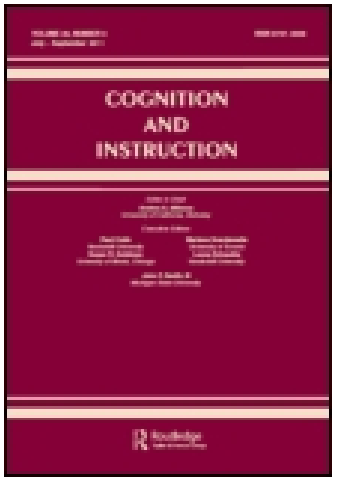

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Representational Translation With Concrete Models in Organic Chemistry

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Representational Translation With Concrete Models in Organic Chemistry

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In representation-rich domains such as organic chemistry, students must be facile and accurate when translating between different 2D representations, such as diagrams. We hypothesized that translating between organic chemistry diagrams would be more accurate when concrete models were used because difficult mental processes could be augmented by external actions on the models. In three studies, the task was to translate between different diagrams of molecules with or without a model. The model groups outperformed control groups, and students who received and used models outperformed those who received but did not use models. Uses of the model suggested that participants were performing external actions to support or replace difficult mental spatial processes. Spatial ability was a much weaker predictor of performance than model use. Results suggest that concrete molecular models can be an effective learning tool but some students need direct instruction to be able to take advantage of models.

Scientists routinely employ many diverse representations in practice, although novices often have difficulty mastering the use of representations in scientific disciplines, such as biology, physics, chemistry, geosciences, and mathematics (Ishikawa & Kastens, 2004; Kastens & Ishikawa, 2006; Kozma, 2003; Novick & Catley, 2007; Schoenfeld, 1992). For example, children as well as adults often fail to understand that a graph is a representation of trends in a data set rather than a picture of its referent (Kozhevnikov, Hegarty, & Mayer, 2002; McDermott, Rosenquist, & van Zee, 1987). Difficulties are compounded when multiple representations need to be related and integrated for meaningful learning (Ainsworth, 2006). Without integrating information across representations, students run the risk of developing disjointed knowledge.

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For students to be successful in scientific disciplines, they must develop the skills of constructing, interpreting, and translating between various representations. Collectively, these skills are important aspects of representational competence in a discipline (Kozma & Russell, 1997, 2005; Kozma, Chin, Russell, & Marx, 2000; Wu, Krajcik, & Soloway, 2001; Nathan, Stephens, Masarik, Alibali, & Koedinger, 2002). More generally, it is beneficial for students to develop meta-representational competence, which includes the ability to understand the advantages and disadvantages of particular representations and to select optimal representations for particular purposes (diSessa, 2004; diSessa & Sherin, 2000). The focus of this article is on representation translation as an essential aspect of representational competence in the domain of organic chemistry.

Chemistry is an ideal domain in which to study representational competence. Chemists rely heavily on multiple external representations, such as chemical formulas, molecular diagrams, and concrete models (Cheng & Gilbert, 2009; Goodwin, 2008; Harrison & Treagust, 2000; Hoffmann & Laszlo, 1991). Each of these representations was created for a specific purpose in the history of chemistry and often preceded major developments in the field (Goodwin, 2008). As the discipline has developed, chemists have created different representations to develop a comprehensive understanding of chemical concepts, for example, molecular structure and reactivity. As such, chemists routinely translate back and forth among different representations while teaching and problem solving, and include multiple different representations in publications of their research (see e.g., Chérest & Felkin, 1968; Summerscales, Cloke, Hitchcock, Green, & Hazari, 2006; Wipf & Jung, 1999).

Students who are enrolled in typical courses in chemistry often struggle with coordinating multiple representations and translating between them (Bucat & Mocerino, 2009; Kozma & Russell, 1997; Stieff & McCombs, 2006). Such difficulties are readily apparent on classroom assessments that include various types of representations (Kozma, 2003) and complex problems that require students to translate between representations, especially spatial representations, such as structural diagrams of molecules (Pribyl & Bodner, 1987; Wu & Shah, 2004; Harle & Towns, 2011; Keig & Rubba, 1993). As students advance through the chemistry curriculum, they are exposed with increasing frequency to new and diverse representations (Ealy, 2004) and are regularly asked to translate newly learned representations into representations introduced earlier in the curriculum.

Many of the representations employed in the chemistry curriculum support thinking and reasoning about spatial relationships within and between molecules (Wu & Shah, 2004). Spatial thinking is an important aspect of chemistry problem solving, because the reactivity of molecules is predicted not just by the number and type of atoms that make up a molecule, but by the spatial configuration of these atomic substituents (i.e., functional groups of atoms). Altering the spatial configuration of substituent atoms can have dramatic and consequential effects on a molecule's reactivity. For example, maleic acid and fumaric acid have the same atomic makeup and differ only in the spatial configuration of their atoms (they are stereoisomers; i.e., they differ in geometric arrangement), yet maleic acid is a potent toxin and fumaric acid is a common food additive.

Chemists use two general types of spatial representations of molecules: concrete models, which are physical 3D models that represent the 3D spatial relations between atoms in a molecule; and 2D diagrams, which use conventions to represent 3D relations in the two dimensions of the printed page (see Figure 1). Although these are all representations, rather than true models, in the philosophical sense (Peirce, 1994; Wartofsky, 1979), we use the term model to refer to concrete

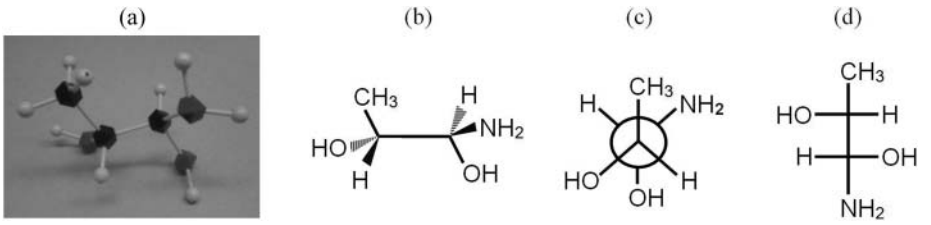

FIGURE 1 Four structural representations of an organic molecule. (a) A concrete (ball-and-stick) model where color is used to denote different atoms. Black is carbon and white is hydrogen. (b) Dash-Wedge diagram, (c) Newman diagram, and (d) Fischer diagram of the same organic molecule depicted in the ball-and-stick model.

models, as this is consistent with chemists' use of the term. We use the term diagram to refer to 2D representations. Expert chemists rely routinely on both concrete models and diagrams in their work and teaching, although computer visualizations of molecular structure are becoming more common (Francoeur & Segal, 2004).

In these studies, we examine how students translate between different diagrams and whether and how they use concrete models in the translation process. In addition to its theoretical importance as a measure of representational and meta-representational competence, the task is ecologically valid for several reasons. First, it tests the degree to which students understand how the various representations depict molecules. Second, asking students to translate between different diagrams of the same molecule is a good test of whether they fully understand the three-dimensional structure of molecules, and therefore it is often used on typical organic chemistry assessments (cf., American Chemical Society, 2010). Third, because different representations are used for different purposes in chemistry, experts often switch between different representations as necessary.

REPRESENTATIONS IN ORGANIC CHEMISTRY

We focus on translations among three types of diagrams commonly used in organic chemistry, which students must master in their first college course in this topic. These are the *Dash-Wedge diagram*, the *Newman projection* and the *Fischer projection*. Multiple diagrams such as these are employed in organic chemistry because they serve different purposes, and each makes salient different features of a molecule's structure. The Dash-Wedge diagram, illustrated in Figure 1b, is effective at depicting the spatial arrangement of substituents within a molecule. In contrast, the Newman projection, illustrated in Figure 1c, was invented to show that with the rotation of a carbon-carbon single bond, the energy of the molecule will vary. These energetic differences are a result of the relationships, and potential strain, between specific substituents on adjacent carbon atoms. A third diagram, the Fischer projection, illustrated in Figure 1d, was invented by chemists to highlight the different stereochemical (3D) relationships between members of the same carbohydrate family. The Fischer diagram makes it easier to illustrate the relationship among various carbohydrates.

Organic compounds have distinctive structures; they commonly consist of a chain of carbon atoms linked with single bonds, referred to as the "carbon backbone," to which substituents are attached. Furthermore, the relative locations of the substituents in 3D space around the carbon backbone determine the physical and chemical properties of a molecule. Dash-Wedge, Newman,

and Fischer diagrams use different conventions to convey this 3D structure, and each presents a view of the molecule from a different spatial perspective. For example, the three diagrams in Figure 1 all represent the same molecule with a 3-carbon backbone. The Dash-Wedge diagram (Figure 1b) shows a side view of the molecule with different symbolisms (i.e., line, wedge, and dash) representing the bonds in three dimensions. The solid lines represent bonds in the plane of the page, the wedges symbolize bonds that are coming toward the viewer and the dashes indicate bonds going away from the viewer. The Newman projection (Figure 1c) offers an end-on view of the molecule. In this representation, the circle represents the molecular bond between two specific carbons within the carbon backbone, and the substituents attached to these two carbons are represented around the circle; the six lines in the Newman projection represent the three substituents attached to each of the carbon atoms. Finally, the Fischer projection (Figure 1d) shows a third perspective of the molecule (i.e., the entire molecule has rotated ninety degrees to present the carbon backbone vertically). In a Fischer projection, horizontal lines represent bonds coming towards the viewer, vertical lines represent bonds going away from the viewer, and intersections between horizontal and vertical lines represent carbon atoms. For the novice in chemistry, it is helpful to think of each of these representations as different orthographic projections of a molecule.

