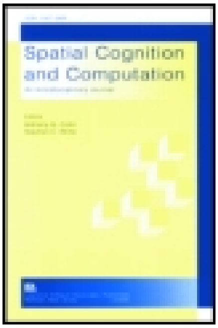

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Expert Algorithmic and Imagistic Problem Solving Strategies in Advanced Chemistry

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Abstract: Visualization and imagistic reasoning appear central to expert practice in science; however, expert use of these strategies on authentic tasks has not been examined in detail. This study documents how science experts use both algorithms and imagistic reasoning to solve problems. Using protocol analysis, we report expert chemists' preferential use of algorithms for solving spatial problems and imagistic reasoning for deducing spatial transformations. We observed experts employ algorithms to solve the majority of spatial tasks while reserving imagistic strategies to solve a class of tasks that required translating between representations. Strategy used varied widely among experts and tasks.

Keywords: mental imagery, spatial reasoning, diagrammatic reasoning, internal and external representations

INTRODUCTION

Advanced problem solving in physical science frequently requires the consideration of interactions between complex three-dimensional objects, such as molecules or forces. Because such objects cannot be directly perceived, expert problem solvers often report using imagistic reasoning to generate solutions. In such cases, experts give accounts of inspecting internal mental images to discern relevant geometric relationships and to mentally simulate potential spatial transformations (Hegarty, 2004). Indeed, several scientists of note have attributed historical discoveries to insights gained from the inspection of mental images; for example, Watson and Crick (Watson, 1968) referenced an important role for mental imagery for characterizing the structure of DNA and Einstein claimed that he frequently thought in terms of images (Schillip, 1949). These self-reports have been supported by several

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studies that indicate mental imagery and other forms of spatial reasoning are involved in problem solving in a wide range of sciences that include physics (Kozhevnikov, Hegarty, & Mayer, 2002), chemistry (Stieff, 2007), geology (Kastens & Liben, 2007), medicine (Keehner, Lippa, Montello, Tendick, & Hegarty, 2006) and meteorology (Trafton, Trickett, & Mintz, 2005).

In all these cases, experts have been observed to use a variety of spatial abilities during problem solving. In chemistry, experts have reported using mental rotation to transform and compare mental images to determine the spatial relationships between similar molecular structures (Stieff, 2007). In medicine, experts mentally assume unique spatial perspectives to inspect imagined anatomical structures during surgery (Keehner et al., 2006). In meteorology, experts claim to mentally animate dynamic spatial transformations of weather maps to predict the trajectory of storm fronts (Trafton et al., 2005). The evidence from each of these scientific domains suggests a primary role for unique spatial abilities with the common strategy of manipulating self-generated mental images of spatial information. In all cases, experts' reliance on internal representations of spatial information appears to be a fundamental characteristic of problem solving in scientific domains.

In addition to the generation and inspection of internal mental images of scientific phenomena, experts also report an important role for the use of external representations when solving problems that involve consideration of three-dimensional spatial information. Such representations include a variety of domain-specific diagrams, models, pictures and computer simulations that emphasize spatial information relevant to the problem. Analysis of expert problem solving has indicated that individuals are able to employ external representations to perceive and manipulate spatial information without the concurrent inspection of mental images (Trafton et al., 2005). In such cases, the formalisms of specific representations appear to make spatial information salient to the expert as well as afford the application of certain algorithms that predict the results of complex spatial transformations (Qin & Simon, 1992).

To some extent the use of such algorithms on domain-specific diagrams are unique to certain representations. For example, Stieff (2007) has shown that expert chemists are able to apply a heuristic to specific symmetrical molecular diagrams that allows determination of spatial relationships without inspecting or rotating mental images. However, when viewing asymmetrical diagrams, these same experts report that the heuristic fails and they must instead employ mental rotation strategies to determine the relevant spatial relationships. Similarly, Trafton et al. (2005) have shown that expert meteorologists report generating complex dynamic mental images of weather maps when viewing static representations of weather data; when provided with computer visualizations of the same data, experts instead systematically refer to the display without interrogating internal mental images.

Although it is clear that imagistic reasoning is an important component of expert problem solving, the extent to which experts rely on the generation and inspection of mental images during problem solving with external spatial representations is unclear. Prior analyses of authentic episodes of expert problem solving in science suggest that advanced problem solving in science involves a complex interaction among imagistic strategies, algorithmic strategies, and domain-specific external representations. The nature of the interaction remains undefined in specific scientific domains, however, and the role of any particular strategy is unknown. For example, given their experience reasoning about spatial information in their relevant domains, experts may excel at and primarily depend upon imagistic reasoning for problem solving. Alternatively, experts may have developed comparable domain-specific algorithms that allow for successful transformation of external representations without the inspection and manipulation of mental images.

Indeed, the availability of alternative strategies and reports of their differential use in laboratory studies indicates that both experts and some novices may choose from both algorithmic and imagistic solution strategies to problem solve successfully (Cooper, 1988; Just & Carpenter, 1987; Schwartz & Black, 1996). Likewise, such studies of strategy choice have also revealed significant individual differences in the extent to which individuals adaptively switch strategies in response to task demands (Schunn & Reder, 2001). Although the nature of the interaction between these two types of problem solving strategies has received some attention in the psychology laboratory, it remains ill defined for authentic science problem solving. Problem solvers' distinction between these alternative strategies has not been examined extensively using authentic episodes of expert science problem solving and individual differences in the use of each strategy remain unknown. Instead, educators have suggested that certain domains, such as the sciences, *require* students and practitioners to engage in the regular use of imagistic reasoning strategies due to the very nature of the domain content (Habraken, 1996).

IMAGISTIC AND ALGORITHMIC PROBLEM SOLVING IN ORGANIC CHEMISTRY

Organic chemistry provides an excellent opportunity to study the role of alternative strategy choice and spatial cognition during authentic problem solving. Historically, imagistic reasoning has been indicated as the primary strategy for problem solving in organic chemistry due to the content of the domain. Organic chemistry takes as a central concern the determination and analysis of spatial relationships within and between molecules in order to determine molecular structure, functionality, and reactivity (Mathewson, 1999; Wu & Shah, 2004). Indeed, a central topic in the domain concerns the relationship between three-dimensional spatial features of organic molecules and their chemical and physical properties. However, a major component of organic chemistry instruction centers on the use of algorithms for manipulating molecular diagrams without regard to spatial information (Stieff, 2004). These latter algorithmic strategies have been understudied in the discipline and their role in spatial thinking in the domain remains poorly understood.

Figure 1 illustrates a common example of how an organic chemist can use either an imagistic or algorithmic strategy to determine if two molecules are identical. Using an imagistic strategy, the expert might invoke a mental image of the first molecule in Figure 1, then mentally rotate and superimpose it on the second molecule to determine their relationship. If the molecules superimpose completely, they are identical. The primacy of this strategy and its correlation with visuospatial ability has been suggested for many organic chemistry tasks in several studies (Barnea & Dori, 1999; Habraken, 1996; Wu, Krajcik, & Soloway, 2001); however, experts can complete the task primarily by applying an algorithm to the diagrams.

Using this second strategy, the expert might examine one of the molecules in the pair to determine if any of the atoms around the central axis are unique. If all four atoms around the central axis are unique, the expert can determine immediately that the molecule cannot superimpose upon its mirror image and the pair contains two different molecules. If the molecules contain two or more identical atoms, the expert can make an immediate decision that the pair contains two identical molecules without the need for generating a mental image of the molecular structure (Stieff, 2007). Thus, using the second strategy the expert can rapidly determine that the third and fourth molecules in Figure 1 are identical.

