign R and S to C3 and C4 . . .** ***She applies the Cahn-Ingold-Prelog naming algorithm to assign R/S into the Fischer projection. . . .*** **I'm going to draw it in dashes and wedges because I can't draw the Newman from here**. *She points to the Fischer.*

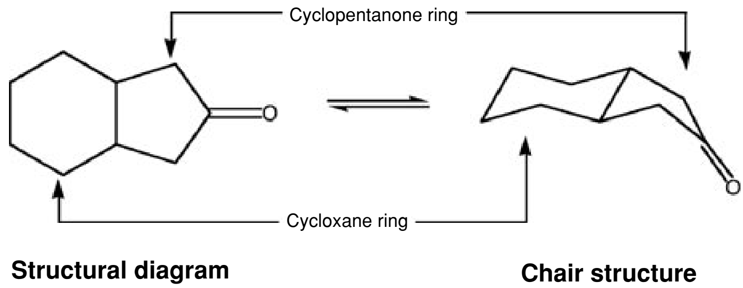
Interviewer: From the Fischer projection?

Malayna: Yeah. ***She duplicates the R/S assignments from the Fischer into the expanded formula and begins to construct a dash–wedge formula***. OK. So this is C3, I'll put the H in the back so that it's easier. So this would be R. So . . . *She pauses for ∼30 seconds.*

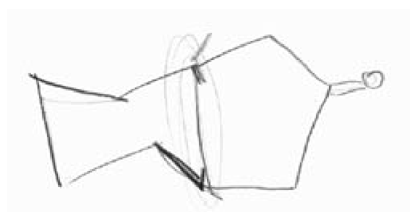
Interviewer: So now what?

Malayna: Well, the rest of this chain is C4 . . . *She designates this by drawing C4-C5-C6. OK, so this over here is C1. She points to the left side of the molecule and adds C1-C6.* Let's see if this worked. ***She applies the R/S algorithm to the dash–wedge as she did in the expanded formula and the Fisher projection. She points to each priority number as she moves through.*** 1–2–3. This is R, so that's right. ***She points to the Fischer then the dash-wedge to compare the R/S labels***. Now we draw C4. ***She repeats for C4 and confirms the R/S labels that she duplicated are correct. Without speaking, she then draws the basic skeleton of a Newman Projection with a circle and six empty bonds. Pointing back and forth from the dash-wedge to the Newman Projection, she duplicates each group individually.***

Notably, elements of this algorithm are highly similar to one strategy seen among experts. Stieff and Raje (2010) reported that experts often completed representational translation tasks by using a "diagram template" strategy with which they would inscribe a basic skeletal structure that had spatial features common to many molecules and subsequently modify the template. Malayna's strategy employs the diagram template strategy near the end of her solution when she inscribes the basic template for a Newman projection and then duplicates the spatial arrangement of atoms from the dash–wedge formula. Although only one other student employed the multiple representation mediator algorithm, the application of the algorithm in both cases highlights the affordances of diagrams to scaffold reasoning about spatial relationships in chemistry. While most students employed imagistic reasoning to solve this task, only one student was successful using imagistic reasoning; the other students who completed the task via imagistic reasoning systematically inverted the spatial relationships in the Newman projection. The use of the algorithm on this task resulted in both students taking approximately 10 times longer to perform the translation than students who reported visualizing the structure mentally; however, both students using the algorithm were ultimately successful.



Expert solution



Karen's solution

Figure 6. The Structural to Chair task requires illustration of implicit three-dimensional features in two dimensions as in this idealized solution. Karen's solution is depicted at the bottom.

