

Expertise & Spatial Reasoning in Advanced Scientific Problem Solving

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Abstract: Visualization and other forms of spatial cognition are considered fundamental to learning and problem solving in science. This assumption is especially prevalent in organic chemistry where imagistic reasoning is considered to be a primary cognitive activity. While previous research has shown that students are aware of several analytical heuristics and imagistic strategies for problem solving, there have been no studies exploring how experts in organic chemistry approach problem solving. Here, we identify problem solving strategies employed by ten chemistry experts to solve undergraduate organic chemistry assessment tasks. Our findings suggest that experts employ a range of imagistic and analytical strategies for reasoning about spatial information and prefer, on average, to use analytical strategies.

Introduction

The role of visuo-spatial reasoning in scientific learning and problem solving, specifically the generation and manipulation of mental images, is generally considered self-evident. Much of the reasoning that must be done in physical science is about the dynamic transformation of objects in three-dimensional space. Students cannot always directly perceive the objects and phenomena under study; therefore, they are often asked to mentally manipulate internal representations constructed from diagrams. This pedagogical practice is especially prevalent in advanced chemistry where some have claimed that imagistic reasoning is a primary cognitive activity (Habraken, 1996; Mathewson, 1999; Wu & Shah, 2004). Yet, a major component of chemistry instruction centers on the use of analytical strategies for manipulating molecular diagrams (Stieff, 2004). When teaching such strategies, instructors employ algorithms and heuristics to reason about spatial transformations of molecular structures. Previously, Stieff (2004) has shown that chemistry students are aware of several analytical heuristics and imagistic strategies that are applicable to a wide range of undergraduate assessment tasks. For example, some students choose to employ a mental rotation strategy to compare asymmetric and symmetric molecular structures while others apply an analytical heuristic that allows them to problem solve successfully on the same task (Stieff, 2005, 2007). Although strategies of the latter sort may obviate the use of imagistic reasoning, they are not necessarily the easier or preferred strategy as students often fail to correctly apprehend their use (Taagepera & Noori, 2000).

Although it may seem obvious that expert chemists might employ similar strategies, there are reasons to suspect this may not be so. Given their long-term experience, expert chemists may excel at the use of imagistic reasoning strategies in their domain. Alternatively, they may have developed even more sophisticated analytical strategies than those induced by their students to problem solve without employing imagery. Finally, experts might freely choose among strategies that have not been previously identified, such as those used by experts in other domains (Craig, Nersessian, & Catrambone, 2002; Nersessian, 2002; Qin & Simon, 1992). Here, we detail the preliminary results from a series of protocol analyses with expert chemists to identify the preferred strategies for expert problem solving in organic chemistry. Our findings suggest that chemistry experts employ a range of imagistic and analytical problem-solving strategies for reasoning about spatial information and prefer, on average, to use analytical strategies when possible. Such strategy use is markedly different from that seen among novices, and implies that instruction in alternative strategies use may be fruitful to novices.

Alternative Approaches to Scientific Problem Solving

The use of alternative strategies for problem solving has been extensively studied outside of science education. Such work has shown that although most students spontaneously develop a range of strategies, they do not switch abruptly from using ineffective strategies to effective expert-like strategies. More often, in the absence of direct instruction students learn to employ expert-like strategies gradually with increasing experience (Siegler & Chen, 2002; Siegler & Svetina, 2006). Frequently, 'experience' refers to extended episodes of problem solving and is characterized by the application of multiple strategies. In science, students undergo a similar trajectory of strategy acquisition (Kuhn, Garcia-Mila, Zohar, & Andersen, 1995). In much of this work, students have been observed to approach problem solving using domain-general strategies (e.g., trial and error, means-ends analysis) for extended periods as they slowly apprehend domain-specific algorithms, heuristics and analytic strategies (Alexander & Judy, 1992). 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). An extension of these prior studies in advanced science appears especially appropriate to reveal whether experts ultimately come to prefer imagistic or analytical strategies.