The Dash-Wedge, Newman, and Fischer diagrams not only show orthographic perspectives, they also represent the molecule at different levels of spatial abstraction. The Fischer diagram does not explicitly display any depth information necessary to show 3D structure; conversely, the Dash-Wedge and Newman projections use different conventions to provide depth information. The Fischer projection includes a further distinction in that it always depicts a molecule in an eclipsed conformation rather than a staggered conformation. A conformation is a spatial arrangement of atoms in a molecule that can come about by rotating the molecular substituents around the bonds without breaking any bonds. In an eclipsed conformation, substituents on adjacent carbons in the backbone occlude each other when viewed end-on, as illustrated in Figure 2. In this example, one must perform a 180° rotation of the back carbon atom and its substituents (DEF in Figure 2) to move between the staggered and eclipsed conformations as illustrated. Dash-Wedge diagrams can also be illustrated in either an eclipsed or a staggered conformation.

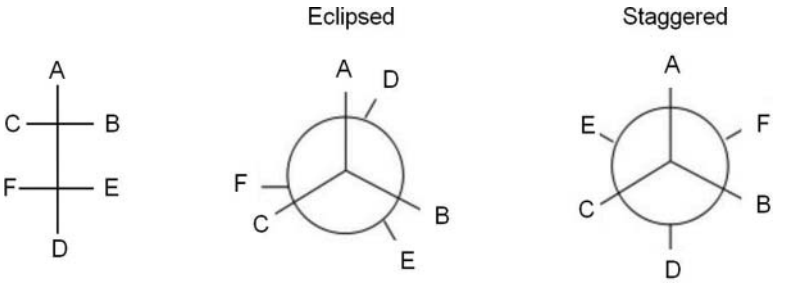

FIGURE 2 A Fischer projection (left) always uses an eclipsed conformation. A Newman diagram can represent either an eclipsed conformation (middle) or a staggered conformation (right). Note: The off-set illustrated in the eclipsed Newman diagram is a convention used to depict the overlap without occluding the substituents on the back chiral carbon. Although not illustrated as such, the substituents of the front chiral carbon (ABC) in an eclipsed conformation should be imagined to completely occlude the substituents of the back chiral carbon (DEF).

In contrast to each of these molecular diagrams, no conventions are required to represent the three-dimensional structure of the bonds in the ball-and-stick model (Figure 1a) because the model itself is three-dimensional and the balls are drilled with holes that constrain the angles between the atoms. However the model incorporates other conventions. For example, even though atoms are made up of subatomic particles, they are represented as colored balls and the molecular orbitals (bonds) between atoms are simplified as solid sticks.

REPRESENTATIONAL TRANSLATION

Students and experts employ a variety of strategies to translate between representations such as Dash-Wedge, Newman, and Fischer diagrams (Stieff & Raje, 2010; Stieff, 2011). The following are two possible strategies, one analytic and one imagistic. First, a student might employ an analytic strategy that transposes the drawn substituents from one diagram to another (Stieff, 2011). For example, translating from the Dash-Wedge diagram in Figure 1b to the Newman diagram in Figure 1c can be accomplished by first moving the three substituents on the left triad of the Dash-Wedge to the front (i.e., 12, 4, and 8 o'clock) of the Newman, while preserving their circular order, followed by moving the substituents on the right triad of the Dash-Wedge to the back (i.e., 2, 6, and 10 o'clock) of the Newman, again while preserving their order. With such a strategy, it may not be necessary to imagine either diagram in three dimensions. However, without an understanding of how the symbol manipulations relate to the underlying three-dimensional structure of the molecule, it may be difficult for novices to remember the exact steps of this procedure, each of which introduces an opportunity for error. Furthermore, translating to a Fischer diagram is more complex, because it involves converting from a staggered to an eclipsed conformation.

Alternatively, employing imagery, translating between a Dash-Wedge and a Newman diagram might include the following cognitive steps. First, one might interpret the spatial conventions of the Dash-Wedge formalism to imagine the 3D structure that it represents. Next, the imagined structure might be mentally rotated to the orientation of the Newman projection, while maintaining the imagined spatial relations between parts of the structure. Finally, the spatial relations between the parts of the rotated image might be transformed into the spatial conventions of the Newman projection to be drawn. Mentally rotating such a complex structure is likely to be effortful and error prone and is probably not performed (Bethell-Fox & Shepard, 1988).

How might a 3D model aid in this translation process? First, a model can represent the three-dimensional structure externally, so that the conventions of a diagram (for depicting the 3D structure of the molecule in the 2 dimensions of the page) do not have to be maintained in working memory. Thus, simply viewing a model may be beneficial. Second, one can physically rotate the model and observe the results rather than mentally rotating, or changing one's perspective of an internal representation, and observe the results. This is an example of what Kirsh (1995a) refers to as a complementary action, that is, an action performed in the world as a substitute for a mental process. While mental rotation is a process in the mind, rotating a model is an action in the world, although the action is guided by cognition and the results of the rotation are observed and encoded by the mind.

Given the potential advantages of a model, we might expect that if students have a model of the relevant molecule available while performing a diagram translation task, they would readily use the model to perform the necessary spatial transformations. Specifically, if using the external

rotation strategy, students should rotate the model to align it to the diagram they wish to draw and reconfigure it if the translation involves a change between a staggered and eclipsed conformation. We predict that the models will be manipulated in this way and used in the course of diagram translation, and not just to check the solution (i.e., after drawing). These predictions are in line with the minimum memory hypothesis proposed by Kirsh (1995b, 1997; Hollan, Hutchins, & Kirsh, 2000), which suggests that when a mental process can be replaced by a physical one, the physical process is performed. Moreover, they are consistent with the general assumption among chemistry educators about use of molecular models (Justi & Gilbert, 2002).

However, it is important to realize that using models to aid in a spatial transformation task may not be easy for everyone (cf. Keehner, Hegarty, Cohen, Khooshabeh, & Montello, 2008), as this strategy involves understanding the correspondence between the model and diagrams, competition with alternative strategies, and meta-representational competence. First, effective use of a model in diagram translation depends on understanding how parts of the model map on to parts of the diagram (e.g., CH_3, maps on to a large black ball with three small white balls attached and H maps on to a single small white ball). Mapping the units of the model and diagram might be particularly difficult when they are not structurally aligned (Gentner, 1983; Markman & Gentner, 2000).

Second, participants may not use models if they have learned analytic translation strategies that do not rely on considering the 3D structure of the molecule (Stieff, 2007; Stieff & Raje, 2010). Under these circumstances, using a model may be perceived to be more effortful than alternative strategies. This possibility is more compatible with the soft constraints hypothesis (Gray & Fu, 2004), which states that complementary actions are not necessarily preferred and the choice between using internal processes and external actions is affected by the comparative ease of using the two strategies. Third, and related to this, strategy selection could be affected by a student's assumptions about the utility or relevance of the models. That is, use of models relies on meta-representational competence to know that and how the models can be used to help accomplish the task. For all of these reasons, students might not use models, despite their potential usefulness for the task.

Finally, spatial ability may also affect the real or perceived usefulness of a model. Success in chemistry problem solving is correlated with spatial ability (see Harle & Towns, 2011 for a review) and spatial ability has been shown to be specifically related to performance in organic chemistry (Bodner & McMillan, 1986; Pribyl & Bodner, 1987), although not always (Keig & Rubba, 1993). Because of the spatial nature of the representation translation task, we expect that performance on this task will be correlated with spatial ability. However, we make no a priori predictions about the interaction between spatial ability and model availability (i.e., how availability of a model might affect the relation between spatial ability and performance). On the one hand, a model can support an internal process (e.g., mental rotation) by replacing or augmenting it with a physical action (rotating the model) so that models might be particularly helpful for students with low spatial ability (who are poor at mental rotation). However, another possibility is that spatial ability is needed to map the units in the model to those in the diagram or to interpret the new view of a model that results from a rotation. In this case, high spatial individuals may be more able to benefit from a model. Finally, it is possible that because of a combination of these factors, models are equally helpful to high-and low-spatial individuals.

This article reports three studies. Study 1 examined whether and how students spontaneously use models to translate between diagrams and assessed the relationship between uses of the

models and success in diagram translation. Study 2 tested whether encouraged use of models versus not having models contributed to success in representation translation. Study 3 tested whether structurally aligning the models with the diagrams (to assist participants with mapping the correspondence between the models and diagrams) contributed to success in representation translation.

STUDY 1

Study 1 was a correlational study that examined how organic chemistry students spontaneously used concrete models while translating between different molecular diagrams and how their use of models contributed to translation accuracy. Participants were organic chemistry students in a research university who had been introduced to the representations (diagrams and models) in their lectures and textbooks.[1] This study established a baseline understanding of whether and how they use models as aids for translating among chemical representations. The following questions were addressed: Do participants spontaneously use concrete models to help them translate molecular diagrams? How do participants use concrete models? Specifically, do participants realign the model with the diagram to be drawn? Is use of concrete models correlated with diagram translation accuracy? Is spatial ability independently related to accuracy in translating between molecules?