This second algorithmic strategy is only one of many approaches that are available to chemistry experts. Indeed, professional chemists have developed formal analytic notation systems to solve many problems without the use of imagistic strategies. These range from nomenclature systems that identify the spatial relationships within a molecule (e.g., Cahn-Ingold-Prelog) to heuristic notations that reduce complex spatial structures to small alphanumeric strings. Previously, Stieff (2004) has shown that both students and instructors are aware of these alternative strategies at several levels of chemistry. Using experimental approaches to identify the use of mental rotation and imagistic

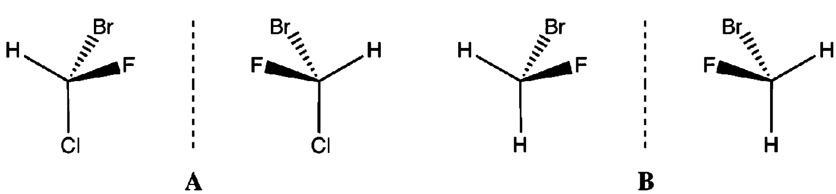


Figure 1. Exemplar comparison tasks from an organic chemistry assessment. 1A contains two spatially unique molecules; 1B contains two identical molecules. Note that the dashed lines indicate bonds below the plane of the page, the bolded lines indicate bonds above the plane of the page.

strategies, these studies revealed that experts employ this second algorithmic strategy as a first step in problem solving; when the strategy fails, experts often claim to generate internal mental images of the structures for comparison (Stieff, 2007). Interestingly, students in that same study instead choose to visualize molecular structures as a first approach and did not employ the algorithmic strategy without direct instruction.

Although it may be argued that the emphasis on spatial characteristics of molecular structures in organic chemistry predisposes experts to use imagistic strategies, it is possible that the opposite is true. That is, the use of diagrams can help to relieve the expert from some of the burden of generating and manipulating an analogical mental image. Although instructors and texts may encourage the use of imagistic strategies, it is unknown whether they personally employ imagistic reasoning or rely on algorithmic strategies for problem solving on authentic chemistry problems. In this paper, we report a first attempt to characterize the interaction between algorithmic strategies, imagistic strategies and external representations during expert scientific problem solving in this highly spatial domain. Through a detailed analysis of expert problem solving during clinical interviews we attempt to answer the question, when do experts employ concurrent and isolated imagistic and algorithmic strategies for successful problem solving in organic chemistry? Our analysis suggests that a variety of alternative strategies are available to the organic chemistry expert and that the generation and inspection of internal mental images is task-specific and also driven by personal preference.

METHODS

To characterize expert problem solving strategies in organic chemistry, we conducted a think-aloud protocol study. This technique allowed maximum flexibility to probe respondents on their self-perceptions regarding the generation and inspection of internal spatial representations of molecular structures. Previously, studies in chemistry (Stieff, 2004) and physics education (Sherin, 2001) have explored students' conceptions and inscription practices to obtain similar insights into participants' understanding and strategy choice as they solve typical science tasks. This approach, which builds on earlier methods for studying problem solving, advocates that attention to utterances, physical behaviors, and inscriptions can provide insight into the underlying conceptions and internal representations that participants use while problem solving. Prior use of this method indicates that the practice of verbally reporting one's own problem solving strategies does not appear to significantly alter or impede performance on complex tasks, although it may extend response time (cf., Ericcson & Simon, 1980; Siegler & Crowley, 1991). As such, it is particularly useful for studying problem solving in organic chemistry where participants frequently generate molecular diagrams.

Participants

Ten experts (8 male, 2 female) were selected from a volunteer population of faculty members from various universities in the mid-Atlantic region of the United States. Participants' years of teaching experience varied from 5 to 30 years ($M = 14.5$, $SD = 8$). Nine of the experts held terminal degrees in chemistry (Ph.D.) and one held a Master's degree in chemistry. All participants have been assigned pseudonyms to protect their identity.

Interview Protocol

Each participant received a stapled packet of 10 tasks at the start of the interview and was asked to complete the tasks while thinking aloud. Participants used either the provided blank worksheets in the task packet or solved problems on an available whiteboard. All tasks were designed by Stieff, in consultation with a practicing organic chemist, using assessment items derived from organic chemistry exams. Briefly, Tasks 1 through 4 required participants to generate a new representation of a given structure depicted on the page. Tasks 5, 6, and 7 included problems (with or without given molecular structures) that required participants to indicate products of a chemical reaction under a certain set of reaction conditions. Tasks 8, 9, and 10 included problems that required the experts to design or explain how to synthesize specific molecular structures.

During each protocol, the interviewer prompted participants to explain their thinking as they worked and also asked clarifying questions to the participants after the problem was completed. After a participant provided a final solution to each problem, the interviewer directly asked each participant whether they had the self-perception of engaging in the generation, inspection, and transformation of a mental image. Due to time constraints, only 3 participants completed all 10 tasks; 2 participants completed 8 tasks, and the remaining 5 participants completed 7 tasks total. Participants were videotaped during problem solving. The tapes were transcribed verbatim with annotation of all participant inscriptions and gestures for later analysis. The transcribed videos and worksheet inscriptions constituted the data corpus. Each participant received USD $50 for completing the interview.

Analytical Framework

We analyzed each task independently as a separate problem solving episode. For the analysis, we included only the 7 tasks that were completed by every participant. Individual transcripts for each task with the corresponding worksheet inscriptions defined the analytical unit. We used participants' verbal utterances with concurrent gestures or specific inscriptions to determine when and how experts employed imagistic reasoning or alternative strategies to problem solve. To determine the experts' problem solving strategy choice, we used a grounded-theory approach with a constant-comparative methodology (Strauss & Corbin, 1994) first to generate a coding scheme that was then applied to dataset. Specifically, the analysis involved developing a well-defined, reproducible coding scheme for participants' verbal utterances, inscriptions and their hand and body gestures. The analytical techniques for each observable behavior (utterance, inscription, and gesture) are detailed below.

We analyzed participant gestures according to the techniques outlined by Trafton and colleagues (Trafton, Trickett, & Mintz, 2005; Trafton et al., 2006) for classifying participants' gesture production. Using frameworks from the analysis of gesture and spatial cognition (e.g., Alibali, 2005; Clement, 2008), our technique identified three types of gestures produced during the protocol: deictic, iconic, and noniconic. Deictic gestures included gestures that involved pointing to specific areas of a worksheet or self-inscribed diagrams while generating solutions.

Iconic gestures included those that involved hand gestures that indicated moving or rotating molecules or imagined bonds within molecules and whole body movements that indicated viewing molecular structures from alternative angles. All other gestures were coded as non-iconic and typically included personal gestures (e.g., touching hair or face) as well as communicative gestures (e.g., shrugging shoulders). Using this technique, the videotaped interviews were first reviewed with the sound turned off, and every occurrence of a gesture was recorded. Following this, the videos were viewed a second time with the sound turned on with a concurrent review of the transcripts. During this second viewing, each noted gesture was classified as deictic, iconic, or noniconic.

The transcripts and videos were reviewed a third time to code participant utterances for specific references to the inspection of imagined spatial relationships relevant to the task. As mentioned previously, verbal reports provide critical insights into participants' perceptions of their own problem solving strategies (Ericcson & Simon, 1980; Sherin, 2001). Verbal reports indicative of imagistic reasoning strategies were quite specific and frequently accompanied iconic gestures. For example, participants made such comments as, "I am imagining this in my mind's eye." We coded all utterances that referenced inspecting an internal image, imagining structures or shapes not present in the diagram, or descriptions of dynamic spatial transformations over time as indicative of imagistic reasoning. Alternatively, utterances representative of alternative algorithmic strategies made specific reference to content-specific strategies, formulas or inscribed diagrams. For example, participants acknowledged routine heuristics with utterances such as, "I am assigning R/S configurations." We coded all utterances that referenced a specific rule for transforming or labeling spatial relationships as algorithmic.