Organic chemistry provides an excellent opportunity to study the role of alternative strategy choice in problem solving. Some have claimed that imagistic reasoning is a primary factor behind student achievement in this domain as students of organic chemistry must often reason about the spatial characteristics of molecular diagrams 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 analytical strategies for manipulating molecular diagrams without regard to relevant spatial information (Stieff, 2004).

Although it may be argued that the use of molecular diagrams in 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. Figure 1 illustrates a common example of how an organic chemist can use either an imagistic or an analytical strategy to determine if two mirror image molecules are identical. Using an imagistic strategy, the expert might invoke a mental image of one molecule, then mentally rotate and superimpose it on the second molecule to compare differences. If the molecules superimpose completely, the expert knows they are identical. The primacy of this strategy and its correlation with visuo-spatial ability has been suggested for many organic chemistry tasks in several studies (Barnea & Dori, 1999; Habraken, 1996); however, experts can complete the task primarily by reasoning analytically from the diagrams. Using this second strategy, the expert might examine one of the molecules for an axis of asymmetry called a *chiral center*, which usually is defined as a carbon atom that possesses bonds to four unique atoms. If such a center is present, then the molecule cannot superimpose upon its mirror image and the pair contains two different molecules (Figure 1A). If any of the four bonds are identical, then a chiral center is not present and the expert can conclude that the pair contains two identical molecules (Figure 1B). Previously, Stieff (2004) has used experimental approaches to reveal that both students and expert instructors are aware of these two strategies for this specific task. Although instructors and texts may encourage the use of imagistic strategies, it is unknown whether they personally employ imagistic reasoning or rely on analytical strategies for problem solving on authentic classroom assessment items.

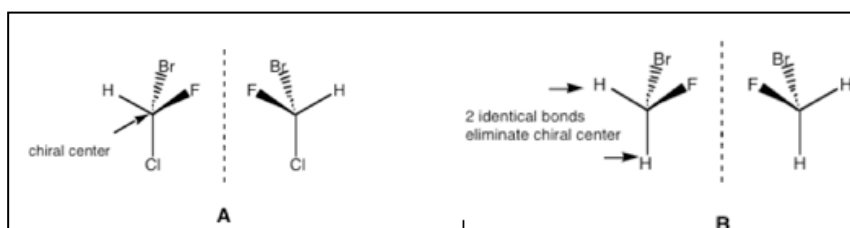


Figure 1. Canonical organic chemistry tasks solved with visuo-spatial or analytical strategies.

Methods

The present study employed clinical interviews to identify expert chemists' strategies for solving canonical undergraduate organic chemistry assessment items. This approach, which builds on earlier methods for studying problem solving (cf., Ericsson & Simon, 1980; Siegler & Crowley, 1991), 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. Such an approach is especially useful to an investigation of problem solving in chemistry: analysis of think-aloud protocols and gestures can provide a more accurate glimpse of when, how and why participants employ specific strategies for problem solving.

Participants

Ten participants were selected from a volunteer population of expert organic chemists including faculty and instructors at primarily research-focused universities in the mid-Atlantic region of the United States. Seven participants were faculty members who practice organic chemistry research and teach college level organic chemistry; three of the participants are instructors involved exclusively in teaching organic chemistry courses. All of the participants held advanced degrees in organic chemistry with a median of 9 years teaching experience.

Interview Protocol

Each participant received a packet of 7 tasks that were derived from undergraduate organic chemistry exams administered at another institution. Each task required the problem solver to explicitly consider internal spatial relationships of specific molecules. Due to space constraints it is not possible to discuss each task; however, we outline a typical strategy on one task that is detailed in the analysis. Participants were instructed to complete each task in order either on paper or using a provided whiteboard. A camera was positioned to record

the participants' inscriptions, gestures, and general body movements for later analysis. Participants sat facing away from the interviewer who asked clarifying questions and encouraged the participant to offer clear explanations of their reasoning on each task. After each task was completed, the interviewer explicitly asked the participant if they had "visualized" three-dimensional molecular structures while solving the problem.