We hypothesized that use of concrete models would be associated with translation accuracy because models allow a difficult internal process to be replaced or augmented by an external action. Specifically, aligning the model to the orientation of the diagram to be drawn should be a predictor of translation accuracy. Second, we expected that spatial ability would be associated with translation accuracy in general, because the task of encoding and translating between structural diagrams is highly spatial. We examined the combined effects of spatial ability and use of models, but we did not make any a priori predictions about how their effects would combine.

Method

Participants. The participants were 30 college students (12 men, 18 women; $M = 20.3$ years, $SD = 1.4$) who had been introduced to the molecular representations in the context of an introductory organic chemistry class (12 were concurrently enrolled and 18 had previously completed the class).[2] Participants received $20 or course credit for their participation.

Materials. The study materials included an informed consent sheet, a diagram description sheet, a set of 12 diagram translation problems (see Appendix A), six concrete ball-and-stick models, a demographics questionnaire, and a spatial ability test.

[1]Students at this campus are not required to own a molecular modeling kit. Although we did not formally ask the students in these studies about model use, other studies have revealed that only about 12% of organic chemistry students at this university own a molecular modeling kit, about 3% own molecular modeling software, and about 23% report that a molecular modeling kit was used in their class, presumably as a demonstration aid for the instructor.

[2]Although our participants differed somewhat in their knowledge of organic chemistry, the representations of interest in this research are all introduced in the first 6 weeks of their first organic chemistry class, and therefore they had all been introduced to these representations. We found no significant differences in any of our studies between performance of those currently enrolled and those who had completed the introductory organic chemistry class.

Diagrams. As illustrated in Figure 1, the three types of diagrams used in this study were Dash-Wedge, Newman, and Fischer, which were familiar to our participants from their course in organic chemistry. The diagram description sheet included a short 67-word paragraph describing the task and an example of each of the three diagrammatic representations to remind students of the names of the diagrams. Because we expected participants to be familiar with the diagrams from their organic chemistry classes, a specific description of each diagram was not provided. A version of this sheet is given in Appendix B.[3]

Diagram Translation Problems. The task for each problem was to translate one diagram of a molecule into a different diagram of the same molecule. Each problem was displayed on an 8.5" × 11" sheet of paper with a diagram of the molecule in one of the three formats (e.g., Dash-Wedge, Newman, or Fischer) at the top of the page and a space for the participant to draw the requested diagram at the bottom of the page. Diagrams of six different straight chain molecules (i.e., molecules with their backbone in a chain and not forming a ring) were each presented twice in sequence, with each given (starting) diagram to be translated into two different diagrams. Thus, there were 12 unique problems, two representing each of six different translation pairs (Dash-Wedge to Newman and vice versa, Dash-Wedge to Fischer and vice versa, and Newman to Fischer and vice versa). Translations to and from specific types of diagrams always involved different molecules (i.e., Dash-Wedge to Newman was of one molecule and its inverse, Newman to Dash-Wedge, was of a different molecule). The starting diagrams, molecule names, and requested target diagrams for these 12 trials are listed in Appendix A in order of presentation.

Concrete Models. An example of a concrete ball-and-stick model of one of the six molecules used in this study is illustrated in Figure 1a. The concrete models were constructed from a commercial molecular modeling kit (HGS Introductory Organic Chemistry Set 1000) that is commonly used in high school and college chemistry courses. The six molecules, named and illustrated in Appendix A, included one 3-carbon molecule, three 4-carbon molecules, and two 5-carbon molecules.

Spatial Ability Test. The Vandenberg and Kuse (1978) Mental Rotation Test (MRT), a 20-item test administered in two 3-minute blocks, was used as a measure of spatial ability. Each item consisted of a row of five block figures. The left-most figure was the goal figure. Two of the four figures to the right of the goal figure were different from the goal figure by a rotation. The other two figures could not be rotated into congruence with the goal figure. The participant's task was to mark the two figures that could be rotated to match the goal figure. Each item was worth four points; a participant's MRT score was calculated by adding one point for each hit or each correct rejection, and subtracting one point for each miss or false alarm. This test of spatial ability was

[3]The information on the instruction sheet in italics was added for later studies due to the results of Study 1, which revealed that participants did not always remember the conventions of the diagrams, something that we did not anticipate in Study 1.

chosen because mental rotation is thought to be a component of the imagistic strategy to solve our translation problems.

Procedure. Participants were tested individually. After giving informed consent, they studied the diagram description sheet at their own pace. This sheet remained available to them throughout the task. Second, participants were given the 12 diagram translation trials, one at a time, and were instructed to translate each of the given diagrams by drawing the target diagram in the blank space at the bottom of the page. The type of diagram to be drawn (Newman, Fischer or Dash-Wedge) was stated above the given diagram. Again, this task was not timed. During each trial, the concrete model of the molecule in question was placed on the table in front of and within easy reach of the participant. The model was placed with its long axis perpendicular to the observer's line of sight in order to minimize viewing occlusions. For each set of two consecutive problems, the given diagram (e.g., a Dash-Wedge diagram of a specific molecule) was the same and participants were asked to draw the other two diagrammatic formats (e.g., a Fischer diagram on one trial followed by Newman diagram on the second trial; see Appendix A). The models were not repositioned between these two consecutive trials. After each pair of trials, the model was replaced with the model of the molecule in the next pair of trials. The Dash-Wedge and Newman projections used in this study were always shown in a staggered conformation (see Figure 2). Participants were neither encouraged nor hindered from viewing or moving the models. Participants were videotaped with their permission. Third, participants completed a short demographic questionnaire. Finally, participants completed the spatial ability test before being debriefed.

Scoring. Drawings were scored as fully accurate if the correct substituents were drawn on the correct chiral carbons and in the correct circular order around both chiral carbons.[4] A system of partial credit was also assigned as follows. Fully accurate diagrams were scored as Level 3 in this system. Diagrams were scored as Level 2.5 if the substituents were connected to the correct chiral carbons but the circular order of substituents was incorrect around one of the chiral carbons. Diagrams with the correct connectivity but incorrect circular order around both chiral carbons were scored as Level 2. Drawings were scored as Level 1 if the correct substituents were included, but were not connected to the correct chiral carbons. Level 0 was assigned to drawings with more serious errors, including drawing the wrong diagram form, omitting substituents, or incorrectly representing substituents (e.g., including atoms that were not in the given molecule). An organic chemistry expert reviewed and ratified the scoring criteria as reasonable. This system of awarding partial credit for drawing performance was used to categorize both individual problem solutions and participants by level of performance. Participants were assigned to a level of performance based on the highest level at which two-thirds or more of their drawings were scored (i.e., Level 2 participants were those for which two-thirds of their drawings were scored Level 2 or above).

Videotapes were coded for three model use behaviors: moving the model to align it in the general orientation of the starting diagram (Align-Start), moving the model to align it with the general orientation of the target diagram (Align-Target), and reconfiguring the model (Reconfigure)

[4]A chiral carbon is a carbon atom in which four different groups of atoms are bonded. All of the molecules used in these studies had exactly two adjacent chiral carbons in their carbon backbone.

by rotating the substituents around their bonds. In addition, each Align-Target behavior was also coded for when it occurred in the drawing sequence (i.e., if the participant aligned the model to the target diagram before, during, or after drawing the target diagram). The drawn diagrams and videotapes were independently scored by two coders. Interrater reliability was high for scores of drawing accuracy ($r = .99$, $p < .001$) and type of model use (Align-Start: $r = .92$, $p < .001$; Align-Target: $r = .89$, $p < .001$; Reconfigure: $r = .99$, $p < .001$). Inconsistencies between raters were resolved by a third rater.

Results and Discussion

Did Participants Spontaneously Use Models? The left section of Table 1 lists the observed model use behaviors along with the proportion of trials (averaged over 30 participants) for which these behaviors were observed. Participants varied in whether and how much they spontaneously used the models while performing the translation task. Notably, less than half of the participants (14 participants or 47%) used the models at all; eight participants (27%) used the models on at least half of the trials; and only one participant (3%) used the models on every trial.

How Did Participants Use the Models? Uses of the models included rotating the model to align it with the orientation of the diagram that they started with (Align-Start) and aligning the model with the orientation of the diagram to be drawn (Align-Target). Align-Start and Align-Target occurred together on 7% of all trials across all participants, with Align-Start preceding Align-Target on 74% of those trials. This behavior would be expected if students first matched the model to the given diagram and then performed an external rotation to replace or augment a mental rotation. The lower frequency of Align-Start suggests that participants accepted that the model and given diagram were representations of the same entity (rather than first verifying the correspondence between the diagram and model) and focused on the essential step of rotating the model to align it with the diagram to be drawn.