Finally, participant inscriptions were analyzed for references to imagined molecular structures. On each task, participants were constantly involved in drawing pictorial representations of molecules while problem solving.

Evidence for the use of imagistic strategies included specific inscriptions that indicated imagined spatial transformations of inscribed structures. Following established symbolisms in organic chemistry, participants used curved arrows to indicate the imagined rotation and movement of individual bonds in molecules. They used straight arrows or sketches of eyeballs to indicate assuming alternative perspectives. Specific inscriptions were coded as indicators of nonimagistic strategies: These included notations such as the use of numerical labels to keep track of relevant spatial features, dashed lines to indicate mirror reflections and canonical diagram templates to sketch skeletal structures.

Each interview task was analyzed along these three levels of analysis independently by each author. The resultant codes applied to each set produced three broad themes that captured the observed strategy used by an expert on each specific task: Algorithmic-Diagrammatic Strategy, Spatial-Imagistic Strategy, and Complex-Mixed Strategy. Representative participant behaviors corresponding to each strategy theme are listed in Table 1. We determined a participant's strategy on each task by determining the consistency between verbal utterances and either gesture or inscription practices. Thus, any task that contained an imagistic utterance code and either an iconic gesture or spatial inscriptions was categorized as solved via a Spatial-Imagistic

Table 1. Coding scheme and representative examples of observable behaviors

	Observable Behavior		
Strategy Theme	Utterances	Gestures	Inscriptions
Algorithmic-Diagrammatic	"That's what we were taught."	Points with pencil or finger at the diagram.	Draws a template of a generic molecule.
	"As I recall."	Points to a generic formula or lists known reactions.	Converts a name to a specific molecular structure procedurally.
	"It's been beaten into my head."	Points to a generic formula or lists known reactions.	Labels spatial information in a diagram.
Spatial-Imagistic	"I can think of it in my mind's eye and rotate it."	Makes a grasping and rotating gesture above the worksheet.	Draws curved arrow showing single bond rotation.
	"I can look down this bond."	Turns self/worksheet 90 degrees.	Draws a stick figure pointing in direction of the bond.
	"Imagine myself looking down that plane."	Slicing hand gesture parallel to worksheet.	Draws an arrow or eyeball in direction of perspective.
Complex-Mixed	Co-occurrence of Analytic-Diagrammatic and Spatial-Imagistic codes		

Strategy. We categorized any task that included algorithmic utterances and either deictic gestures or non-spatial inscriptions as solved via an Algorithmic-Diagrammatic Strategy. We classified any task that was coded with both imagistic and analytical codes as solved via a Complex–Mixed Strategy. At least two of the three coded behaviors were observed on every task.

Comparison of the two authors' utterance, gesture, and inscription codes for the entire data set established interrater reliability ($\kappa = 0.95$). All disagreements in coding assignments were resolved via discussion and collaborative review of each task. Under the cautious assumption that participants might engage in an imagistic reasoning strategy without observable behaviors, or appear to use algorithmic strategies while mentally rotating molecules, we deliberately triangulated evidence from utterances, gestures, and inscriptions to increase the likelihood of capturing imagistic reasoning.

We attempted to confirm our strategy assignments by analyzing participant responses to direct questions about whether they mentally imagined the molecules at any time after each task was completed. In all cases participant's self-reports agreed with our analysis. Although participant's self-reports of imagistic reasoning are potentially misleading, our decision to accept these reports at face-value was motivated by reference to the prior literature that suggests a primary role for imagistic reasoning in chemistry (Mathewson, 1999; Wu & Shah, 2004) as well as the growing literature that shows a strong correlation between iconic gesture production, imagistic reasoning and self-report (Alibali, 2005; Clement, 2008; Hegarty, Mayer, Kriz, & Keehner, 2005; Trafton et al., 2005, 2006).

RESULTS

Our analysis of the data corpus yielded unexpected results with respect to our assumptions regarding expert use of imagistic reasoning strategies for problem solving. Given previous studies implicating a primary role for imagistic reasoning by experts in this domain, we were surprised that our analysis revealed a more nuanced role for imagistic reasoning for supporting a variety of learned heuristics and algorithmic strategies. Indeed, we rarely observed experts engage in the exclusive use of imagistic reasoning to solve organic chemistry problems. Instead, they reported that they used imagistic reasoning selectively for imagining specific molecular structures or for evaluating the quality of their proposed structures. The participants appeared to rely most heavily on the correct application of a known algorithm or heuristic to reason about a given diagram and generate novel structures for further consideration. Thus, our analysis suggests that advanced problem solving in organic chemistry involves a complex interaction between imagistic reasoning and algorithmic strategies that experts can apply in unique ways. Specifically, we observed experts approach each task with one of five specific strategies that involved imagistic reasoning to varying degrees. Below, we illustrate the frequency of expert use of Spatial-Imagistic, Algorithmic-Diagrammatic, and Complex-Mixed Strategies followed by illustrative cases of the unique strategies we observed in the dataset.

Frequency of Expert Strategy Choice

Figure 2 summarizes the observed frequency of strategy use across the 7 tasks solved by all 10 experts. A repeated-measures ANOVA indicated that there were significant differences in the use of each strategy among the experts, $F(2, 69) = 4.72$, $p < 0.001$. None of the given tasks were solved routinely using imagistic strategies. On only two tasks (Task 1 and Task 4) did we observe an expert use of a Spatial-Imagistic Strategy to generate a solution without concurrent use of analytical heuristics or algorithms. Of note, these two tasks both require the expert to construct a specific chemical representation (i.e., Newman Projection) to generate an answer. In this way, these tasks were unique in that they each required the problem solver to generate a novel molecular diagram that was illustrated from a perspective that was orthogonal to the perspective in the given diagram.

In contrast, the experts employed a range of diagrammatic strategies to manipulate their inscriptions using heuristics and learned algorithms on each task in the data corpus. By far, experts applied Algorithmic-Diagrammatic strategies ($M = 4.5$, $SD = 1.1$) more frequently than Spatial-Imagistic strategies ($M = 1.0$, $SD = 1.1$) in the data corpus, $F(1, 29) = 30.12$, $p < .001$. In particular, experts reported that for Task 2 an analytical manipulation of their inscriptions was sufficient to generate an answer without consideration of any of the spatial relationships in the given structure.

Of note, we observed a complementary role for imagistic and diagrammatic strategies across several tasks in the data corpus that were classified as

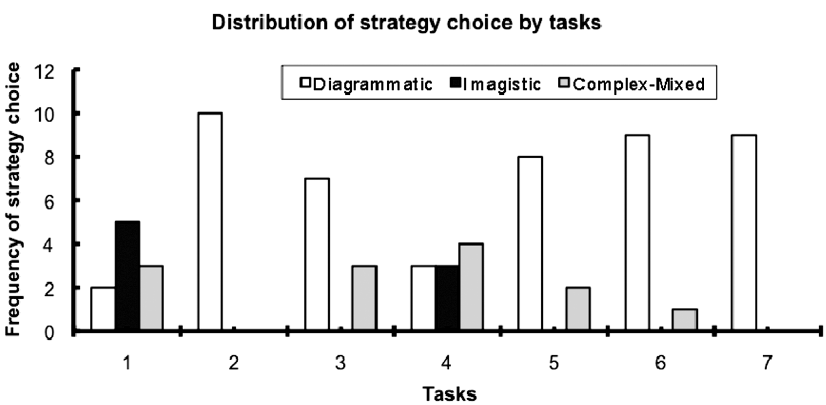


Figure 2. Frequency of strategy codes for each interview task.

solved via a Complex-Mixed Strategy. In such cases, experts appeared to rely on the generation and inspection of mental images at certain stages of problem solving prior to and following the application of a learned heuristic. These interactions were nonuniform and the experts reported using imagistic reasoning in several unique ways. In some cases, an expert's first step in a strategy was to mentally imagine a given structure to develop a solution pathway. In other cases, an expert employed an algorithmic strategy to generate a novel inscription and then evaluate the quality of the inscription by inspecting an imagined three-dimensional structure. Even more complicated, some experts reported mentally transforming imagined structures that they then inscribed, followed by the application of a heuristic to modify the inscription before inspecting a new mental image of the most recent inscription.

