Chemistry Education Research and Practice

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Journal:	*Chemistry Education Research and Practice*
Manuscript ID:	RP-ART-08-2014-000169.R2
Article Type:	Paper
Date Submitted by the Author:	07-Nov-2014
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Examining the Relationship between 2D Diagrammatic Conventions and Students' Success on Representational Translation Tasks in Organic Chemistry

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Abstract: Two-dimensional (2D) diagrams are essential in chemistry for conveying and communicating key knowledge about disciplinary phenomena. While experts are adept at identifying, interpreting, and manipulating these representations, novices often are not. Ongoing research efforts in the field suggest that students' effective use of concrete and virtual manipulatives can support their development of representational competence in the domain. However, as these affordances are not always present within the learning environment, it is imperative that educators evaluate the influence diagrammatic conventions have on student success in the discipline, specifically on tasks requiring translation between two, 2D diagrams. In this study, we adopt a quantitative approach to examine students' accuracy at translating between Dash-Wedge and Newman projections, as well as Dash-Wedge and Fischer projections when the conventions of each of these representations are varied (e.g., staggered vs. eclipsed conformation of the Dash-Wedge diagram, rotation of the Newman Projection). Results indicate two important findings. First, students perform significantly better on Dash-Wedge to Newman tasks when the Newman projection has undergone no rotation (i.e., when the two representations are exact conformers of one another) compared to simple or complex rotations. Second, students' degree of success on Dash-Wedge to Fischer translation tasks is directly related to the conformation and spatial arrangement of substituents on the Dash-Wedge diagram, with poorer performance noted on tasks in which the visuospatial conformation of the Dash-Wedge representation is both staggered and inconsistent with the participants' preferred viewing perspective. Together, these data reaffirm the need to explore in greater detail how 2D diagrammatic conventions impact novices' ability to successfully translate between representations in Organic Chemistry.

Keywords: Organic Chemistry, Undergraduate, Diagrammatic Conventions, Representational Translation, Diagrams, Representations

Introduction

Diagrams are an integral component of chemical discourse and are utilized routinely in the discipline to convey knowledge about the micro- and macromolecular world. The pervasive use of these representations within the field necessitates that novices and experts alike possess the skills required to identify, interpret, and translate between different diagrammatic forms – skills characterized as constituting an individual's level of representational competence in the domain (Kozma & Russell, 1997; Gilbert, 2005). While experts are traditionally adept at employing these skills, the same cannot be said for novices. Instead, research suggests that novices tend not only to focus almost exclusively on the superficial features of these representations (e.g., the size and shape of atoms), but also to see these diagrams as being static rather than dynamic illustrations of the phenomenon they are meant to depict (Grosslight *et. al*, 1991; van Driel & Verloop, 2002; Boukhechem *et al.*, 2011). To some degree, this latter misconception is perpetuated by the manner in which molecules are portrayed in chemistry textbooks and media (Kumi *et al.*, 2013), as well as by instructional practices that result in students simply being "shown" 2D diagrams in fixed conformations rather than being actively engaged in translating between various conformations of a molecule illustrated as either a Dash-Wedge representation, Newman projection, or Fischer projection (Olimpo, 2013).

In addition, it is well acknowledged in the literature that Organic Chemistry is a heavily spatial domain. Students are frequently (and simultaneously) required to understand and access chemistry knowledge, as well as construct and manipulate mental models of molecules – tasks that, together, confer significant cognitive demands. In their examination of Algerian pre-service teachers' acquisition of stereochemical knowledge, Boukhechem and colleagues (2011) showed,

for instance, that while participants had made an effort to utilize stereochemistry concepts to solve the series of visuospatial and representational translation items presented to them in the course of the study, they were often unsuccessful in doing so accurately. These inaccuracies, the authors argued, were attributable to the fact that participants lacked the spatial awareness and representational competence to complete the tasks.

Similar studies have shown that students' difficulty understanding these representations is often further exacerbated by the fact that the conventions adopted by each diagram are rather abstract and intangible in nature. For example, Kuo and colleagues (2004) administered a battery of stereochemical tasks to organic chemistry students that required them to assign *R* and *S* configurations to the molecule presented in each problem. The types of representations used in these tasks included both physical and computer models, as well as pseudo-3D and 2D diagrams. The authors found that students performed significantly better on tasks involving physical and computer models, where representational conventions and spatial relationships were more apparent, than on problems depicting pseudo-3D and 2D diagrams, where the same characteristics were more obscure. Such findings continue to highlight the important need for educators to attend to students' understanding of the structural and spatial relationships inherent of molecular representations as a means of supporting student success in the domain.