Reconfiguring the models (i.e., rotating the bonds within the models) was observed less commonly. This behavior is most relevant when translating to a Fischer diagram from one of the other two diagrams, because the Fisher diagram uses an eclipsed conformation. However, reconfiguring the model was not only exhibited on these trials. Participants reconfigured the models more often when translating to a Fischer diagram (38% of all reconfiguration behaviors) and to a Dash-Wedge diagram (38% of all reconfiguration behaviors) than to a Newman projection

TABLE 1
Incidences of Types of Uses of the Concrete Models During Representation Translation

	Study 1		*Study 2*		*Study 3*	
Model Use Behaviors	*Percentage of Participants*	*Mean Proportion of Trials M (SD)*	*Percentage of Participants*	*Mean Proportion of Trials M (SD)*	*Percentage of Participants*	*Mean Proportion of Trials M (SD)*
Align to Start	40%	.09 (.16)	81%	.24 (.24)	na	na
Align to Target	43%	.23 (.31)	75%	.35 (.36)	90%	.54 (.38)
Reconfigure	17%	.07 (.16)	47%	.22 (.34)	47%	.16 (.23)

TABLE 2
Means and Standard Errors for Drawing Accuracy (Level 3) and Spatial Ability Measures for Models and No Models Conditions and for the Use Models and Have Models Subgroups of the Models Condition

Study	*Group*	*n*	*Drawing Accuracy M (SE)*	*Spatial Ability M (SE)*	*Experience M (SE)*
Study 1	Models	30	.31 (.45)	38.73 (3.01)	1.67 (0.16)
Study 2	Models (all)	32	.40 (.05)	43.44 (3.57)	1.63 (0.15)
	Use	13	.66 (.06)	50.62 (4.93)	1.46 (0.22)
	Have	19	.23 (.05)	38.53 (4.08)	1.74 (0.18)
	No Models	32	.26 (.04)	38.94 (2.79)	1.50 (0.14)
Study 3	Models (all)	30	.33 (.04)	29.87 (2.72)	2.17 (0.13)
	Use	18	.45 (.05)	34.78 (3.39)	2.28 (0.17)
	Have	12	.16 (.06)	22.50 (4.15)	2.00 (0.21)
	No Models	29	.24 (.04)	31.03 (2.67)	2.19 (0.14)

Drawing accuracy is measured in proportion correct, spatial ability is the raw value out of a maximum of 80, and experience is measured in the number of college organic chemistry courses attended.

(25% of all reconfiguration behaviors), but these frequencies were not significantly different (X^2 (2, $N = 30$) = 3.23, $p = .20$). Reconfiguring a model independently of the need to convert from an eclipsed to a staggered conformation (or vice versa) may reflect exploratory behavior or an attempt by the participant to produce the most energetically efficient conformation of the molecule. Although this was not a requirement of our task, it is a common task in organic chemistry classes.

Is Use of Models Correlated With Drawing Accuracy? The frequency of fully accurate (Level 3) drawings was low overall ($M = .31$, $SD = .25$, see Table 2). However, the analysis of levels of accuracy (see Table 3) indicates that the majority of all drawn diagrams ($M = .72$, $SD = .25$) were scored as Level 2.5 or higher. In addition, Table 4 shows that while

TABLE 3
Percentage of All Trials at Each Level of Accuracy Grouped by Study and Condition

Study	*Group*	*n*	*Level 0*	*Level 1*	*Level 2*	*Level 2.5*	*Level 3*
Study 1	Models	30	6	10	13	**41**	31
Study 2	Models (all)	32	3	11	11	34	**40**
	Use	13	2	5	9	19	**66**
	Have	19	4	15	13	**44**	23
	No Models	32	2	11	12	**50**	26
Study 3	Models (all)	30	5	8	11	**43**	33
	Use	18	6	2	10	38	**45**
	Have	12	5	16	12	**52**	16
	No Models	29	3	7	13	**54**	24

The most frequent level is marked in bold font for each condition.

TABLE 4
Number of Participants Performing Consistently at Each Level of Accuracy Grouped by Study and Condition

Study	*Group*	*n*	*Level 0*	*Level 1*	*Level 2*	*Level 2.5*	*Level 3*
Study 1	Models	30	1	4	2	18	5
Study 2	Models (all)	32	0	2	8	13	9
	Use	13	0	0	3	2	8
	Have	19	0	2	5	11	1
	No Models	32	0	2	5	24	1
Study 3	Models (all)	30	0	3	1	22	4
	Use	18	0	0	1	13	4
	Have	12	0	3	0	9	0
	No Models	29	0	3	1	24	1

Participants were assigned to a level of performance based on the highest level at which two-thirds or more of their drawings were scored (i.e., Level 2.5 participants were those for which two-thirds of their drawings were scored Level 2.5 or above).

only five participants performed consistently at Level 3, eighteen of the 30 participants performed consistently at Level 2.5 or above and only seven of 30 performed consistently below this level. Importantly, the distinction between a Level 3 and a Level 2.5 score is a single spatial error of reversing the circular order of substituents around one side of the drawn diagram, indicating that participants had a good understanding of the connectivity of molecular substituents, but often failed to correctly depict their three-dimensional configuration.

The correlations between model use and drawing accuracy are listed in the left section of Table 5. Drawing fully accurate (Level 3) diagrams was positively and significantly correlated with participants' reconfiguration of the model and alignment of the model to the target diagram. Regression results ($b = .42$, $R^2 = .28$) indicate that for each additional Align-Target manipulation (the behavior most highly correlated with drawing accuracy) there was an increase of 0.42 correct drawings. Thus, as predicted, using models helped students to draw the correct three-dimensional structure of the molecules.

TABLE 5
Correlation of Types of Uses of the Concrete Models During Representation Translation With Drawing Accuracy and Spatial Ability

	Study 1		*Study 2*		*Study 3*	
Model Use Behaviors	*Drawing Accuracy r (p)*	*Spatial Ability r (p)*	*Drawing Accuracy r (p)*	*Spatial Ability r (p)*	*Drawing Accuracy r (p)*	*Spatial Ability r (p)*
Align to Start	.35 (.06)	.29 (.12)	.54 (.001)	.27 (.14)	na	na
Align to Target	.52 (.004)	.35 (.06)	.84 (.001)	.33 (.07)	.71 (.001)	.38 (.04)
Reconfigure	.42 (.02)	.31 (.10)	.66 (.001)	.40 (.03)	.53 (.003)	.13 (.49)
Spatial Ability	.58 (.001)		.32 (.01)		.32 (.01)	

Correlations between spatial ability and drawing accuracy were computed for the combined Model and No Model groups, whereas all other correlations included only the Model group.

Is Drawing Accuracy Predicted by Spatial Ability? As predicted, accuracy on the diagrammatic translation task was positively correlated with spatial ability, as shown in Table 5. This table also shows that spatial ability had marginally significant correlations with measures of model use (Align-Start, Align-Target, and Reconfigure). A simultaneous multiple regression analysis was conducted to examine effects of spatial ability and measures of model use on drawing accuracy (Level 3). Together, these four predictors explained 49% of the variance in drawing accuracy ($R = .70$; $F(4,25) = 6.01$, $MSE = .213$, $p < .01$). An examination of the partial regression coefficients revealed that spatial ability ($\beta = .43$, $p = .006$, $sr^2 = .16$) and Align-Target ($\beta = .45$, $p = .026$, $sr^2 = .09$) were both significant predictors of drawing accuracy after controlling for the other variable. Neither Align-Start ($\beta = –.31$, $p = .25$, $sr^2 = .03$) nor Reconfigure ($\beta = .28$, $p = .20$, $sr^2 = .04$) were significant predictors of drawing accuracy after controlling for the other variables.

When do Students Use the Models? If students are using external actions to replace or augment a mental process (e.g., mental rotation) as part of the translation process, then the external actions should be performed before drawing their solution to a problem. Alternatively, they might perform the external action as a check on a solution derived by some other strategy. To examine these possibilities, we coded when participants first aligned the diagram to the target, that is, whether they did so before, during, or after drawing the diagram. We focused on the Align-Target behavior in this analysis, because this behavior was most highly correlated with accuracy. Align-Target was typically performed before (36% of all instances of Align-Target) or during (55%) the act of drawing, rather than after the diagram was drawn (9%) indicating that manipulating the models was part of the solution process, and not just a check.

In summary, Study 1 indicated positive correlations between use of a model and drawing accuracy. The most common type of model interaction, and the one most highly correlated with accuracy, was to rotate the model to the orientation of the target drawing, as one might expect if participants performed an external action that replaced or augmented a mental process (e.g., mental rotation). Importantly, aligning the model with the target typically occurred before or during the drawing of the target diagram and rarely occurred after completing the drawing, suggesting that it was part of the solution process and not just a check on the answer.

Even though performance was generally poor, with less than one third of drawings fully correct (Level 3), a majority (72%) of participants' drawings were accurate in terms of the connectivity between substituents but incorrect in terms of the configuration of substituents in 3D space (Level 2.5). Importantly, this 3D configuration determines the molecules' reactive properties, so this small error in spatial terms is a large error in chemical terms, as it means that the participants drew a molecule with very different reactive properties to the one they should have drawn (e.g., maleic acid and fumaric acid). This common error could occur because students did not appreciate the importance of the 3-D spatial arrangements, because they were unable to preserve the correct spatial configuration in their translations, or because they did not remember how the conventions of the diagrams represent this 3D configuration. A possible benefit offered by the models in developing students' representational competence (including learning the diagram conventions) is that they transparently represent both the connectivity and the 3D configuration of substituents.

In spite of the benefit of models, their use was not common in this study. Students might not have used models because they were unable to establish the correspondence between parts

of the diagram and parts of the model, or because they preferred to use analytic translation strategies. Alternatively, they might not have realized how the models could be used to help with the translations, indicating untrained meta-representational competence.

However, unanticipated methodological limitations of Study 1 might also have somewhat restricted the use of models. Because the goal of Study 1 was to observe spontaneous use of models, model use was neither encouraged nor discouraged. In post-task informal interviews, some participants reported that they were not sure if they were allowed to pick-up the models during the task. Others reported that because they had not used models in their classes, they did not understand which colors represented which atoms, (although illustrations using these color conventions are used pervasively in their textbooks). In Study 2 we addressed these unanticipated limitations of Study 1 by improving our instructions to remind students of the diagrammatic conventions and making it clear that they were not just allowed but encouraged to pick up and use the models.