Our finding that Algorithmic-Diagrammatic Strategies that involved heuristics for transforming inscribed diagrams occurred most frequently in the data corpus motivated us to examine individual differences in strategy use between our expert participants. To do this, we aggregated the frequency of imagistic and analytic strategies for each participant across all tasks. Figure 3 shows the distribution of strategy choice for all 10 experts. As illustrated, individual experts rarely relied on one exclusive approach to problem solving. Among the experts, only Participant 2 reported using algorithmic strategies alone to solve all of the problems in the interview. More common was the application of both Algorithmic-Diagrammatic and Spatial-Imagistic Strategies as needed to solve specific tasks. Eight of the 10 experts reported using imagistic and diagrammatic strategies interactively to generate solutions for specific tasks. As mentioned before, the concurrent application of both strategies was nonuniform and the participants appeared to use these strategies in unique ways to meet goals established early during problem solving.

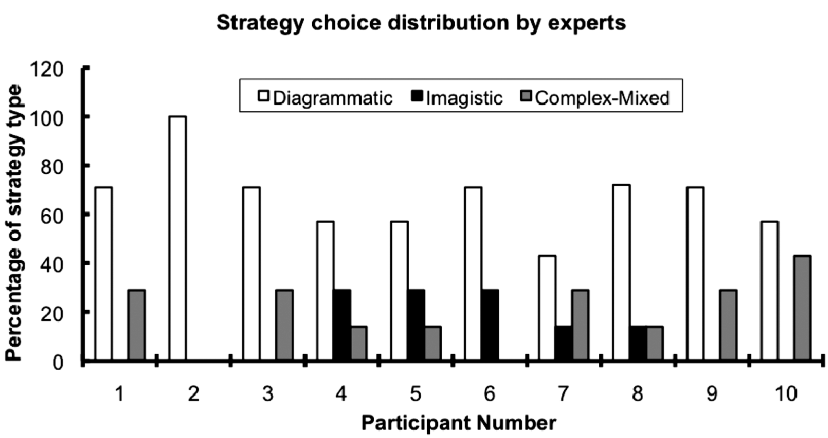


Figure 3. Distribution of expert problem-solving strategies across all tasks.

The descriptive statistics provide a general overview of the relative frequency of the observed strategies across both the tasks and the experts. Although they do not illustrate the specific role of each strategy, they do suggest the potential task-specificity of some strategies as well as the role of personal preference in strategy choice. Namely, our expert participants used imagistic strategies primarily for tasks that involved translating between representations (Tasks 1, 3, and 4). However, for problems that involved predicting reaction products (Tasks 5, 6, and 7) and identifying isomers (Task 2), the experts reported the exclusive use of analytic strategies. Likewise, the analysis of individual expert's strategy choice suggests that while all experts were experienced in the use of algorithmic strategies for manipulating molecular diagrams, some experts displayed a preference for applying imagistic strategies either in isolation or in tandem with learned heuristics.

Next, we attempt to illustrate the nature of each of these strategies with descriptive cases of problem solving. First, we offer examples of two Algorithmic-Diagrammatic Strategies and one Spatial-Imagistic Strategy used alone followed by two unique examples of Complex-Mixed Strategies. In each episode, critical utterances and behaviors that we used as evidence of specific strategy choice are indicated in bold in the transcript. Asterisks (***) represent omitted text that contains technical jargon not critical to the episode.

Case 1: Use of a Diagram Template to Generate a New Structure (Algorithmic-Diagrammatic)

In the case presented here, we highlight how one expert used an Algorithmic-Diagrammatic Strategy exclusively to solve a task that mandates reasoning about complex three-dimensional spatial relationships. To solve the problem, "Bob" employed a known template structure initially that he then modified as he generated a solution. Indeed, the entire body of experts revealed a familiarity with several relevant molecular diagram templates that they would occasionally inscribe to solve certain problems. Like Bob, once they had inscribed the basic skeletal template, they would proceed to add the required spatial information or atomic structures unique to the given problem. Although several experts were familiar with this strategy, not all of them used it for problem solving. We observed the use of this "Diagram Template Strategy" 10 times in the data corpus on Tasks 1, 3, and 4. In the following excerpt, we will present our analysis of Bob's verbal utterances, gestures, and inscriptions to highlight the potential of using diagram templates as a problem solving strategy on Task 4.

Bob: (***Bob draws two circles immediately on the white board, Figure 4a.***) Ok, in this case I am going to—You have again asked for the Newman projection. You have not mentioned again anything whether it is thermodynamically lower or not, but I am going to assume it is and I am going to . . . (***Bob completes a generic Newman Projection; Figure 4b. He***

A **B** **C**

Figure 4. Bob's use of an example diagram template strategy.

then inspects the given diagram and adds the indicated methyl groups to his generic diagram to generate a final solution, Figure 4c.) ***

I: Ok—

Bob: Right now I have to make sure my stereochemistry is right. I have the 1 on the methyl on the same plane as my 3. (***Bob makes a slicing gesture with his hand to indicate a horizontal plane on top of the diagram.***) And I have . . . and the rest are hydrogens so I put these back here—I did actually the opposite.

I: What do you mean?

Bob: So you showed with the methyls up (*He points to the given diagram in the worksheet.*) and if I were to—depending on how you wanted to define the plane. (***He traces a plane with his hand that is parallel to the board and which roughly passes through the centers of the two circles in his final drawing.***) I have the two methyls down but it's the same molecule, right?

I: Ok why did you choose to—?

Bob: So I did that . . . as I set up—I tried to do the first time—I **set up the Newman projection first making all the staggered confirmation and then I figured I would fill all the substituents later**. So, this (*He points to his inscription.*) is a—I made basically the chair form of the cyclohexane with the two staggered and then I said, "Where do I put the methyls? ***

I: So again when you are solving this sort of a problem are you picturing the three-dimensional relationships as to which side of the rings things were on that this one was the opposite of the original?

Bob: Um . . . like I said, **"Let's get the skeleton right first." Get a skeleton and then attach things to the skeleton**.

In the preceding excerpt, Bob reveals an intimate familiarity with the basic template of a Newman Projection. He begins the task by drawing two circles as shown in Figure 4a. Next, he proceeds to draw in lines on top of the Newman projection, shown in Figure 4b, to represent the connecting bonds. Given this basic template diagram, he indicates that any Newman projection can be constructed by amending it with the constituent atoms of any specific molecule. After the template is in place, Bob proceeds to fill in the relevant atoms to complete the task. He acknowledges this by stating, "I set up the

Newman projection first making all the staggered confirmation and then I figured I would fill all the substituents later."

As he proceeds toward a solution, Bob realizes that his final answer to the task has been rendered as if it were rotated 180 degrees from the given molecular structure by stating, "I did actually the opposite." That is, the methyl groups in Bob's final inscription (shown by "Me" in the given Figure 4c) indicate groups of atoms that are projecting below the plane of the paper. The given task, however, indicates these same groups should project above the plane of the paper. Although initially concerned, Bob immediately concludes his structure is correct because the internal spatial relationships have been preserved in his final solution. He emphasizes the accuracy of his diagram by placing his hand against the whiteboard to illustrate that the relevant groups are on the same side of the molecule as they are in the given diagram. Ultimately, Bob concludes that his diagram is a faithful Newman projection of the initial structure without the need for engaging in mental transformations or imagined gestalt rotations of the structure to make a comparison. As Bob states, generating the solution does not require one to consider a mental image of the molecular structure, one has only to "get a skeleton and then attach things to the skeleton."