In an effort to promote students' development of representational competence in chemistry, recent research in this area has focused largely on the benefits afforded to students when they are provided with access to manipulatives – whether concrete or virtual in nature – for use in translating between diagrams (Copolo & Hounshell, 1995; Wu *et al.*, 2001; Stull *et al.*, 2012; Stull *et al.*, 2013). Though of implicit importance, few of these studies have focused exclusively on students' interpretation of diagrammatic conventions as they complete translation tasks, particularly when models are not present in the learning environment. The work presented here adopts a quantitative approach to address this need through evaluation of the following central question:

What impact do 2D diagrammatic conventions have on a novice's ability to translate from a Dash-Wedge diagram to either a Newman projection or Fischer projection?

Specifically, we examined students' ability to translate between Dash-Wedge and Newman diagrams when the Dash-Wedge representation was depicted in either a staggered or an eclipsed conformation and when the Newman projection had undergone various levels of rotation (no rotation, 120° rotation of the front carbon, or 120° rotation of both the front *and* back carbons). We hypothesized that as the complexity of the degree of rotation of the Newman projection increased, student performance on Dash-Wedge to Newman translation tasks would decrease. Furthermore, we anticipated a significant main effect to be found for Dash-Wedge conformation and an interaction effect between Dash-Wedge conformation and degree of rotation of the Newman projection to be observed due to empirical evidence demonstrating that students are frequently shown the above representations depicted in only one conformation (typically staggered) (Kumi *et al.*, 2013).

For Dash-Wedge to Fischer translation tasks, we again presented the Dash-Wedge diagrams in either a staggered or eclipsed conformation, though we also varied the orientation of substituents on the C2 carbon and the question item format (multiple-choice vs. open-ended response items). We hypothesized that students would perform better on the multiple-choice tasks than on the open-ended response items because only a limited number of answers were

provided, one of which was the exact conformer of the initial Dash-Wedge diagram. Similarly, we believed that students would exhibit greater accuracy in completing tasks (regardless of question type) in which the Dash-Wedge representation was shown in an eclipsed versus staggered conformation and with an inverted versus upright C2 Y-template (see Figure 1, left panel), as this would provide for a more direct translation between the Dash-Wedge diagram and the Fischer projection (which, conventionally, is always shown in an eclipsed conformation).

Representations and Translation between 2D Diagrams in Organic Chemistry

Representations in Organic Chemistry

The advent of virtual visualization and modeling technologies has revolutionized the way in which we have come to "see" and explore the chemical world. Despite these advancements, however, research suggests that the two-dimensional (2D) diagram remains the most prevalent form of representation in the field (Bodner & Domin, 2000). Within the context of the research presented here, we focus on three 2D diagrams that novices are asked to use routinely throughout the course of their studies in Organic Chemistry, namely: the Dash-Wedge (DW) diagram, the Newman projection (NP), and the Fischer projection (FP). These representations are illustrated in Figure 1 below.

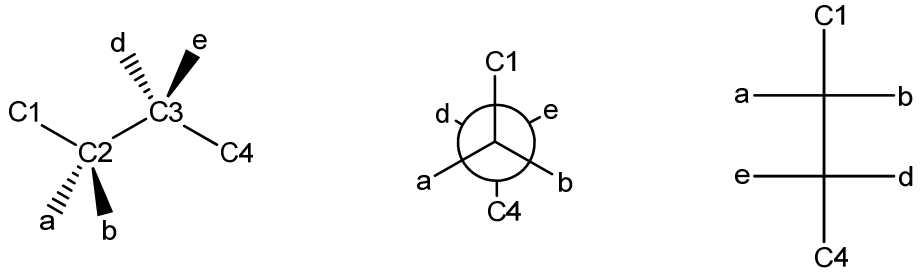

Figure 1. Common 2D diagrams in Organic Chemistry. The Dash-Wedge diagram is at the left, the Newman projection is center, and the Fischer projection is at the right. The spatial relationships of substituents on each diagram are indicated. In the Dash-Wedge diagram, the C2 carbon possesses an inverted Y-template, while the C3 carbon possesses an upright Y-template.