STUDY 2

Study 2 examines whether providing and encouraging participants to use models offers an advantage over not receiving models. Study 2 addressed the following questions: Is translation accuracy affected by availability of a model? Is use of models predictive of translation accuracy when their use is encouraged? How is model use affected by spatial ability under these circumstances? What are the relative effects of model use and spatial ability on translation? We predicted that participants who received models would use them to perform better on the representation translation task and that model use and spatial ability would independently predict translation accuracy.

Method

Participants. The participants were 64 college students (27 men, 35 women; $M = 19.6$ years, $SD = .77$) who had not participated in Study 1 but were recruited in the same manner. All participants had been introduced to the molecular representations in the context of an introductory organic chemistry class (37 concurrently enrolled; 27 had previously completed the course). Participants were paid $10 or received course credit for their participation. Thirty-two participants served in the models group and 32 in the control group.

Materials. The study materials were identical to those in Study 1 except that the number of translation problems was increased, written descriptions of the three diagrams were added to the instructions, and written and verbal encouragement to use the models was given to participants in the model group. There were 18 translation problems in this study. Diagrams for nine different straight chain molecules were each presented twice in sequence to be translated from the same diagram into two different diagrams, which created 18 unique problems. Translations to and from diagrams were always of different molecules (i.e., Dash-Wedge to Newman was one molecule, and its inverse, Newman to Dash-Wedge, was a different molecule). The nine molecules included

three molecules with each of three lengths of carbon backbone (3-, 4-, and 5-carbon molecules) and are listed in Appendix C by their chemical name and dash-wedge diagrammatic form.

Appendix B presents the written instructions given to the model group in Study 2, which differed from the instructions in Study 1 in that they included a sentence encouraging use of the models. In addition, one paragraph for each of the three diagrams was added to provide explicit descriptions of how to interpret the diagrammatic conventions used to represent the arrangement of substituents. Italics in Appendix B mark the text unique to Study 2. As in Study 1, a video camera was used to record uses of the model and spatial ability was measured with the Vandenberg and Kuse (1978) Mental Rotation Test (VK-MRT).

Procedure. The procedures were identical to Study 1 except that participants were alternately assigned to either the control (No Models) group or Models group. All participants were reminded of the conventions for all three molecular diagrams. Participants in the Models group were also informed about the color conventions for the atoms used in the models and were explicitly given written instructions (see Appendix C) and oral encouragement to use the models (i.e., "You are welcome to move, manipulate, adjust, alter, or do whatever you need to do to this model to help you solve this problem"). The participants were then given the 18 diagram translation trials. Scoring of drawing accuracy and model use behaviors from videotapes also followed the same procedure as Study 1. Interrater reliability was high for scores of drawing accuracy ($r = .99$, $p < .001$) and type of model use (Align-Start: $r = .94$, $p = .001$; Align-Target: $r = .98$, $p < .001$; Reconfigure: $r = .99$, $p < .001$).

Results and Discussion

The Models and No Models groups did not differ in spatial ability as measured by the mental rotation test, $t(62) = .99$, $p = .33$, or in experience as measured by the number of organic chemistry courses taken, $t(62) = .63$, $p = .53$). Descriptive statistics are listed in Table 2.

How did Participants Use the Models? The middle section of Table 1 lists the percentage of participants who exhibited each type of model use and the proportion of trials (averaged over 32 participants) for which these model uses were observed. As in Study 1, type of model use varied widely between participants, but model use was generally more common in Study 2 (see Table 5), presumably due to the written and verbal instructions, which encouraged their use. Only four participants (13%) performed no actions with the models, compared to 53% in Study 1. As in Study 1, the most common types of model use were to align the model with the start diagram (24% of trials) or the target diagram (35% of trials). These model uses occurred within the same trial on 16% of the trials, with Align-Start preceding Align-Target approximately 87% of the time.

Does Providing Models Improve Accuracy? As predicted, participants in the Models group drew more accurate (Level 3) diagrams than those in the No Models group, $t(51.8) = 2.24$, $p = .029$, $d = .56$, but as in Study 1, the frequency of fully accurate diagrams was low in general (see Table 2). As before, the most common error, which occurred in 34% of drawings for the Models

group and 50% of drawings for the No Models group, indicated that students understood the connectivity of substituents but not their 3D configuration (Level 2.5). Importantly, the majority of solutions for the Models group were fully accurate (Level 3) while the majority of solutions for the No Models group were at Level 2.5 (see Table 3). In addition, as indicated in Table 4, 9 of the 32 participants in the Models group performed consistently at Level 3 while only 1 of the 32 participants in the No Models group performed at this level. This difference was statistically significant (X^2 (2, $N = 32$) = 70.84, $p < .01$).

Is Using a Model Predictive of Drawing Accuracy? To assess the benefit of *using* a model rather than just *having* a model, the Models group was categorized into two groups based on how often participants aligned the model to the target. Means and standard errors for drawing accuracy and spatial ability are listed in Table 2. Participants who aligned the model to the target on 50% or more of the trials were classified into the "Use Models" group. Participants who aligned the model to the target on less than 50% of trials were in the "Have Models" group. These three groups did not differ significantly in organic chemistry experience, $F(2,61) = .65$, $MSE = .42$, $p = .52$, or spatial ability, $F(2,61) = 2.30$, $MSE = 726.03$, $p = .11$, although the Use Models group had marginally higher spatial ability than the Have Models group, $t(61) = 1.89$, $p = .06$. A post hoc analysis was conducted to compare these two model sub-groups to the control (No Models) group. The three groups (Use Models vs. Have Models vs. No Models) differed significantly in a one-way ANOVA, $F(2,61) = 18.59$, $MSE = .878$, $p < .001$, $\eta_p^2 = .38$. Pair-wise comparisons with Bonferroni corrections revealed that the Use Models ($N = 13$) group significantly outperformed the No Models ($N = 32$), $t(61) = 5.65$, $p < .001$, $d = 1.52$, as well as the Have Models group ($N = 19$), $t(61) = 5.47$, $p < .001$, $d = 1.69$. The Use Models group drew more than twice as many correct diagrams as the No Models control group and the performance of the Have Models group was not significantly different from the No Models group, $t(61) = .41$, $p < 1.0$. While it is perhaps not surprising that students received no benefit from the models if they did not align them to the target diagram, it is worth noting that just seeing the 3D spatial arrangement of substituents, which is represented transparently by the models, does not offer any benefit to performance.

Is Drawing Accuracy Predicted by Spatial Ability? The correlations between model use, drawing accuracy, and spatial ability for the models group are given in the middle section of Table 5. As predicted, spatial ability and measures of model use were positively and significantly correlated with drawing accuracy (see Table 5). A simultaneous multiple regression analysis was conducted to examine effects of spatial ability and model uses on drawing accuracy (Level 3). Together, these four predictors explained a notable 72% of the variance in drawing accuracy ($R = .85$; $F(4,27) = 16.90$, $MSE = .55$, $p < .01$). An examination of the partial regression coefficients revealed that Align-Target was a strong predictor of drawing accuracy after controlling for spatial ability and the other types of model use ($\beta = .82$, $p < .01$, $sr^2 = .27$). In contrast, spatial ability ($\beta = .01$, $p = .92$, $sr^2 < .01$), Align-Start ($\beta = -.16$, $p = .32$, $sr^2 = .01$), and Reconfigure ($\beta = .17$, $p = .32$, $sr^2 = .01$) were not significant predictors after controlling for other predictors. In contrast with Study 1, spatial ability did not uniquely predict drawing accuracy in this study after controlling for aligning the model to the target diagram, possibly because spatial ability was somewhat correlated with this model use behavior (see Table 5).

A question that arises from this analysis is whether availability of a model moderates the correlation of spatial ability with performance. The simple correlation between drawing accuracy and spatial ability was very similar in the Models ($r = .30$, $p = .09$) and No Models ($r = .30$, $p = .10$) groups, indicating that model availability did not significantly affect this relationship. This result is important in that it indicates that models were equally helpful for low and high spatial ability individuals.

When do Students Use the Models? As with Study 1, we coded when participants first aligned the diagram to the target, (i.e., before, during, or after drawing the diagram). Align-Target was typically performed before (34% of all instances of Align-Target) or during (62%) the act of drawing, rather than after the diagram was drawn (4%), which supports our hypothesis that students use models in the process of deriving a solution and not just to check their solution.

In summary, Study 2 indicated that performance was better when models were provided than when they were not. However, for the models group, performance was better only for those who aligned the models to the target diagram while performing the translation. Viewing models without aligning them to the target diagram did not affect accuracy, suggesting that participants are not able to extract effectively the necessary information from visual inspection of a model without first placing it in the orientation of the diagram to be drawn. Although overall accuracy was low, as in Study 1, again the most common error was in preserving the circular order of the substituents around the central carbon atoms of the molecule. Participants who aligned the models to the targeted diagram were less likely to make this error, which suggests that the models help with resolving the correct 3D circular ordering of substituents.

Use of models was more common in Study 2 than in Study 1 (see Table 1), presumably due to the oral and written encouragement to use the models and the added explanation of the diagrammatic conventions given in this study. In contrast, the correlation of spatial ability with performance was lower in this study and spatial ability did not predict performance independently of model use. Finally, the simple correlation between drawing accuracy and spatial ability was very similar in the Models and No Models groups, indicating that model availability did not moderate the correlation between spatial ability and accuracy. In sum, the results suggest that models are beneficial when they are actively aligned to the diagram to be drawn, and aligning models in this way is much more predictive of performance than is spatial ability.