Case 5: Visualization of a Diagram Template to Re-Render a Diagram (Complex-Mixed). The final case of problem solving with "Karen" illustrates how some participants employed a spatial-imagistic strategy in tandem with an algorithmic-diagrammatic strategy to complete a translate task. In such cases, students were seen to inscribe diagrams to generate partial solutions before engaging in imagistic reasoning. This practice was commonly seen among experts in Stieff and Raje (2010) but was only observed in 11 of the problem-solving episodes in the data corpus. The correctly solved task is illustrated in the top of Figure 6. As with the other translation tasks, the *Structural to Chair* task concerns the accurate representation of three-dimensional relationships in the target molecular diagram that are not illustrated in the two-dimensional structural diagram. The correct solution requires the student to depict the three-dimensional relationships in the target representation using the formalism of the two-dimensional chair structure. To achieve this, typical instruction encourages students to perceive both internal bond rotations and a gestalt rotation of the entire structural diagram out of the plane of the page for a successful translation (e.g., Ege, 2003).

In the excerpt below, Karen engages in several behaviors that suggest a central role of imagistic reasoning for completing the task. When asked to complete the *Structural to Chair* task, Karen first states that she has memorized the structure of a basic cyclohexane ring chair diagram, which she inscribes immediately (Figure 6, bottom). Given her inscription of the cyclohexane ring, Karen then attempts to add the cyclopentanone ring onto the chair. She finds the task unexpectedly difficult and mentions that she tries to visualize the molecular models she has used previously in class. Concurrent with her model references, Karen also gestures to indicate spatial arrangements of the bonds extending from the ring, as below:

Interviewer: Can you re-render this molecule as a chair?
Karen: 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.**

She points to the cyclopentanone ring. How would I do that . . . Well, **this is just the old cyclohexane chair—*She draws out the cyclohexane chair while speaking*.** Now I don't know if this bond—*She points to one of the cyclohexane bonds in her inscription*—is supposed to represent this—*She points to the bridging bond between the rings in the given diagram. She erases her inscription of the cyclohexane chair and then draws it again to more closely resemble the accepted chair*.

Interviewer: Why are you erasing?

Karen: 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.

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

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

Interviewer: From class?

Karen: **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. *With her right hand, she points up to the ceiling and then down to the floor*.**

Interviewer: Which?

Karen: **Like the molecules when you put them together like in the cyclohexane, it will go up and down, up and down. *She puts down the pencil, extends both hands side-to-side. From this position, she extends her thumbs toward the ceiling and her index fingers toward the floor. She focuses her gaze on her extended fingers while slowly twisting her wrists in an up- down motion*.**

Karen's excerpt illustrates a common sequence of events that characterized students' interactive use of diagrammatic reasoning and imagistic reasoning in tandem, as seen among experts. On many tasks, students relied on canonical molecular diagrams to represent and preserve important spatial relationships. Karen illustrates such practices by inscribing the chair diagram at the outset of the task. Her immediate inscription and subsequent correction suggests that she does not engage in imagistic reasoning until she is faced with the additional task of illustrating the spatial relationships in the structure. Imagistic-reasoning strategies occurred most frequently when students reached such impasses during a translation. Here, they frequently reported visualizing molecules "in the head" or referenced picturing their molecular models from class to make progress. It appeared that imagistic reasoning helped students move beyond the impasse by providing additional information about three-dimensional relationships implied by the diagrams.

This excerpt indicates a fundamental shared impact of both imagistic reasoning and diagram use for solving tasks that required students to perceive and manipulate embedded three-dimensional information in a given or constructed diagram. To accomplish such a task, students often first inscribed learned molecular diagrams to initiate the solution strategy, as Karen did when she first drew the basic chair structure. When the diagram template failed to provide an adequate solution, students employed an imagistic-reasoning strategy to clarify spatial relationships, which were then inscribed in a subsequent diagram. On translation tasks, at least, it appears that the interplay between imagistic reasoning and reasoning from diagrams helped to drive problem solving for all students, independent of chemistry skill.