Individually, these diagrams afford the user unique advantages, particularly when considering aspects of molecular structure and stereochemistry. In the Dash-Wedge convention (Figure 1, left, also known as a Cram representation), for instance, the chemical bonds linking each atom within a molecule are commonly illustrated either as a solid line, wedge, or dashed-line. The bonds that are solid lines are within the plane of the page, whereas the dash formalism indicates bonds going into the plane of the page, and the wedge indicates bonds that are coming out of the plane of the page. For this reason, the Dash-Wedge diagram is suggested to provide the user with the greatest amount of three-dimensional (3D) information about the molecule in comparison to the other 2D diagrams that will subsequently be discussed (Loudon, 2008).

Alternatively, the Newman projection (Figure 1, center) offers the viewer an opportunity to more ready visualize the spatial relationships of substituents on adjacent carbons, as it provides an end-on view of the entire molecule. Given that these substituents can rotate around

internal carbon-carbon sigma bonds, Newman projections are typically used to determine the lowest-energy, or most stable, conformation of a molecule (Newman, 1955). According to standard convention, the circle represents the electron density between the two carbon atoms that form the bond the person is looking down, and the substituents on the front and back carbons are placed around the circle. Much like the Dash-Wedge representation, the Newman projection precludes that the spatial arrangement of atoms and molecules within the compound is dependent upon the specific bonds linking these groups and the relative position (i.e., bond angle) of these bonds in relation to the entire compound. In other words, as full rotation around the carbon-carbon sigma bond occurs, alternate conformers of both the Dash-Wedge and Newman diagrams are created. This leads to the formation of staggered and eclipsed conformers in which substituents are either offset from one another or overlapping, respectively (Figure 2).

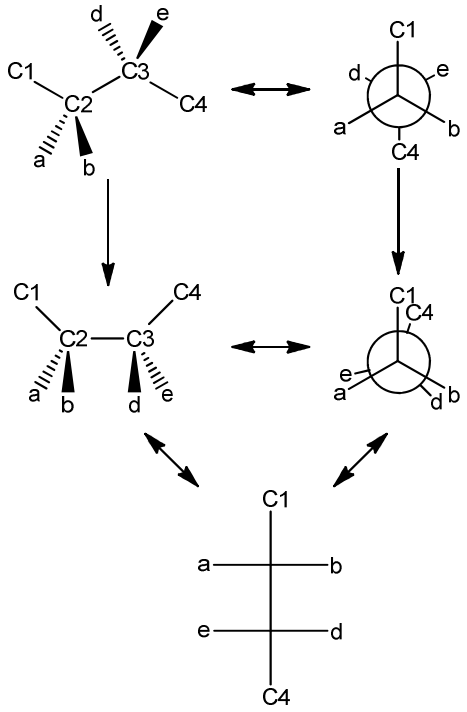

Figure 2. Different conformations of the same molecule. The top left diagram shows a Dash-Wedge representation of a staggered molecule. The top right diagram is an exact conformer of this molecule depicted as a Newman projection. An eclipsed conformation of the molecule is presented in the middle series of illustrations as a Dash-Wedge diagram (left) and Newman projection (right). This eclipsed conformation is shown as a Fischer projection in the bottom illustration. Note that in the Newman projection of the eclipsed molecule, the front and back substituents are slightly offset so as not to occlude the identities of the substituents on the back carbon.

Unlike both the Dash-Wedge and Newman representations, the Fischer projection (Figure 1, right) must be depicted using an eclipsed conformation, limiting its ability to capture any three-dimensional information regarding alternative conformations of the molecule itself. An

affordance of this caveat is that the Fisher projection allows one to assign stereochemistry for given carbon atoms within the molecule with relative ease (Loudon, 2008). Diagrammatically, substituents within the molecule are arranged on opposing ends of either horizontal or vertical bonds, which project toward and away from the viewer, respectively. These relationships must be inferred, however, as there is no distinctive cue (as there is in the DW diagram) to indicate those bonds coming out of versus going into the plane of the page – a characteristic of the FP that students often find confusing (Olimpo, 2013). Due to the nature of the representation itself, and resultant from Fischer's own professional interests, the Fischer projection is most frequently used in Organic Chemistry and Biochemistry courses to depict carbohydrates (Robyt, 1998).