STUDY 3

In the previous studies, the models were presented to participants in an orientation that was not aligned with the given diagram. Without structural alignment (Gentner, 1983; Markman & Gentner, 2000), students may not have been able to see the correspondence between the model and the given diagram, and this may have inhibited model use. The purpose of Study 3 was to test the benefit of models when participants were actively encouraged to use them, when the models were placed in their hands, and when the models were presented in the orientation corresponding to the given diagrams.

We expected that availability of a model would be positively associated with drawing accuracy, but only if students rotate the model to the orientation of the diagram they are required to draw (Align-Target), as in Study 2. We examined whether aligning the model to the given diagram

influenced use of the model. A possible reason for the non-use of models in Studies 1 and 2 was that students could not appreciate how the model could help because they could not see the correspondence between the model and diagram when they were misaligned. If this is a reason for lack of model use, then students should use models more often when they are aligned. In contrast, if inability to map the model to the diagram is not a source of difficulty, or if students have other reasons for not using the models, then providing aligned models should not lead to increased model use or improved drawing accuracy. We acknowledge that spontaneous alignment of the model with the given diagram by students was not a strong predictor of performance in Studies 1 and 2. However, for students who do not understand the affordances of the models, it is possible that seeing the model and given diagram in alignment would enable them to realize that the models can be used and how they can be used to help accomplish the task.

Method

Participants. The participants were 59 college students (22 men, 37 women; $M = 20.0$ years, $SD = 1.14$) who had not participated in the previous studies but were recruited in the same manner. All participants had been introduced to the molecular representations that we studied in the context of an introductory organic chemistry class (4 concurrently enrolled in the class; 55 had previously completed the class). Participants were paid $20 or received course credit in psychology for their participation. Thirty participants served in the model group and 29 in the control group.

Design. The experiment had two levels of model availability (Models vs. No Models) as a between-subjects variable. The proportion of diagrams drawn at each of the five levels and the three coded model use behaviors were the dependent measures.

Materials and Equipment. The study material and experimental task were the same as in Study 2. The same video recorder and measures of spatial ability were also used.

Procedure. The procedures were the same is in Study 2 except that the 18 drawing trials were presented in a random order. In addition, the relevant model for each trial was placed in the participants' hands in the Models group so that the orientation of the model, with respect to the participant's line of sight, corresponded to the orientation of the given diagram. Participants were given the following verbal instructions: "As it is put in your hand, the model will be aligned with the orientation of the given diagram." They were also encouraged to use the models both in writing and orally (see Appendix C).

Scoring. Drawn diagrams were scored as in Study 2. Because participants were handed the models in the aligned orientation, Align-Start was no longer relevant, so the coded model uses were Align-Target and Reconfigure. Interrater reliability was high for scores of drawing accuracy

($r = .98$, $p < .001$) and type of model use (Align-Target: $r = .97$, $p < .001$; Reconfigure: $r = .99$, $p < .001$).

Results and Discussion

The Models and No Models groups did not differ in spatial ability, $t(57) = .30$, $p = .77$, as measured by the mental rotation test, or in experience as measured by the number of organic chemistry courses taken $t(57) = .21$, $p = .84$. Descriptive statistics are given in Table 2.

How did Participants Use the Models? The right section of Table 1 lists the percentage of participants who exhibited each type of model use and the proportion of trials (averaged over 30 participants) on which these uses were observed. Although all participants in the Models group were encouraged to use the models, and this use was initiated by placing the models into their hands, several participations accepted the models only to ignore them by placing them to the side (9 participants on 33% of their trials) or by holding them off to the side in their non-writing hand (9 participants on 43% of their trials). Participants aligned the models with the target diagrams more frequently in this study than in Studies 1 or 2 but reconfiguring the model was intermediate in frequency (see Table 1). As in the previous studies, there was large variance in type of model use within the Models group.

Is Use of the Models Predictive of Drawing Accuracy? Although the trend was for the Models group to be more accurate than the No Models group, this trend did not reach statistical significance $t(57) = 2.04$, $p = .16$ in this study. To assess the benefit of *using* a model rather than just *having* a model, the Models group was categorized into a Use Models group, and a Have Models group (i.e., non-users) using the same criterion as in Study 2. Model users had higher spatial ability ($t(56) = 2.29$, $p = .03$, see Table 2) suggesting that spatial ability was related to the ability to see the relevance and take advantage of the models. The three groups (Use Models vs. Have Models vs. No Models) differed significantly on drawing accuracy in a one-way ANOVA, $F(2,56) = 7.44$, $MSE = .363$, $p = .001$, $\eta_p^2 = .21$. As in Study 2, pair-wise comparisons revealed that the Use Models group ($n = 18$) significantly outperformed the No Models control group ($n = 29$), $t(56) = 3.12$, $p = .009$, $d = .84$, as well as the Have Models group ($n = 12$), $t(56) = 3.54$, $p = .003$, $d = 1.51$ (see Table 2). The Use Models group drew nearly twice as many correct diagrams as the No Models control group and the drawing accuracy of the Have Models group was not significantly different from the control group, $t(56) = 1.11$, $p = .82$. These results are reinforced by a review of the levels of accuracy for the three groups. A majority of trials were scored as Level 3 in the Use Models group but in the Have Models group the majority of trials were at Level 2.5 (see Table 3).

Is Drawing Accuracy Predicted by Spatial Ability? Table 5 lists the correlations between the types of model use and drawing accuracy (number of completely correct, i.e. Level 3 diagrams) and between model use and spatial ability. As in Studies 1 and 2, spatial ability, Align-Target, and Reconfigure were significantly correlated with drawing accuracy. Align-Target (but not Reconfigure), was also significantly correlated with spatial ability. A simultaneous multiple regression analysis was conducted to examine the effects of spatial ability and the two types of

model use on drawing accuracy. Together, these three predictors explained a notable 53% of the variance in drawing accuracy, $R = .73$; $F(3,26) = 9.89$, $MSE = .322$, $p < .001$. An examination of the partial regression coefficients revealed that Align-Target was a strong predictor of drawing accuracy after controlling for spatial ability ($\beta = .57$, $p < .001$, $sr^2 = .19$). In contrast, neither spatial ability ($\beta = .09$, $p = .55$, $sr^2 < .01$) nor Reconfigure ($\beta = .20$, $p = .24$, $sr^2 = .03$) were significant predictors after controlling for Align-Target. Similar to Study 2, spatial ability and reconfiguring the models do not independently promote drawing accuracy.

As in Study 2, there was no evidence that availability of a model moderated the correlation of spatial ability with performance. The simple correlations between drawing accuracy and spatial ability were again extremely similar in the Model group ($r = .33$, $p = .07$), and in the No Model group ($r = .34$, $p = .07$) suggesting that high and low spatial individuals benefit equally from models.

When do Students Use the Models? As with Studies 1 and 2, we coded whether participants first aligned the diagram to the target before, during, or after drawing the diagram. Align-Target was typically performed before (52% of all instances of Align-Target) or during (45%) the act of drawing, rather than after the diagram was drawn (3%), suggesting that participants used models as external aids to augment their problem-solving processes rather than as a check of their solutions after the fact.

Post-Hoc Comparison Across Experiments. Study 3 replicates the main results of Study 2, but accuracy was lower in Study 3 and effects of model use were weaker, although the models were aligned and placed in participants' hands in the latter study. There were some differences between the participants in the two studies in that spatial ability was lower in Study 3 ($M = 30.4$, $SD = 14.8$) than in Study 2 ($M = 41.2$, $SD = 18.1$), $F(1,121) = 12.85$, $MSE = 3545.6$, $p < .001$, $\eta_p^2 = .10$, and experience (number of organic chemistry courses taken) was higher in Study 3 ($M = 2.2$, $SD = .73$) than in Study 2 ($M = 1.6$, $SD = .79$), $F(1,121) = 20.45$, $MSE = 11.95$, $p < .001$, $\eta_p^2 = .15$. To better understand the differences in results across studies, we conducted a post hoc ANCOVA of the effects of Models (Use Models vs. Have Models vs. No Models) and Study (Study 2 vs. Study 3) on drawing accuracy, with spatial ability and experience as covariates. Model use, $F(2,115) = 20.15$, $MSE = .934$, $p < .001$, $\eta_p^2 = .26$, but not Study, $F(1,115) = 1.97$, $p = .16$, or their interaction, $F(2,115) = 1.65$, $p = .20$, significantly affected drawing accuracy after controlling for these variables. In this analysis spatial ability was a significant predictor, $F(1,115) = 5.79$, $MSE = .268$, $p = .02$, $\eta_p^2 = .05$, but experience was not, $F(1,115) = .15$, $p = .70$. This analysis reveals that the differences in performance across studies can be accounted for by differences in the spatial ability of the participants, and that differences in organic chemistry knowledge (beyond the minimum necessary for participants in this study) are not predictive of performance.