Case 2: Algorithmic Transformation and Inscription of a Structure (Algorithmic-Diagrammatic)

Although the majority of expert problem solving strategies observed across the interviews involved the use of a diagram template or the spatial transformation of imagined spatial representations and external inscriptions, in many cases experts were able to generate solutions solely via algorithmic transformations of self-inscribed external representations. Unlike the use of a diagram template, this Algorithmic-Diagrammatic Strategy permitted experts to quickly generate novel molecular structures by the use of a specific algorithm. Using an algorithm, the experts reported that they had learned a particular "rule" that allowed them to create spatially unique structures without directly considering the spatial relationships in a given structure. These strategies were most extensively observed for solving Task 2, which required participants to generate multiple molecular representations of spatially unique molecules from a given two-dimensional diagram. We observed the use of Algorithmic Transformation strategies 27 times across Tasks 2, 6, and 7. Next, we illustrate how "Irene" employed a "Flipping Strategy" that involved the algorithmic transformation of her self-generated inscription to solve the task without imagistic reasoning.

Irene: (*Reading aloud.*) Please draw the stereoisomers of the following amino acid isoleucine. So I'll look for the chiral centers—so there're two of them *(She points to two carbon atoms in the given molecule)*. **So since there're 2 we'll have 4 stereoisomers so we can draw this out, draw**

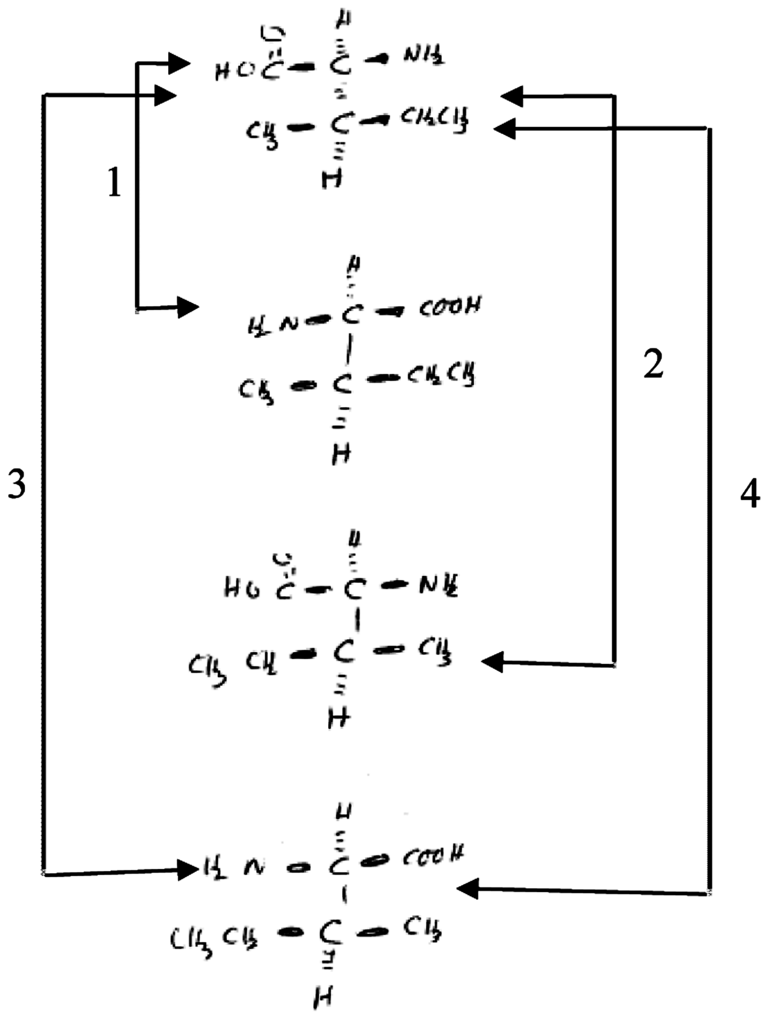


Figure 5. Irene's depiction of four stereoisomers to solve Task 2.

it out very simply if you like, like this (*She draws the top perspective diagram in Figure 5*) … we can draw it like that **and then we can just switch things around. So basically, I just switched one of the bonds to switch the configuration and we can do it again and draw the other two. So now I am just switching things around to make all the possibilities** (***She quickly draws the next three diagrams in succession by duplicating the previous diagram and reversing the location of specific groups of atoms***).

I: So when you said you just switched it, did you imagine this to be switching things in your head or did you just switch them on paper?

Irene: Um ... it really was only necessary to switch them on paper—they don't have to be ...
I: Ok. Do you think you need to visualize these things in 3D to solve these kinds of problems?
Irene: **Um, I don't think that you have to visualize to do it for this kind of a problem.**

Irene begins the task by stating, "I'll look for the chiral centers." She immediately notes that there are two of them and uses a formula (i.e., 2^n, where n equals the number of chiral centers) to determine that four unique structures are required to solve the problem. Notably, she makes this determination without consideration of the possible spatial relationships within the molecule via an imagined spatial representation. She proceeds to inscribe her solution by depicting the first diagram in Figure 5.

Using this first diagram, Irene is then able to apply a heuristic to create the three additional structures in the figure. To do this she notes that she has only to "just flip things around" to generate the new structures. Thus, she creates the second diagram by duplicating a portion of the first diagram and then reversing the position of the COOH and NH_2 groups on the uppermost carbon atom indicated by Line 1. Irene quickly inscribes the third and fourth diagram using the same heuristic to reverse the position of substituents on the lower most carbon and then the substituents on both carbon atoms, respectively (shown with Lines 2, 3, and 4 in the figure).

As with the Diagram Template Strategy, experts used the Algorithmic Transformation Strategies to generate spatially unique molecular structures without directly considering the spatial relationships relevant to the task. In the preceding episode, Irene confirms that imagistic reasoning is not necessary for the problem by stating, "I don't think that you have to visualize to do it for this kind of a problem." Indeed, every expert participant stated unequivocally that imagistic reasoning was not necessary on Task 2 and that the application of the "Flipping Strategy" heuristic was sufficient to generate the solution. Several experts also applied the heuristic as part of more complex strategies to quickly generate one or more stereoisomers on other tasks in the packet. In this way, experts inscribed all potential stereoisomers that were possible from a proposed reaction by simply reversing the relative position of two substituents around an axis of asymmetry. Thus, our experts revealed that they rarely employed imagistic reasoning to compare the three-dimensional spatial relationships between stereoisomers.

Case 3: Mental Transformation and Inscription of a Visualized Structure (Spatial-Imagistic)

As with the isolated application of Algorithmic-Diagrammatic Strategies, such as the Diagram Template and Flipping Strategies, we observed several experts employ Spatial-Imagistic Strategies exclusively on specific tasks. In each case, the expert reported the perception of imagined molecular structures that they inspected or transformed to generate a solution prior to making an inscription. The nature of such transformations were varied and ranged from the simple generation of a three-dimensional internal representation of a molecular structure to more complex operations that involved mentally rotating molecules, perspective-taking and simulated spatial rearrangement of specific bonds or atoms. When using these "Imagistic Strategies," individual experts frequently verbally reported seeing the molecule (e.g., "I can think of this ... in my mind's eye") and gestured above the workspace as if they were grasping and manipulating an imagined structure. We observed experts use Imagistic Strategies 8 times specifically on Tasks 1 and 4. Here, we detail "Dan's" use of imagistic strategies involving to solve Task 4.