Analytical Framework

The transcribed interviews were analyzed for verbal utterances using established techniques (Ericsson & Simon, 1980) and for gestural behaviors using techniques described by Feyereisen & Havard (1999) and Clement (2005). Briefly, construction of the analytical framework for identifying specific instances of visuo-spatial and analytical strategy use began with a review of each interview with careful attention to participants' utterances as they generated inscriptions. In brief, critical utterances of behaviors indicative of imagistic reasoning strategies included verbal references regarding molecular structure and physical attempts to gain new perspectives on diagrams. For example, participants were quick to refer explicitly to their own attempts to "imagine a molecule" or "visualizing models in their mind's eye".

The videotaped data was also concurrently analyzed for participants' gesture production. Specifically, the researchers noted participants' use of iconic or representational gestures (Feyereisen & Havard, 1999). The use of such gestures for reasoning about spatial information in chemistry has been illustrated recently by Becvar, Hollan & Hutchins (2005) among expert researchers. This work has revealed that experts employ distinct gestures that include such acts as the rotating or twisting of hands or pointing to empty space immediately above the work area when reasoning about spatial information in molecular structures. Because of their unique nature, the framework identified iconic gestures both with and without concurrent utterances regarding spatial information as indicative of imagistic reasoning. This decision was based on linguistics studies that report individuals employ iconic gestures frequently when engaged in tasks involving mental imagery (e.g., Hadar & Butterworth, 1997) and studies in science education that have examined gestural behavior during physics problem solving (Clement, 2005; Narayanan, Suwa, & Motoda, 1995).

Using a grounded theory approach (Strauss & Corbin, 1994), we attempted to identify the problem-solving strategies used by experts inductively from the dataset. Each task was reviewed as an independent unit, and each participant's utterances and behaviors were analyzed in toto to identify strategy use. We annotated each expert's approach to individual tasks to develop a narrative description of their strategy. These descriptions were then analyzed for common themes and behaviors and grouped into categories with similar participant behaviors. We then reviewed individual videotaped episodes in each group in parallel to determine whether different experts were employing similar strategies. After the initial identification of a strategy, a second analysis of each episode was conducted to elaborate the character and role of the proposed strategies. Finally, we generated a set of descriptive statistics to illustrate the relative frequency of experts' use of each strategy.

Results

As indicated in Table 1, our analysis of the data corpus shows that expert chemists employed 8 unique strategies for completing authentic organic chemistry assessment tasks. By far, the majority of problem-solving approaches were characterized by analytic strategies that included parsing diagrams into sub-structures, duplicating spatial relationships and employing heuristics to generate intermediate diagrams. Expert strategies also included an array of imagistic approaches. Such strategies included the use of both ego- and exocentric perspective-taking, mental rotation, and simulated spatial transformations. While there were several common approaches to solving particular tasks, the experts displayed a wide variety of individual differences in their approaches: each expert employed imagistic and analytical approaches to varying degrees on similar tasks.

Table 1: Major expert problem-solving strategies in organic chemistry.

Strategy	Occurrences
<i>Imagistic Strategies</i>	
Visualization of Spatial Relationships to Generate a New Structure	21
Visualization of a Given Structure to Understand the Problem	11
Visualization to Explain a Solution to the Interviewer	10
Visualization of a Self-Inscribed Structure to Verify the Answer	3
<i>Analytical Strategies</i>	
Basic Recall of a Known Structure/Reaction Mechanism	47
Use of a Diagram Template to Generate a New Structure	20
Analytical Spatial Transformation to Generate a New Structure	9

As a group, the experts employed analytical strategies on the majority of interview tasks. Frequency counts indicate that 81 (64%) of the strategies used by experts were analytical strategies. Such strategies corresponded to recalling known answers, reasoning from basic template structures, application of discipline-based algorithms (e.g., naming systems), and simple heuristics (e.g., alternating carbon bond positions to generate isomers). Although as a group, the experts applied analytical strategies in the majority of cases, these trends were not apparent on the individual level: some experts were observed to use only analytical strategies while others applied imagistic strategies more extensively. Conversely, the experts employed imagistic strategies on 45 (36%) of the tasks. Such strategies were characterized by the self-reported inspection and mental transformation of a mediating internal spatial representation. We observed the experts engage in this strategy for a variety of purposes including the initial analysis of a problem, generation of novel structures, evaluation of final proposed structures and explanation of spatial relationships to the interviewer.