Translation between 2D Diagrams

The task of translating between DW, NP, and FP diagrams is a common one, and novices are routinely asked to do so on both in-class assessments and standardized exams (American Chemical Society, 2010). Furthermore, because different representations serve unique purposes in the field, success in chemistry (as measured by achieving expert-level knowledge in the domain) rests in part upon switching between these different visualizations as necessary (Stull *et al.*, 2012).

Research suggests that novices utilize a wide array of strategies when translating between representations, though these strategies can largely be categorized as being either imagistic or analytic in nature (Stieff & Raje, 2010; Stieff, 2011). Using an imagistic approach, for instance, one might attempt to translate between a Dash-Wedge diagram and Newman projection by creating a mental model of the DW diagram and then envisioning it rotating, holistically, to adopt the conformation of a NP, all the while maintaining proper spatial positioning of substituents in the molecule. Alternatively, taking the same task of translating from a DW to a NP, individuals employing an analytic strategy might first draw the template for the Newman projection and then transpose substituents on the left side of the DW diagram to the front face of the NP, preserving spatial orientation. Finally, substituents on the right side of the DW diagram would be transposed to the back face of the NP, again preserving spatial orientation, completing the task (Stieff & Raje, 2010).

While each strategy theoretically leads to the same outcome, they are both potentially error-prone for several reasons. In the case of adopting an imagistic approach, for instance, one must cognitively grapple with chemistry content and spatial manipulation simultaneously (Bethell-Fox & Shepard, 1988). In the event that the molecule has to undergo a conformational change (i.e., staggered conformation to eclipsed conformation), additional mental manipulation would be required, further complicating the task.

This same concern – that of *accurately* preserving the spatial arrangement of substituents when transposing from one representation to another – holds true for students adopting an analytic approach. Furthermore, this technique can be fallible if students inappropriately apply the strategy, such as "flattening" a Dash-Wedge or Newman projection to form a Fischer projection as a result of either failing to remember that the FP must be in an eclipsed conformation or a belief that DWs and NPs represent fixed structures that cannot be rotated (or both) (Boukhechem *et al.*, 2011; Kumi *et al*., 2013).

Regardless, aberrant alteration of the spatial arrangement of substituents when translating from one representation to another will commonly lead to the formation of stereoisomers – molecules that have the same molecular formula and sequence of bonded atoms, but that differ in the three-dimensional arrangement of substituents in space (Loudon, 2008). In molecules with

two or more chiral centers, a *diastereomer* is formed when the bonding arrangement of two substituents on one center is changed. The *enantiomer*, a mirror-image stereoisomer of the chiral molecule, can be formed if such a change occurs on both chiral centers (assuming a molecule has only two chiral centers; see Figure 3).

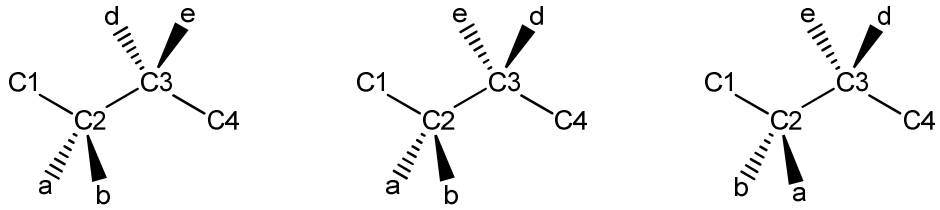

Figure 3. Rearrangement of bonds creates new molecules. The center molecule is the diastereomer of the left molecule, in which the arrangement of substituents on the C3 carbon have been reversed. The right molecule is the enantiomer of the left molecule.

Recent reports suggest that students perform these types of errors on translation tasks as frequently as 76% of the time, depending on the experimental context (Stull *et al.*, 2012). These findings reinforce the importance of attending to students' interpretation of diagrammatic conventions when considering their success at translating between 2D representations in Organic Chemistry.