> Dan: Ok what I always do is—What is it ... comes from *Caddyshack*, right? **"Make yourself the ball."** So instead of worrying about this **I always try and put myself** ... **mentally at this point address** ... **I want to look down a bond I think what it would look like from the perspective if I were sitting on this sheet of paper here** *(Dan points toward the molecule from the side of paper)* **looking down that specific bond what would I see?** Alright and so if we're going to do C1-C6 and this is always a nice way to do things so there's C1 for me. *(He draws in the basic circle of a Newman projection and its specific atoms from the given diagram).* It's a Newman projection. I am looking down that bond so what I can

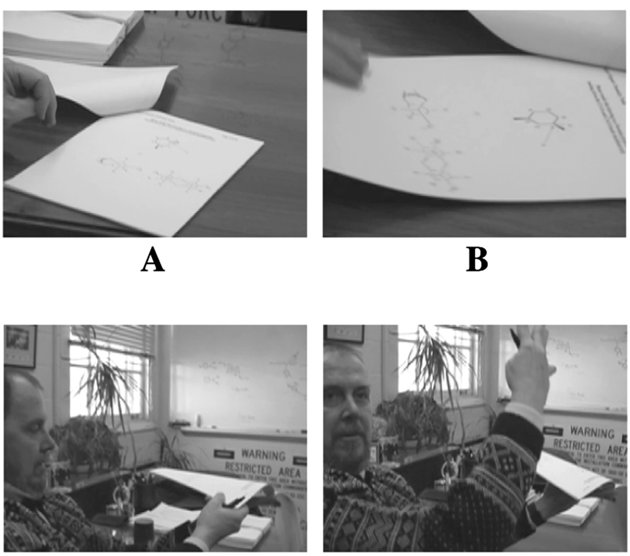


Figure 6. Dan's use of an imagistic reasoning strategy on Task 4.

tell you from looking at this is—I am going to have the H down because the methyl group is up. ***

Dan: You're looking down C1-C6 **so I have sort of put myself in this position** (***He draws an eyeball with an arrow pointing from it toward the C1 atom.***) **looking down that bond** so there's the equivalent of that . . . so that's the way I always do it . . . **be on the paper and be the paper.** Then what do you want me to do? C3-C4 simultaneously . . . then I could go back over here and then play with this . . . (*Dan proceeds to draw in the second part of the Newman projection and quickly completes the task without further comment.*) ***

I: Just one question before you are done . . . so did you imagine yourself looking down that plane . . . when you drew that eyeball . . .?

Dan: In fact you'll see me do that in class a lot of times. I'll actually take the paper like this. (***Dan turns the packet clockwise in Figs. 6a and 6b. He then lifts the paper to the level of his gaze in Fig. 6c so that his eyes are parallel with the arrows he drew previously.***) **Then I'll look down like this to give me the right perspective** and I encourage them [students] to do that because if they know that this means if this is sticking up then that's down, then they'll kind of remember . . . if they see something sticking up and sticking down (***He points his hand upward then downward relative to the lifted task packet in Fig. 6D.***) and then they get a feel for this . . .

In this excerpt, Dan illustrates how he employed an Imagistic Strategy to complete the translation task. Dan's first step toward a solution involves the generation of a mediating internal spatial representation for inspection. Using an analogy to a popular movie, Dan explains to the interviewer that he tries to "put myself mentally at this point address." He emphasizes that he mentally assumes an imagined spatial position by stating "if I were sitting on this sheet of paper here" and "so I have sort of put myself in this position" and inscribing a pair of eyeballs pointing at the given diagram from another perspective. These utterances and inscriptions are indicative of a perspective-taking strategy where Dan uses imagistic reasoning to move himself on the sheet of paper. In doing so, Dan is able to view the structure *from within* to determine the relevant spatial relationships that he later illustrates in the Newman projection. Once he has determined which atoms and bonds should be explicitly detailed in the solution, he quickly and accurately inscribes his final answer. After completing the task, Dan explains his reasoning further. To clarify his strategy, he physically rotates and lifts up the task packet (as in Figure 6C–D) to illustrate the imagined perspective-taking strategy he employed to complete the problem.

Case 4: Evaluation of a Diagram Template via Visualization

Although the majority of tasks were solved via the isolated use of a single strategy, several experts employed a combination of Spatial-Imagistic and

Algorithmic-Diagrammatic strategies to problem solve. Across all interviews, the experts relied heavily on the use of known diagram templates, as noted, to reason about complex three-dimensional spatial relationships. Once this "skeleton" structure was inscribed, the expert would then proceed to amend the diagram by adding spatial information or atomic structures unique to the molecule given in the task. As noted in Case 1, the experts appeared for the most part to solve problems without relying on visualization of the relevant molecular structures to solve the task. In a few cases, however, the experts indicated that visualization of an imagined molecular structure was critical for evaluating their final inscribed structure. In this way, the experts appeared first to use templates to inscribe a novel structure, which they then visualized, to evaluate the quality of their answer. Next, we illustrate one example case of such problem solving. We observed the sequential use of a diagram template followed by imagistic evaluation in this "Template Visualization Strategy" eight times in the data corpus, specifically on Tasks 3 and 4.

Bob: ***Bob draws the chair template depicted in Fig. 7a*** . . . **So I am drawing the chair because that easiest and then I am going to connect it and this to that.** ***He draws the five-membered ring attached to the initial template, as in Figure 7b without the two indicated hydrogens.***

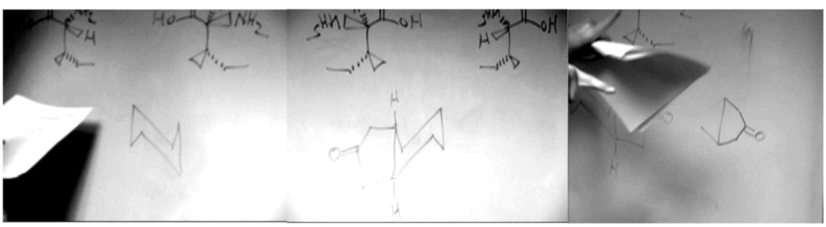
I: So as you've drawn it, can you say . . . are the two bonds that are coming off the cyclohexane into—(*Bob draws the hydrogens to indicate their relative orientation*) that's what I wanted to know . . .

Bob: So they are both um . . . equatorial.

I: Why have you chosen that?

Bob: **To tell you the truth when I drew this I just connected five bonds to this I didn't really think of the stereochemistry.** You certainly . . . one could have axial equatorial but it would be harder for me to draw it **so I just drew it to make the connections, not to think about stereochemistry**. Again, you asked me for the chair form of this; you didn't tell me you wanted the most stable form or what you wanted there so I didn't worry about it.

I: So as it's drawn would that be the most stable form of this molecule?



A B C

Figure 7. Bob's rendering of a diagram template followed by visualization of the structure.

Bob: Um ... I don't know unless I work out the structure of what I am torquing this (*he points to the five-membered ring he has drawn on the board.)* right now ... certainly it allows ... Equatorial substituents we teach is the most stable and it depends on whether we put strain on this five-membered ring and I don't know that unless I have to spend some time thinking about this, which I could do if you want me to or we could go to the next.

I: Actually could you walk us through a little bit about how you would figure that out?

Bob: Well, I'd probably try to draw things a little more accurately and so I would just look at this and I would remember that so that goes down (***Bob begins to inscribe the new structure indicated in Figure 7c by first drawing an isolated bond***) and that goes up (***he draws a second isolated bond***) and then we got (***he connects the two isolated bonds to complete the five membered ring depicted in Fig 7c.***)—let's see that's 4—and then we need one more ... Yeah, so I would say that *is* the most stable. **I mean, I try to think about a model (*Bob places is hands next to each other and points both index fingers in opposite directions to illustrate the angles of the original bonds he drew, as in Figure 7c*) of what it would look like in my head that seems quite doable without adding too much strain at all.** Again, it would prefer to have essentially the *cis* orientation.