Given space constraints, we are unable to detail each of the identified strategies here. However, we offer two case studies of unique expert problem-solving strategies on one specific task from the corpus. The first task exemplifies an analytic strategy that was characterized by the recall and inscription of a diagram template that allowed the expert to make explicit complex three-dimensional relationships between atoms within a molecule without engaging in imagistic reasoning. The second case depicts an imagistic reasoning strategy that a second expert used to imagine the view from inside a molecular structure to generate a novel diagram.

Representative Interview Task

Both case studies below describe expert problem solving on the fourth task in the interview protocol. The task and its solution are illustrated in Figure 2. For this task, participants were asked to draw a specific molecular representation, a Newman Projection, of the given structure. Generally speaking, chemists use Newman projections to display the spatial relationships between adjacent bonds that are responsible for the overall conformation of a molecule. Ostensibly, students must be able to imagine how the indicated molecule appears when viewed from an alternative perspective (indicated by the arrows in Figure 2) and render that view in the Newman projection. Additionally, one must understand the basic structure of a cyclic molecule, the formalisms of the given diagram which imply, but do not show, relevant atoms, and the representational constraints of the desired Newman Projection. Because the task requires participants to consider complex three-dimensional relationships and illustrate those relationships in a unique two-dimensional diagram success on such a task does appear to be highly dependent upon a persons' ability to visualize the given structure. Thus, we were primarily concerned with examining whether experts did indeed use imagistic strategies on such a task.

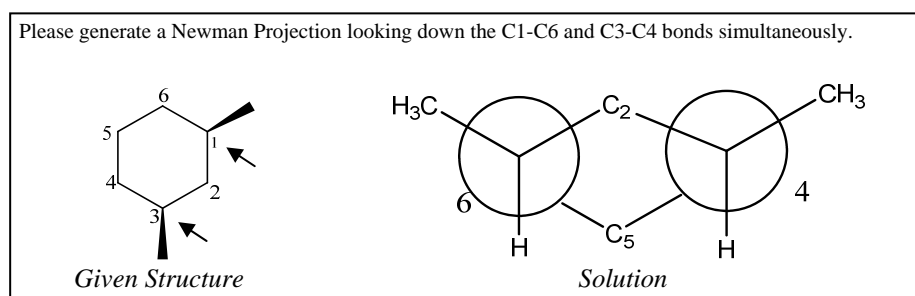


Figure 2. "Newman Projection Task" and its solution.

Use of a Diagram Template to Generate a New Molecular Structure

The first case of problem solving that we present illustrates experts' preference for using known diagram templates to reason about complex three-dimensional spatial relationships. Across tasks, experts revealed a familiarity with several template molecular diagrams that they often employed to represent generic molecular structures. 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. Each expert displayed familiarity with this strategy; however, not all experts employed the strategy across all tasks. We discuss the transcript from one expert's protocol below to illustrate the application and potential of using diagram templates. Utterances and behaviors used to determine strategy are indicated in bold in the transcript.

Bob: (*Bob draws two circles immediately on the white board, Figure 3A.*) 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 3B. He then inspects the given diagram and adds the indicated methyl groups to his generic diagram to generate a final solution, Figure 3C.*)

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 is my 3. (*Bob makes a slicing gesture with his hand to indicate a horizontal plane cutting through 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 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.**