These results also indicate that placing the models in participants' hands did not have significant effects on translation accuracy compared to merely encouraging students to use the models in Study 2. Interestingly, this was true even though participants aligned the model to the target more frequently in Study 3 than in Study 2, $F(1,58) = 6.87$, $MSE = .888$, $p = .01$, $\eta_p^2 = .11$ (see Table 1). The comparison of the two studies indicates that aligning the model with the diagram to be drawn is not sufficient for accurate translation performance, because even after the model is so aligned, there is additional work to be done in translating the final orientation of the

diagram to the required 2D diagram. In sum, while matching the orientation of the model to the drawn diagram increases drawing accuracy, it is not a sufficient condition for drawing an accurate diagram.

Together the two studies also indicate that providing models and encouraging their use does not necessarily induce all students to use models. Even with the stronger experimental manipulation of aligning the models and placing them into the participants' hands, several participants did not consistently use models. In post-task interviews, some participants reported that they did not understand how to use the models, suggesting that orienting a model to match a starting orientation was not sufficient to help them understand how the models could be used. It is also possible that some students preferred analytical strategies (cf., Stieff & Raje, 2010), but it appears that in the context of these studies, these alternative strategies were not as effective as using models.

In summary, the positive correlations between types of model use and drawing accuracy in Study 3 replicate those of Studies 1 and 2, which further strengthen the conclusion that active and intentional use of concrete models helps with the diagrammatic translation task. Again, analyses of drawing errors showed that most participants drew diagrams that were nearly accurate in terms of spatial relations but depicted molecules with very different reactive properties. Students who used models were more likely to draw fully accurate molecules and model use did not moderate the correlation between spatial ability and accuracy; both low spatial and high spatial individuals received a benefit from model use.

GENERAL DISCUSSION

This research was motivated by the hypothesis that using concrete models can lead to improved performance on challenging representation translation tasks in organic chemistry because concrete models can directly represent the three-dimensional structure of the molecular substituents and because they allow difficult mental processes to be replaced or augmented by actions on the models (cf. Kirsh, 1995a; Kirsh & Maglio, 1994). In support of our hypothesis, model use was positively correlated with translation accuracy in all three studies. Furthermore, the results of Study 2 and 3 also indicate that just seeing a model is not sufficient to promote translation accuracy. Participants who saw the models, but who did not physically interact with them, performed no better than participants in the control condition who did not see models. Spatial ability was associated with translation accuracy, but model use did not moderate the correlation between spatial ability and drawing accuracy. Low-spatial and high-spatial individuals benefitted equally from model use.

How are Models Beneficial?

Two main types of interactions with the models were associated with more accurate performance: rigid rotations of the whole model into the general orientation of the given or target diagram, and reconfiguring the models by rotating substituents around bonds within the models. Rotating the whole model, especially to align it with the orientation of the target diagram, was highly correlated with drawing accuracy. A possible explanation of this result is that people have difficulty imagining and then mentally rotating or shifting their perspective around a structure as

complex as the molecules used in our studies. Alternative strategies can involve piecemeal mental rotations (cf. Bethell-Fox & Shepard, 1988) or transposition of components following a learned algorithm (Stieff, 2011; Stieff & Raje, 2010). However, in these strategies, the spatial relations between separately processed parts must be maintained, and so these strategies can be demanding of working memory, and at least in the case of a piecemeal mental rotation strategy, failure to apply the same transformation to the pieces can be a source of error (Just & Carpenter, 1985). The common error found in these studies, in which the molecular substituents were configured correctly on one side of the molecule but not on the other side (i.e., accuracy Level 2.5) is suggestive of a piecemeal strategy in which the same transformation was not applied consistently to the different pieces of the representation. In contrast, a physical rotation of a model is holistic and because the model is rigid, it maintains the spatial relations between its components when the whole model is rotated. Thus, a physical rotation of the model concretizes a task by placing desirable constraints on the process and maintains the structural integrity of the represented entity. These reasons explain why external rotations of models were particularly effective for inferring transformations of complex molecules.

Reconfiguring the substituents within the model was also significantly correlated with representation translation accuracy, although this behavior did not uniquely predict accuracy after controlling for the effects of aligning the main axis of the molecule. Reconfiguring the models is an external behavior that represents changing a molecule's conformation and is relevant for diagram translations that end with a Fischer projection because of differences between the Fischer's required eclipsed conformation and the Dash-Wedge and Newman's presented staggered conformation. (Reconfiguration is not necessary when beginning with a Fischer diagram, because participants were allowed to draw translations of eclipsed Dash-Wedge and Newman diagrams, but it is more conventional to represent these as staggered conformations.) However, reconfiguration was also observed even when participants translated between Newman and Dash-Wedge diagrams, which did not require changing conformations. This result might be explained by cross-over with learned information from students' courses in organic chemistry. Some conformations of molecular components are more thermodynamically stable than others, and a common task in organic chemistry courses is to find the most energy stable conformation. We speculate that students may have been trying to optimize the energy conformation of the drawn molecule, although this was not a requirement of our task (see also Raje & Stieff, 2009).

We predicted that models would help participants while translating diagrams, by allowing them to use external actions to replace or augment difficult mental processes. Analyses of the timing of model use behaviors with respect to drawing the diagrams is consistent with this interpretation in that model use more commonly occurred before or in the course of drawing. Thus, participants used models to help perform the translation rather than merely to check their answer.

Why did Some Students Not Use the Models?

Although aligning models with the diagram to be drawn improved performance, this action was performed on a minority of trials. Matching the target occurred spontaneously on only 23% of trials in Study 1, with encouragement it occurred on 35% of trials in Study 2, and when the models were structurally aligned and placed into the hands of the participants in Study 3, it occurred on a little more than half of the trials (54%).

There are many potential reasons why students did not commonly use the models. First, students may *choose* not to use models for a variety of reasons. For example, several participants reported that they did not think that using the models would be helpful. Others reported that they did not look to the model for help because they did not need to, or did not wish to depend on models because such aids would not be provided on their exams (see also, Bowen, 1990). More specifically, the models might not have been used because some participants used an algorithmic strategy for translating between two diagrams without imagining the three-dimensional nature of the molecule (Stieff, 2011; Stieff & Raje, 2010). Although such strategies can be effective, and using these strategies is consistent with the comments of some participants in their post-study interviews, students who used these strategies in the current studies were less successful than those who used models productively. Finally, lack of model use may be an indication that these students are not distinguishing between a diagram as a representation and the reality that is represented (Bucat & Mocerino, 2009). In such cases, these students are working at a superficial level performing steps in the translation between two diagrams without seeing the relevance of the model with its transparent 3D structure.

A second set of reasons for not using the models can be attributed to *inability* to use them effectively. Some students in Study 1 did not remember the conventions of the models (e.g., what the colors mean) or the correspondence between the models and the diagrams, although these conventions are explained in their textbooks (students were reminded of these conventions in Studies 2 and 3). It is also possible that students were unable to establish the correspondence between the models and diagrams, in other words, to chunk the model units that are identified as chunks in the diagram. For example, "H" is a unit in the diagram that corresponds to a single visible unit in the model where as "CH_3" can also be a unit in the diagram but corresponds to a configuration of several visible units in the model. Related to this point, some participants reported that the models were too complex and that they could perform the necessary manipulations more easily by gesturing with their hands as simplified representations. These students sometimes held their hands over molecular substituents and, when queried afterward, reported that they were trying to identify the carbon backbone. They appeared to be addressing the complexity of the representations by isolating relevant parts while physically occluding other parts with their hands. A more complete account of these gestures is an important priority for future research but outside the scope of the present study.

Finally, establishing the correspondence between the model and diagram is not sufficient for using the model effectively, as emphasized by the results of Study 3 in which model use was relatively high, but performance was relatively low. To understand this, consider the steps a typical participant appeared to take when using a model to translate between diagrams. These include (a) interpreting the conventions of the given diagram to encode the 3D configuration of components, (b) rotating the model in correspondence with the encoded configuration (align to start), (c) rotating the model to align it with the target diagram to be drawn (align to target), and (d) converting the new alignment and conventions of the model to that of the target diagram. Putting the model into the hands of the participant and aligning it with the given diagram is just one step in this process. The research presented in this article gives us insight into which of these steps are critical for successful task performance. There is strong evidence that aligning the model with the target diagram is important. In all three experiments this behavior was highly correlated with drawing accuracy. Moreover, viewing a model (i.e., by non-users) did not improve task performance if the student did not place the model in alignment with the target diagram.

There is also evidence in Study 3 that converting the aligned model to the target diagram is an important and error prone step, because some students successfully aligned the model but did not correctly draw the diagram. Logically, the first two steps, encoding the given diagram and aligning the model with that diagram, are unnecessary and performing this alignment for the students in Study 3 was ineffective. However, even though aligning the model to the starting diagram was ineffective, it is notable that many students in Study 1and the vast majority of students in Study 2 still performed it at least once. It is possible that this initial alignment served a bootstrapping function in enabling the students to recognize the potential of the model for helping accomplish the task.

Our studies provide evidence that using a concrete model can be an effective strategy in problem solving, but we acknowledge that this strategy might not be optimal for all individuals and under all circumstances. Although the minimum memory hypothesis of Kirsh and Maglio (1994) proposes that performing actions in the world takes priority over internalizing actions in memory, the soft constraints hypothesis (Gray & Fu, 2004; Gray, Sims, Fu, & Schoelles, 2006) recognizes that substituting external actions for internal processes is not always easier, obvious, or more efficient. The results of the present studies are strikingly similar to a recent study by Keehner et al. (2008) that involved using a computer model as an aid in drawing the cross-section of a three-dimensional object. In both studies, people who used models effectively had better performance on the task, yet many participants did not use the models. These studies highlight the fact that using an external model is not necessarily obvious or easy for all individuals, and depending on the availability and apparent relevance of other strategies, may not be the optimal strategy for all individuals.