In the above excerpt, Bob first inscribes a basic diagram template of a cyclohexane chair molecule, as indicated in Figure 7a. The template depicts a basic six-membered ring that represents one part of the structure in the original diagram. After considering the template for a moment, Bob quickly adds on the five-member cyclopentanone ring on the left side of the diagram. Bob appears satisfied with his answer until the interviewer asks him to depict the bonds that define the relative spatial relationship between the two rings. At this request, Bob clearly states that he had not considered those spatial relationships when constructing the diagram. Similar to his work on other tasks, Bob reveals that he relied on a Diagram Template to solve the problem and explicitly notes that he tries "not to think about stereochemistry." When asked to clarify the relationship, however, Bob changes his strategy. First, he points to his inscribed structure and notes that he needs to decide if the structure he proposed would result in "torquing" or twisting of the relevant bonds.

To make a final determination, he draws a new structure, again carefully working from a known template by stating that he remembers that specific bonds should be drawn at specific angles. After drawing each relevant bond deliberately in isolation, he pauses to consider his final diagram. At this point he raises both of his hands and points his index fingers at angles similar to the bonds he has drawn. While looking at his hands and twisting his index fingers relative to one another he states that is considering a "model of what it would look like in my head." From this mental evaluation, he reasons that his proposed structure is a valid solution because it does not depict spatially constrained bond angles. Thus, he appears satisfied with his response only after the generation and inspection of an internal mediating spatial representation of his work.

Case 5: Inscription and Subsequent Mental Transformation of a Diagram Template

As mentioned previously, many experts relied on the use of diagram templates as part of their initial problem-solving steps. In some instances, the diagram template was sufficient to complete a problem, while in others experts appealed to imagined structures to evaluate the quality of the inscribed diagram template. On 15 occasions, we observed a more complex interaction between the use of diagram templates and imagistic strategies. At least one expert used a Complex-Mixed strategy on each task except Task 7. In these instances, experts reported using a diagram template to make initial progress on a task before they appealed to mental simulations of spatial transformations of the diagram template. In effect, the experts appeared to gain critical insights into the task by considering their structures from new imagined perspectives or from altering spatial relationships in the molecule via visualizing rotating bonds or entire molecules. Below, we illustrate one of these complex mixed strategies used by Caroline to transform a given molecular representation into a novel representation.

> Caroline: Please render the drawing as a Newman projection looking down the C3-C4 bond. So this is C3 and this is C4 (*she labels each carbon atom as she speaks*), so a Newman projection is going to look different depending on whether it is R or S stereochemistry. *** I know that Newman projections will look different depending on if it is R or S stereochemistry. **Now is this racemic**? No, it's not . . . so we'll go . . . **so what I would probably first do is draw a dash-wedge version of this Fischer projection so I will say this is C3 and this is C4 and I would assign stereochemistry because I want to make sure it is internally consistent.**

Caroline begins Task 4 by first acknowledging that she can most easily draw a Newman Projection if she first draws another intermediate representation (e.g., dash-wedge perspective formula) of the given Fischer Projection. Notably, the task does not require the use of these additional representations as given. She first looks for planes of symmetry in the diagram as indicated by her rhetorical question, "is this racemic? No, it's not." To accomplish this, she constructs a basic template of a dash-wedge perspective formula and transcribes the atoms depicted in the given diagram onto her template, as in Figure 8a. She expresses concern over whether she has preserved the given spatial relationships and executes an algorithm to determine the spatial relationships in her dash-wedge perspective formula.

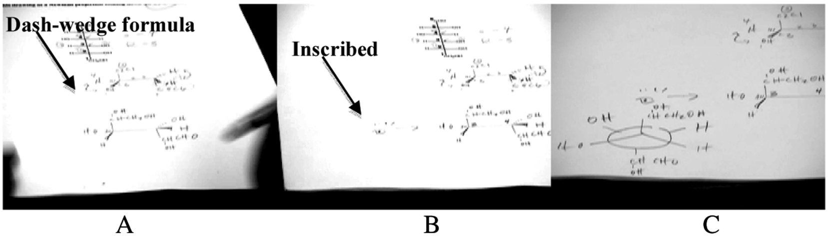


Figure 8. Caroline algorithmically transforms a diagram template and then spatially reorients her frame of reference using imagistic reasoning.

Specifically, she applies a discipline-specific naming convention that makes the spatial relationships within both the given diagram and her dash-wedge perspective formula explicit. Her application of the algorithm produces the same name for both structures and she expresses confidences that she has preserved the necessary spatial information. Next, Caroline draws a basic template of a Newman Projection and then pauses to consider her dash-wedge perspective formula and the blank Newman template. She notes the position of each atom in the dash-wedge perspective formula by repeatedly pointing to each atom and then pointing to different parts of the Newman Projection template. She gestures to the right and left sides of her own body briefly and then completes the Newman Projection in Figure 8b by placing the atoms in their correct spatial locations. Caroline explains her strategy in response to a question from the interviewer.

I: Um hmm . . . And could you explain when you say you have a clear way of drawing a Newman projection from a dash-wedge, what do you mean by that? What is the clear way? ***

Caroline: So, my methodical approach is I have taught students many times how to draw an exact Newman projection, meaning the exact stereoisomer from a dash wedge model and so coming to a dash wedge model when I am taking it from this perspective (**she inscribes a small eyeball pointing at the dash-wedge perspective formula as in Figure 8b**) I know that anything that's on the wedge is on the right and anything that's on the dash is on the left (**she gestures to each side of her body**) and so it's pretty clear then how everything is going to orient itself spatially within the Newman projection and therefore I am maintaining the stereochemistry that's inherent to the molecule that you actually asked me to draw before.

I: And when you draw the eyeball, does that mean . . . are you imagining that you are actually looking down there?

Caroline: That's exactly right. So the eyeball is out here because it's clear for you, the camera, or the student to see that I am looking from this way. But I actually teach the students that you are actually sitting right here and if you were sitting right here . . . **(She re-**

peatedly points to a carbon atom in the dash-wedge perspective formula).

I: Where is that?

Caroline: Right here on this dot, right at this carbon, if I were this carbon right above me **(she gestures above her head)** is this group to my right and down is the H **(she points toward her right foot)** and to my left and down is the OH **(she points toward her left foot)** that's exactly where I am standing so even though I draw the eyeball right out there, when I initially teach in my class remember you are right here so you have a very ... So it's like standing in a city I can imagine myself standing in the city and I can see all the skyscrapers above me and all the even-numbered apartments on my right and all the odd-numbered apartments on my left, so that's exactly how I do it.

In her explanation Caroline describes a complex strategy that involves an interaction between both an Algorithmic-Diagrammatic strategy and a Spatial-Imagistic Strategy. As she states she is completing the task "methodically" by first using her algorithm to construct a stereoisomer using the dash-wedge formula without engaging in imagistic reasoning. Following this, she mentally positions herself within the molecule. She accompanies her self-report of viewing the molecule from within, as if she were sitting on the carbon atom, by inscribing a small eyeball next to the dash-wedge formula and gesturing in space around her body. Using her hands, she indicates the relative position of the atoms in the dash-wedge formula as if they surrounded her where she was sitting. When asked to clarify her imagined spatial position, she makes a spatial analogy to a cityscape that contains the same spatial relationships she is attempting to depict in the model. Like several of the experts, Caroline's strategy to complete Task 4 reveals a significant and complicated role for both imagistic reasoning and algorithmic strategies to generate new structures as proposed solutions. In sum, by inspecting a mental image of an analytically transformed structure, she was able to generate her final solution to the task.