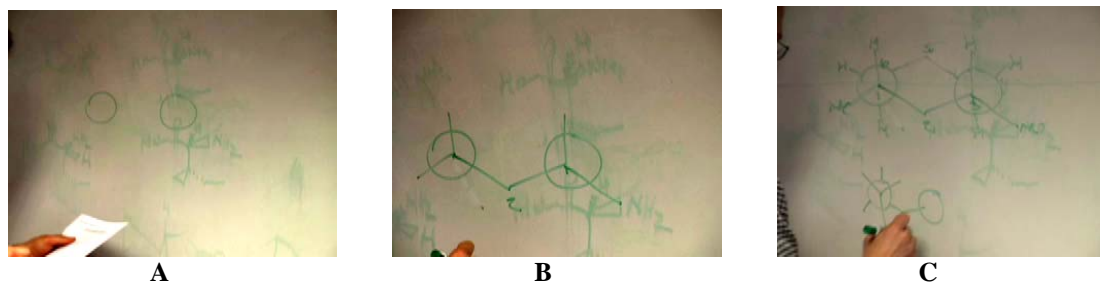


Figure 3. Bob’s use of an example diagram template strategy.

In the above excerpt, Bob reveals an intimate familiarity with the basic structure of any Newman Projection, which he immediately inscribes upon reading the task. As shown in Figures 2 and 3, all Newman projections are based on a circle-and-stick formalism. In the Newman projection, the dots in the center of each circle represent the first carbon atoms one would see when looking at the molecule from an oblique angle (C1 and C3) and the circle represents the carbon atoms immediately behind (C6 and C4). The sticks or “spokes” of the circle represent the three atoms connected to each carbon under consideration. Given this basic template diagram, any Newman projection can be constructed by amending it with the constituent atoms of any specific molecule. 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.”

As he proceeds toward a solution, Bob realizes that his final solution 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 black wedges in the given diagram (Fig. 2) indicate groups of atoms that are projecting above the plane of the paper. Bob, however, has drawn a Newman projection that indicates these same groups would project below 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. As he indicates with his slicing hand, he has drawn the relevant groups on the same side of the molecule as they were indicated in the given diagram. Therefore, Bob concludes that his diagram is a faithful Newman projection of the given diagram without the need for engaging in mental transformations or gestalt rotations of the structure to make a comparison.

Reasoning About Spatial Relationships Via Imagistic Reasoning

In contrast to the analytical strategy exemplified by Bob above, some experts instead preferred to employ an imagistic strategy to reason about spatial information on this task and others in the corpus. Using

such strategies, experts often reported the perceived experience of “seeing” the three-dimensional structure implied in the two-dimensional diagrams. In many cases, the perception of the three-dimensional features of the molecules preceded an imagined mental transformation (e.g., translation, rotation, distortion) that the experts executed to gain new insights on the structure. Such operations appeared to be distinct from other expert’s self-reported experience of imagining themselves viewing the molecule from new angles or from within an imagined three-dimensional image of the molecule. Here, we detail one expert’s successful use of this latter strategy.

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 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. 4A and 4B. He then lifts the paper to the level of his gaze in Fig. 4C 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 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. 4D.*) and then they get a feel for this ...

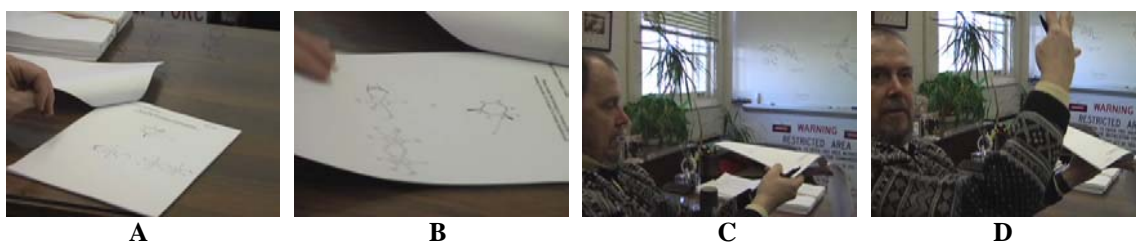


Figure 4. Dan’s example use of an imagistic reasoning strategy on Task 4.

In this excerpt, Dan illustrates how he personally employs imagistic reasoning to complete the given 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’. 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 the interviewer. To clarify, he physically rotates and lifts up the task packet to illustrate the imagined perspective-taking.