What is the Role of Spatial Ability?

Organic chemistry is a spatially complex discipline and our research is consistent with previous studies (summarized by Harle & Townes, 2011; Wu & Shah, 2004) in demonstrating that it places demands on spatial ability. A common feature shared by this domain and other science, technology, engineering, and mathematics (STEM) disciplines, is that it requires the representation of 3D entities in diagrams that must be represented using the two dimensions of the printed page. For example, students in biology, medicine, and geology have difficulty understanding cross-sections, which are also 2D representations derived from 3D objects, and this is particularly true of students with poor spatial abilities (Kali & Orion, 1996; Keehner et al., 2008; Liben, Katens, & Christensen, 2011; Rochford, 1985).

As in these previous studies, performance on our representation translation task was related to spatial ability. However, although spatial ability was quite predictive of performance in Study 1 ($r = .58$) this correlation was reduced when students were encouraged to use models in Studies 2 and 3 ($r = .32$ in both studies) and model use was much more predictive of performance in these studies. Furthermore, although there were trends for those who used the models to have higher spatial abilities, there was no evidence that providing models moderated the effect of spatial ability on accuracy. If models were more helpful to high spatial individuals, then the correlation of spatial ability with performance should have been higher in the models conditions. In fact, the observed correlation between spatial ability and performance did not differ for the Models and No Models groups, indicating that high and low spatial individuals were equally able to benefit

from models. This supports the conclusion that a focused training program that teaches students to use models effectively might overcome challenges faced by low spatial learners in spatially rich STEM domains like chemistry and also enhance the performance of high spatial learners.

What are the Implications for Instruction?

Students have difficulty translating between different structural diagrams in organic chemistry, even though this task is important in the domain (Harle & Towns, 2011; Keig & Rubba, 1993; Pribyl & Bodner, 1987; Wu & Shah, 2004). Our results suggest that using models can aid in this process by allowing difficult internal processes to be replaced or augmented by external actions on models. An implication of our research is that students should be encouraged to use models in organic chemistry, at least in the beginning stages when they are first developing their understanding of the 3D structure of molecules and of molecular representations.

Notably, not every student used the models even with strong encouragement, although those who used the models performed more accurately. This suggests that more emphasis should be placed on using models within the curriculum and in developing techniques to train students to use them effectively. It may not be sufficient for instructors simply to recommend using models or even to demonstrate how to use models for a specific task. Rather, instructors might make clear value statements about the benefit of models both in the classroom and in their own practice. From such social modeling practices, students may better learn to appreciate the utility of concrete models in the chemistry classroom and in other science disciplines, which may, in turn, improve their representational competence in chemistry and meta-representational competence more generally.

Our study revealed that most students made errors in the spatial ordering of substituents around one of the central carbon atoms in the model. In contrast, they showed good understanding of the molecular structure in terms of the connectivity of the substituents. From these results, it seems clear that instructors should place more emphasis on the importance of the spatial ordering of substituents. Again, models can help with this instruction. Our study revealed that when using models effectively (e.g., using the model during the translation), students often avoided this error.

Although chemistry is a spatially challenging discipline, our research shows that model use is a better predictor of performance than students' spatial ability in at least one spatially complex tasks studied here. This is an important outcome and strengthens our suggestion that model instruction should be integrated into the curriculum. Rather than focusing on spatial ability as a barrier to success in science, our research suggests that providing focused instruction on spatial representations should enhance opportunities for all students to succeed in science.

In summary, the observed benefit of using concrete models in a representation translation task in organic chemistry suggests that using physical objects to enact and support cognitively difficult tasks can enhance problem solving. However, the general lack of model use by some low-performing participants suggests that a model-use strategy is not necessarily readily discovered or understood as relevant. Lacking the necessary experience with models, individuals might be less likely to rely on such external aids even when they are available and more likely to utilize other, more error-prone cognitive strategies. Future research should investigate the ways in which individuals can be taught to use models effectively in chemistry and other representation-rich disciplines.

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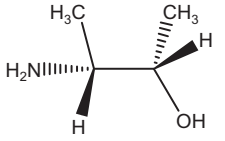
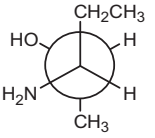
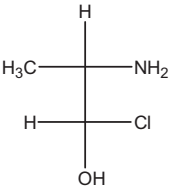
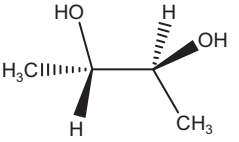
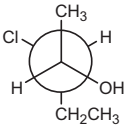
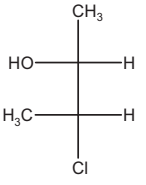
APPENDIX A

Trial	*Start Diagram*	*Molecule Name*	*Start*	*Target*
1		3-aminobutan-2-ol	Dash-Wedge	Newman
2				Fischer
3		3-aminopentan-2-ol	Newman	Dash-Wedge
4				Fischer
5		2-amino-1-chloropropan-1-ol	Fischer	Dash-Wedge
6				Newman
7		2,3-butanol	Dash-Wedge	Newman
8				Fischer
9		3-chloropentan-2-ol	Newman	Dash-Wedge
10				Fischer
11		3-chlorobutan-2-ol	Fischer	Dash-Wedge
12				Newman

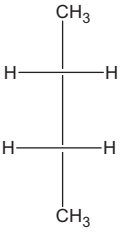
APPENDIX B

Instructions

For each of the following 18 worksheets you will be given a Fischer, Newman, or Dash-Wedge projection of a molecule as well as a physical model of that molecule. Your task is to draw a different projection for each molecule. The text at the top of each page will describe which projection you are to draw. *Please hold and manipulate the physical model to help you with each task*. Some of the transformations may be difficult but please try your best.

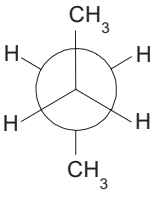
Here are examples of the three different projections that you will be expected to draw. All three use different conventions to illustrate the 3D shape of the molecule. The same molecule is illustrated in all three projections:

Fischer



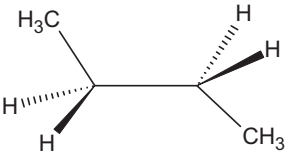
The Fischer projection to the left illustrates a 4-carbon molecule. The atoms at the right and left of the horizontal lines are coming out of the page (above the plane of the paper) and the atoms at the top and bottom of the vertical line are going into the page (below the plane of the paper). The two backbone carbons are located where the horizontal lines cross the vertical line. These carbons are on the plane of the paper.

Newman



In a Newman projection, the molecule is oriented with one backbone carbon in front of the other. The front carbon is located at the intersection of the 3 lines (noon, 4 o'clock and 7 o'clock around the circle). The atoms at the ends of these three lines are attached to the front carbon. The rear carbon is behind the circle. The atoms at the ends of the shorter lines connected to the circle (2 o'clock, 6 o'clock, and 10 o'clock around the circle) are attached to the rear carbon.

Dash-Wedge



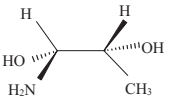
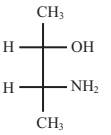
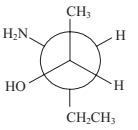
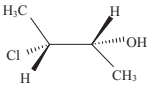
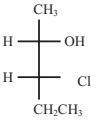
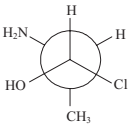
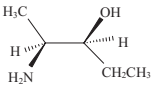
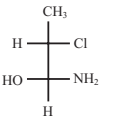
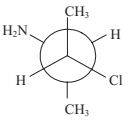
In a Dash-Wedge projection, the molecule is oriented with the backbone carbons at the two 4-way intersections of lines on the left and right of the diagram. Dashed lines represent bonds to atoms that are going into the page (below the plane of the paper). Wedge lines represent atoms that are coming out of the page (above the plane of the paper). Solid lines represent bonds to atoms that are on the plane of the paper.

Take a moment to visualize how each projection represents the three-dimensional structure of the molecule. Compare and contrast the three projections because you will need to draw each in the following activity.

In addition, you will be given a ball & stick model of each molecule that you are asked to draw. The atoms on the models will be colored to indicate different atoms. Carbon is black, hydrogen is white, nitrogen is blue, oxygen is red, and chlorine is green.

Please let the experimenter know if you have any questions.

APPENDIX C

Study 2 Trial	*Study 3 Trial*	*Diagram*	*Molecule Name*	*Start*	*Target*
1	9		1-aminopropan-1,2-ol	Dash-Wedge	Fischer
2	4				Newman
3	3		3-aminobutan-2-ol	Fischer	Dash-Wedge
4	10				Newman
5	1		3-aminopentan-2-ol	Newman	Dash-Wedge
6	15				Fischer
7	13		3-chlorobutan-2-ol	Dash-Wedge	Fischer
8	16				Newman
9	5		3-chloropentan-2-ol	Fischer	Dash-Wedge
10	2				Newman
11	14		2-amino-1-chloropropan-1-ol	Newman	Dash-Wedge
12	17				Fischer
13	11		2-aminopentan-3-ol	Dash-Wedge	Fischer
14	6				Newman
15	12		1-amino-2-chloropropan-1-ol	Fischer	Dash-Wedge
16	8				Newman
17	18		2-aminobutane-3-chloride	Newman	Dash-Wedge
18	7				Fischer