DISCUSSION

The results of the protocol analysis indicate that the use of imagistic reasoning in advanced scientific problem solving, specifically organic chemistry, is more nuanced than suggested by prior studies in the field (e.g., Ferk, Vrtacnik, Blejec, & Gril, 2003; Habraken, 1996; Wu & Shah, 2004). Although the domain of organic chemistry clearly takes the consideration of spatial information as a central concern, expert problem solvers in the domain have a variety of strategies available that involve imagistic reasoning to varying degrees. Some strategies appear to obviate imagistic reasoning completely by allowing experts to generate inscriptions that depict spatial transformations by analyzing and transforming diagrams. Other strategies appear to involve the inspection and manipulation of perceived mental images in order to identify critical spatial features of molecular structures. A few strategies involve the sequential application of both algorithmic and imagistic reasoning strategies in unique ways to produce intermediary inscriptions as well as to evaluate structures after a problem has been solved.

Despite the variety of strategies we observed across the data corpus, an interaction between strategy choice and task demands was apparent in the data set. Although the expert participants employed a range of strategies on each task, some strategies were task-specific. Broadly speaking, experts relied heavily on imagistic reasoning to complete tasks that required the generation and inscription of molecular representations that depicted a given structure from novel spatial perspectives. Seemingly, the experts were able to predict the appearance of the structure from alternative perspectives by generating mental images of the given structures that were either mentally rotated or inspected by imagining unique views from within or behind the structure. In contrast, tasks that required experts to generate all possible stereoisomers of a compound were solved exclusively through the application of an algorithm. In such cases, the experts applied a known algorithm to rapidly generate a series of inscriptions that depicted structures with unique spatial features while stating explicitly that the inspection or spatial transformation of mental images was not useful.

Distinct individual differences in strategy preference between the participants were observed in the interviews. Although some experts relied more extensively on imagistic reasoning than others, the majority of participants applied both imagistic reasoning and algorithmic strategies while problem solving. In only one case did an expert apply algorithmic-diagrammatic strategies exclusively to solve all of the problems given during the protocol; yet even this expert indicated he might use imagistic problem solving strategies when reasoning about molecules that had more complex spatial structures than those included in interview. We believe this observation is especially interesting, given previous work that has aimed to classify problem solvers as either "visual" or "verbal" problem solvers (e.g., Kozhevnikov, Kosslyn, & Shepard, 2005). While this protocol analysis cannot be generalized beyond the population of organic chemistry participants, the findings suggest that individuals rarely rely exclusively on one approach to problem solving and that expertise affords the application of multiple strategies to problem solve effectively.

With respect to the use of these strategies, it is important to note that we classified our experts' problem solving strategies as either imagistic or algorithmic and that we have not indicated a role for spatial reasoning for problem solving in this domain. Previously, Hegarty (2004) has noted a distinction between problem solving strategies that involve the inspection of mental images and those that involve the manipulation of domain-specific diagrams. In her framework, Hegarty notes that both of these approaches involve the analysis of spatial information and the consideration of possible spatial transformations. Here, all of the experts' strategies, whether algorithmic or imagistic, involved the careful analysis of the spatial features of a molecular structure as well as transformations of those features. Thus, our analytical framework treats both algorithmic problem solving strategies as well as imagistic spatial transformations of diagrams as examples of spatial reasoning in the domain. That is, our analysis suggests that spatial thinking in organic chemistry involves a variety of strategies that include, but are not limited to, reasoning via mental imagery.

We note that there are several limitations to the present study that suggest a need for further research on the interaction between imagistic and algorithmic strategy choice (both in chemistry and other high-spatial disciplines). First, our use of observable behaviors (i.e., gestures, utterances, and inscriptions) as evidence for the generation and inspection of mental images does not provide clear evidence for a functional role of mental imagery. We do not attempt here to address the ontology of mental imagery during problem solving and we acknowledge that it may indeed be epiphenomenal; however, we aimed to focus on participants' self-perceptions of the use of imagistic reasoning and other strategies during episodes of authentic problem solving and we conclude that the functional role of mental imagery in chemistry problem solving remains unclear from this work.

Of greater concern is the extent to which our expert participants are representative of the larger population of expert chemists. Each of the experts in the present study had several years of experience teaching within the domain of organic chemistry, and the impact of this experience on their problem solving approach should not be underestimated. It is possible that daily episodes of teaching problem solving to students made our experts aware of alternative strategies that are rarely used by expert chemists who are not engaged in teaching. The current data set cannot rule out this possibility and we suggest that future analyses of chemists working outside of academic institutions might provide complementary data on the prevalence and generalized use of these strategies among experts.

We also note that our analytical approach does not provide evidence about whether problem solvers inspect static mental images prior to inscribing spatial diagrams or whether they engage in imagistic reasoning covertly. As discussed above, we limited our analysis of imagistic reasoning to strategies that involved the generation and dynamic spatial transformation of mental images of molecular structures. Future work will be needed to clarify whether experts' engage in the inspection of transient mental images during problem solving and whether inspecting such images is task-specific. Likewise, the degree of correspondence of observable behaviors to underlying strategies remains unknown here. For example, we interpreted Bob's slicing gesture in Case 1 as a noniconic gesture that highlighted the spatial relationships in his diagram; however, it is possible that the gesture might indicate Bob is projecting a mental image of a plane into the diagram. In cases such as this, as well as others, we believe that triangulation of gestures with participant utterances and self-reports of strategy are necessary to clarify gestures that might have multiple meanings.

Despite these limitations, the results of our analysis appear to support studies in other domains that propose a central role for imagistic reasoning in advanced scientific problem solving such as physics (Clement, 2008; Hegarty, Keehner, Cohen, Montello, & Lippa, 2006), medicine (Keehner, Lippa, Montello, Tendick, & Hegarty, 2006) and meteorology (Trafton et al., 2005). Consistent with the reports of these other studies, our own analysis suggests a highly specific role for imagistic problem solving strategies in organic chemistry. Namely, experts appear to employ imagistic reasoning to approach tasks in the domain that require the consideration of alternative perspectives of molecular structures as well as complex three-dimensional interactions between two or more molecular structures. In cases where algorithmic manipulation of a diagram or inscription is possible, imagistic reasoning appears to play a supportive role for deducing spatial information or evaluating the quality of a spatial transformation predicted by the use of an algorithm. In no cases did we observe an exclusive dependence on imagistic reasoning for advanced problem solving in organic chemistry.

Although our work did not involve the examination of novice or journeyman chemists, we wish to conclude with some instructional implications that follow from our analysis of experts. Given the availability of alternative strategies to experts, novice students may benefit from instruction and activities that help them choose between imagistic reasoning and appropriate algorithmic strategies for problem solving. Our findings contradict previous calls for training only imagistic reasoning strategies in chemistry (Ealy, 2004; Ege, 2003; Ferk et al., 2003). Although we do not deny an important role for such strategies, our findings suggest that instructors might also reflect on their own preference for employing imagistic strategies for some specific tasks and algorithmic strategies on others. Rather than teaching the limited use of either strategy, new approaches might include specific lessons on how to perceive spatial information embedded in unique molecular representations by using diagram templates or labeling atoms when translating or re-rendering representations.

Likewise, instructors might employ a formative assessment rubric based on our analytical framework to attend to students' utterances and gestures and guide them to use different reference frames or to adopt an algorithmic strategy when imagistic reasoning is not effective. As Stieff (2004) has previously shown, students are capable of using both imagistic and algorithmic strategies to perceive spatial information and re-render representations. Similarly, enhancing students' facility to analyze molecular diagrams for recurrent structures, spatial relationships, and composition can support students' use of algorithmic strategies on a wide variety of tasks. To successfully employ alternative strategies such as those used by our expert participants is likely to require extended practice within the domain; however, the observed distribution and task specific use of the strategies certainly cast doubt on the need for reasoning exclusively with either imagistic or algorithmic strategies alone in this domain.

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