Dan’s strategy is markedly different than the analytical strategy employed by Bob. Although it is clear that Dan is also familiar with the basic skeleton structure of a Newman projection, he does not simply inscribe the skeleton and make amendments to it. Rather, Dan displays a preference for imagining how the given structure would be viewed if he himself were to perceive it in three dimensions. To gain this information, he mentally “views” the structure as if he were facing the diagram 30 degrees from his seated position, which he illustrates by pantomime at the end of the interview. With the same conviction Bob displayed for using a

template strategy, Dan is adamant that for him an imagistic strategy is necessary for successful problem solving and that he actively teaches students to employ his strategy as well.

Conclusion & Implications for Instruction

We consider the results of this work to offer a preliminary description of the problem-solving strategies that expert chemists employ to reason about authentic classroom assessment tasks. Foremost, we have shown that experts, like students, are able to employ analytical strategies to complete tasks that ostensibly require imagistic reasoning. Thus, we question prior claims that suggest imagistic reasoning is the requisite strategy for successful problem solving in chemistry. The small sample of experts in our study revealed that they have available several strategies for reasoning about spatial relationships in molecular structures *without* engaging in the generation and inspection of internal mediating spatial representations. Likewise, the present analysis addresses lingering assumptions in the public about who can succeed in science. Claims persist in various public forums (e.g., Fogg, 2005) about the critical need for highly developed visuo-spatial skills for general success in advanced science. By documenting which tasks truly require imagistic reasoning or other forms of spatial cognition, we hope to marginalize the role of individual or group differences in visuo-spatial ability in science.

Our identification of the alternative analytical and imagistic reasoning approaches here also offers tentative implications for pedagogy in undergraduate chemistry. First, the successful application of the analytical strategies we observed required a strong familiarity with the formalisms of molecular diagrams. In the above excerpt, Bob was able to avoid imagistic reasoning by first inscribing a known template diagram that depicted important spatial relationships by its very nature. To successfully employ such a strategy students need extensive training in the constraints and affordances of the available spatial representations in chemistry beyond current practices. Typically, less than one month of yearlong instruction in organic chemistry is devoted to developing students' ability to understand and translate between molecular representations. The bulk of coursework is devoted instead to direct instruction about the structure and reactivity of several organic substructures. We instead advocate for more extensive training in the depiction of and translation between different molecular representations to achieve representational competence in math and science as advocated elsewhere (Kozma & Russell, 1997; Nathan, Stephens, Masarik, Alibali, & Koedinger, 2002).

Second, student understanding and achievement may benefit from instruction and activities that help them choose between imagistic and analytical strategies. This contrasts with a suggested emphasis on training imagistic reasoning skills in chemistry (Ealy, 2004; Ege, 2003; Ferk, Vrtacnik, Blejec, & Gril, 2003). Instead, instructors might reflect on their own preference for employing imagistic strategies for some specific tasks and analytical strategies on others. Rather than teaching the limited use of either strategy, new approaches might instead make students aware of the alternative strategies. Likewise, instructors may employ a formative assessment rubric such as our analytical framework to attend to students' utterances and gestures and guide them to use different reference frames or to adopt an analytical strategy. Undoubtedly, analytical strategies like "basic recall" can be achieved only through practice and expertise in the discipline. Nevertheless, students may benefit from specific lessons on how to perceive spatial information embedded in unique molecular representations by using templates or labeling atoms when translating or re-rendering representations, as identified in some of the expert strategies. As Stieff (2004) has previously shown, students are capable of using both imagistic and analytical 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 analytical strategies on a wide variety of tasks.

In conclusion, the common approaches to problem solving shared by our participants suggest that the role of imagistic reasoning in organic chemistry, and other science disciplines, should be reconceived by both educators and researchers. That many tasks and concepts in science concern imperceptible three-dimensional objects and their interactions is without question; however, the presence of such spatial information in these domains does not necessitate the exclusive use of imagistic reasoning for successful problem solving. Rather, the above analysis of expert problem solving in organic chemistry, which takes spatial relationships within molecular structures as a central concern, illustrates that imagistic reasoning is only one of several strategies experts employ. Future investigations and pedagogical approaches must take care to avoid privileging the role of imagistic reasoning in science at the cost of ignoring the alternative avenues to success available to students.

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