DISCUSSION AND IMPLICATIONS FOR TEACHING

The results of the analysis provide evidence supporting a task-specific role for imagistic reasoning in chemistry that is highly interactive with heuristics and algorithms for manipulating diagrams. Students were inclined to visualize three-dimensional mental images of molecular structures when they needed to translate or re-render a given molecular representation. On the majority of such tasks, students routinely generated, inspected, and translated internal mediating spatial representations of molecules to gain insight into spatial relationships relevant to the task. Conversely, students rarely engaged in imagistic-reasoning strategies on tasks that did not require representation translations specifically. Rather, students instead used systematic alteration and duplication of given diagrams to generate new molecular structures under the apparent assumption that such actions would produce or preserve the spatial information in the task. The relative use of such strategies are similar to those used by expert organic chemistry instructors on each type of task (Stieff & Raje, 2010). In contrast to experts who used multiple strategies while problem solving in that study, students in the present study appeared to rely on one primary strategy alone for solving each task.

By far, students preferred strategies for reasoning about spatial relationships in the extended problems included the two algorithmic-diagrammatic heuristics discussed above. Each of these strategies, the holistic duplication and localized transformation heuristics, allowed students to solve a variety of tasks by using the affordances of molecular diagrams to scaffold spatial thinking. In this manner, the students were able to make significant progress on many tasks without direct reference to spatial content in the task. These practices are suggestive of students' reliance on a general means-ends analysis approach to organic chemistry tasks in which they compare the superficial features of given and target representations. A common feature of each practice was the use of duplication strategies to copy geometric shapes, structures, and internal spatial relationships between inscriptions without detailed considerations of dynamic three-dimensional spatial relationships or the conceptual underpinnings of the tasks.

Indeed, students seemed dependent on their inscriptions as they progressed toward a solution: Any errors inadvertently made when generating an inscription halted progress toward a solution or was carried forward in the solution as each diagram was duplicated. This practice occurred even when the students were correct with regard to the underlying concepts relevant to a task. For example, students often verbalized the correct reactivity of functional groups and mechanistic categories of specific reactions despite drawing incorrect structures or mechanism arrows, as seen with Cassie. Surprisingly, students were more likely to acknowledge that they were explicitly distorting accepted chemistry concepts to agree with faulty diagrams than they were to search for and correct diagram errors. This is in marked contrast to experts who systematically check generated diagrams for mistakes as they work on a task (Stieff & Raje, 2010). Thus, students in the present study relied more on the direct perception of given or generated inscriptions than they did on consideration of the represented spatial relationships.

Although the present analysis does not attempt to describe a developmental pathway for the use of these strategies, it sets the stage for such work with a description of some common student approaches to problem solving in organic chemistry in comparison to those seen among experts. Namely, the present work suggests that novice students infrequently consider the shape or structure of organic compounds during problem solving on genuine tasks. Moreover, they fail to consider the dynamic spatial relationships represented by the variety of molecular diagrams available. Rather students appear to manipulate molecular diagrams with heuristics that reify the diagrams instead of recognizing them as representations of the molecular world. The implicit reference to three-dimensional relationships in any chemical representation and the abstract relationship between a representation and a given molecule appears unrecognized by students. Indeed, the affordances of heuristics and algorithms, such as those employed by students in the present work, encourage students to reason in such ways given that they often lead to successful problem solving. Despite the fact that students may generate an accurate structure as a solution to organic chemistry assessment tasks such as these, the transformations of spatial relationships that occur in a particular problem go unnoticed by the student: They are simply redrawing two-dimensional diagrams as they problem solve.

The common exception to this dependence on diagrams seen in the present work occurred on translate tasks. Translate tasks required students to consider three-dimensional relationships represented by a given two-dimensional molecular diagrams to produce a new diagram. Presumably, the explicit goal of re-rendering or re-representing a molecular structure from different angles or perspectives encouraged students to consider the spatial relationships embedded in the given structure. To do this, students employed imagistic-reasoning strategies that included mental rotation and perspective taking to identify spatial relationships and draw new representations. Remarkably, some students were seen to avoid such strategies on even these tasks by using an algorithm to create multiple representations. Both students who used this strategy were vocal about their inability to visualize molecular structures and their need to find alternative approaches to solve such problems. Although this approach increased the length of problem solving time, it proved to be highly accurate.