Methods

Participant Sampling and Treatment Allocation Procedures

Participants (n = 49) were selected at random from all students currently enrolled in an Organic Chemistry I course at a large, research-intensive university in the eastern United States. Upon consent, participants were quasi-randomly assigned to one of two treatment conditions based on their seat location in the classroom (students first selected their seat, and assessments were subsequently distributed in alternating order). Specifically, these conditions were: completion of a 24-item, multiple-choice Newman projection assessment followed by completion of a 16-item, mixed-response Fischer projection assessment (n = 23); or vice versa (n = 26). Because of the quasi-experimental nature of the study, a counterbalanced design was utilized to account for any mediating influence assessment order would have on student performance. Both assessments were untimed, and students were asked to complete the diagnostics individually. Students were instructed not to write directly on the assessments, forcing them to adopt a mental modeling problem-solving strategy. It is important to note also that while all participants taking part in this study had received prior instruction on the Dash-Wedge, Newman, and Fischer diagrams, none had received specialized instruction (i.e., instruction above and beyond the standard course curriculum) on how to interpret the diagrammatic conventions of these three diagrams to translate between representations.

Diagnostic Instruments

Newman Projection Assessment. The Newman Projection Assessment (NPA) consisted of 24 multiple-choice items, each depicting an initial, unique, 4- or 5-carbon straight chain molecule in the form of a Dash-Wedge (DW) diagram. These diagrams were presented in either a staggered or eclipsed conformation, with molecule conformation being randomized equally across the assessment to avoid presentation bias. The rationale for including both staggered and eclipsed Dash-Wedge diagrams was two-fold. First, representing molecules in this way is more realistic because it reinforces the notion that molecules are dynamic (i.e., that they can adopt more than one conformation). Second, we were interested in assessing the impact DW conformation had on students' success on the NPA, especially given research indicating that novices tend to perceive molecules as static in nature (Grosslight *et al.*, 1991; van Driel & Verloop, 2002). Items on the diagnostic were adapted from Stull and colleagues' (2012) *Representational Translation Tasks* assessment and were evaluated by three chemistry and chemistry education experts prior to their inclusion on the NPA to ensure they were of equal and appropriate difficulty. All items were presented individually on an 8.5" x 11" piece of paper.

Immediately below each of the 24 initial diagrams were five answer choices representing various NPs that could potentially correspond to the Dash-Wedge diagram depicted in the given task. One of these NPs was an exact conformer of the Dash-Wedge diagram. The other answer choices designed as distractors included the C2 and C3 diastereomers of the molecule, the enantiomer, and a molecule in which the substituents on the C2 and C3 chiral centers had been rearranged on the molecule at random.

In eight of the problems, all of the five NPs were illustrated having undergone no rotation. In other words, it was theoretically possible for students to perform a direct translation between the DW and NP diagrams with little mental manipulation, as the NP was an exact conformer of the original Dash-Wedge representation. Eight additional problems contained NP answer choices that had undergone a simple rotation in which the front carbon had been rotated 120°. The last group of eight problems depicted NPs that had undergone a complex rotation in which both the front *and* back carbons had been rotated 120° in opposite directions (Figure 4). Because the order of DW presentation was randomized, the type of NP shown in each problem was likewise randomized, the end result being four problems with staggered DWs containing answer choices where the NP had undergone no rotation, four problems with eclipsed DWs containing answer choices where the NP had undergone no rotation, etc., with these problems being randomly distributed throughout the assessment.

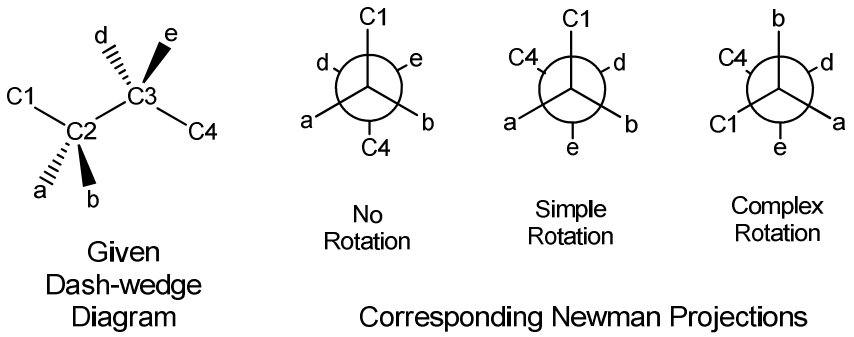

Figure 4. The C2-C3 Newman projections corresponding to the Dash-Wedge diagram at the left are shown having undergone no rotation, simple rotation, and complex rotation.