While the limited number of classrooms and participants in this study prohibits broad generalizations, the common approaches to problem solving do suggest three potential practices for supporting students' use of imagistic reasoning and other strategies in organic chemistry. First, and perhaps most immediately realized, the results suggest that students need more training to develop representational competence in organic chemistry. This implication agrees with the emphasis on representational competence advocated more broadly in chemistry (Kozma & Russell, 1997) as well as in mathematics (Nathan, Stephens, Masarik, Alibali, & Koedinger, 2002) and science in general (American Association for the Advancement of Science, 1990). Currently, accepted pedagogical practices in organic chemistry follow the "functional group approach." That is, little instructional time is devoted to developing students' ability to understand and translate between molecular representations. Although instructional practice was not a focus of the present work, each instructor's classrooms was observed on a daily basis and both instructors were consistent in their teaching methods, which involved drawing prepared solutions on the blackboard for students to copy. Of the 150 hours of classroom observed, 2 hours of instruction was devoted in each class to discussing perspective taking and translating between representations. Student responses in this study indicate that they were attending to the functional groups within a molecule as instructed; however, the focus on functional groups often caused them to overlook diagram errors and spatial transformations elsewhere in a molecule. By devoting more attention to enhancing students' ability to translate between different molecular representations, instructors may improve students' ability to perceive such errors and select the best representation to solve a particular task.

Second, students' understanding and achievement may benefit from instruction and activities that highlight an interactive role for imagistic reasoning and diagrammatic reasoning on specific tasks. Instructors might capitalize on students' tendencies to employ imagistic-reasoning strategies for translating molecular representations and diagrammatic-reasoning strategies for extended problem solving. The performance of students in this study indicates that organic chemistry students in general may benefit from specific instruction on how to visualize molecular structures or how to assume different perspectives when translating or re-rendering representations. For example, systematic instruction in which direction to rotate a molecule when performing a translation might benefit a student such as Jamie. Conversely, enhancing students' facility to analyze molecular structures for recurrent structures, spatial relationships, and composition can support students' preferred diagramming strategies for extended problem solving, such as David's. Moreover, students appear to need more training in perceiving molecular diagrams as *representations* of the molecular world with explicit attention to the impact of inscription errors on problem solving. Students rarely detected such errors despite the fact that even minor mistakes in drawing a bond or rotating a structure dramatically impacted progress toward a solution.

Finally, students' preference for visualizing changes in their perspective of molecular diagrams instead of visualizing and mentally rotating molecular structures suggests new directions for the design of computer-based learning environments. Designers of educational software for chemistry have already realized the potential of software for enhancing students' use of imagistic reasoning and visualization at all levels and domains of chemistry (Dori & Barak, 2001; Stieff & Wilensky, 2003; Wu, Krajcik, & Soloway, 2001). The results of the present work agree with the predilection of designers for incorporating such tools in chemistry. However, new designs might depart from the historic goals of using such software so that students learn to appreciate the overall size, shape, and structure of particular molecules. Instead, new software tools for chemistry might support learning by offering alternative imagistic-reasoning strategies for specific tasks. This might include the option of altering viewing preferences that place either the student or the diagram as a frame of reference to support both egocentric and exocentric frames of reference. Likewise, novel software might improve students' diagramming practices by highlighting the similarities between different molecular diagrams in a series of problem-solving steps as well as possible sources of inscription errors.

Regardless of the future developments in technology and instructional practice, the present work illustrates that students approach problem solving in organic chemistry with a variety of strategies that both make use of and neglect imagistic reasoning for solving distinct tasks. The range of strategies employed by these students reflect those used by expert organic chemistry instructors; students do indeed attempt to employ expert strategies that they likely apprehend in textbooks and classrooms. No one strategy to problem solving appeared most effective, as at least one student was able to employ any given strategy successfully. Ultimately, the students' protocols indicate that novices, like experts, are able to evaluate and choose strategies depending on their self-perceptions of ability and the constraints of a task: Imagistic reasoning is employed almost exclusively to translate between representations. More importantly, the availability of such alternative strategies suggests that the presumed fundamental need for advanced visuospatial ability to succeed in chemistry should be reconsidered and further research on improving students' use of all available strategies is warranted.

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