For each problem, students were asked to select the response they believed best illustrated the correct conformer of the DW diagram presented to them in the task. Student responses were scored as either correct ('1') or incorrect ('0'), and then entered directly into SPSS® for data analysis purposes.

Fischer Projection Assessment. The Fischer Projection Assessment (FPA) consisted of 8 multiple-choice and 8 open-ended response items, each depicting an initial, unique, 4- or 5-carbon straight chain molecule in the form of a Dash-Wedge (DW) diagram. These diagrams varied both in conformation (either staggered or eclipsed) as well as orientation of substituents on the C2 carbon (resulting in the formation of either an upright Y-template at the C2 position or an inverted Y-template at the C2 position; refer to Figure 1). Conformation and C2 Y-template orientation were randomized equally across the assessment to avoid presentation bias. Likewise, the carbon chain of the DW was numbered so that students' ability to assign priority to the molecule was not a potentially confounding factor. The construction of problems in this manner and the inclusion of 8 open-ended questions instead of 8 additional multiple-choice questions on this diagnostic was done intentionally based on research suggesting that students have greater difficulty in both selecting and drawing FPs *de novo* from either a Dash-Wedge diagram or Newman projection than in performing translations between DWs and NPs (Stull *et al.*, 2012). Items on the diagnostic were adapted from Stull and colleagues' (2012) *Representational Translation Tasks* assessment and were evaluated by three chemistry and chemistry education experts prior to their inclusion on the FPA to ensure they were of equal and appropriate difficulty. Each item was presented individually on an 8.5" x 11" piece of paper (see Appendix A for an example of a close- and open-ended item).

Within the multiple-choice section of the assessment, students were asked to select, from a list of five answer choices, the FP they believed best illustrated the correct conformer of the DW diagram presented to them in the task. Students were informed prior to beginning both sections of the assessment that the C1 carbon of the DW molecule should be shown at the top of the FP and the C4 carbon shown at the bottom. In addition to the exact conformer, answer choices included both the C2 and C3 diastereomers of the DW, the enantiomer, and a molecule in which the C1 and C4 carbons of the Fischer projection were not located at the top and bottom of the diagram, respectively. Student responses were scored as either correct ('1') or incorrect ('0'), and then entered directly into SPSS® for data analysis purposes.

Student responses on the open-ended questions were coded using the same categories as the available multiple-choice answers, namely: exact conformer, enantiomer, C2 diastereomer, C3 diastereomer, and other (a category that included any incorrect response not evaluated as a diastereomer or enantiomer of the DW diagram). Each question was coded independently by two research assistants, with 100% agreement between raters observed ($\kappa = 1.0$, $p < 0.001$). As was the case for questions on the multiple-choice portion of the FPA, student responses were then also scored as either correct ('1') or incorrect ('0') and transferred directly into SPSS® for future data analysis.

Results and Discussion

A series of independent t-tests was performed to assess for potential biases introduced due to order of presentation of the diagnostics used in this study on student performance

outcomes on both the NPA and FPA. No significant differences in student performance were observed either for the NPA ($t(47) = 0.185$, $p = 0.854$) or the FPA ($t(47) = 0.318$, $p = 0.752$), suggesting no effect due to order of presentation of the instruments. Q-Q plots identified five participants who were extreme outliers on the FPA, with scores three times greater than the upper quartile score. These individuals were removed from the FPA analysis. Remaining assumptions for performing parametric tests were confirmed prior to data analysis.

Student Performance on the NPA is influenced only by the Degree of Rotation of the Newman Projection

In an effort to examine how variation in the diagrammatic conventions of both Dash-Wedge and Newman diagrams influenced students' ability to translate between these representations, a 2x3 Repeated Measures Analysis of Variance (RM ANOVA) procedure was performed. Dash-Wedge Molecular Conformation (staggered vs. eclipsed) and Degree of Rotation of the Newman Projection (no rotation, simple rotation, complex rotation) served as within-subject variables in this analysis.

Results indicated that while the molecular conformation adopted by the Dash-Wedge diagram did not significantly impact student performance on the NPA ($p = 0.121$), the degree of rotation of the NP did (Table 1). No interaction between DW molecular conformation and degree of rotation of the NP was observed. Subsequent post-hoc analyses with Bonferroni correction revealed that students' accuracy was greatest on tasks in which the NP had undergone no rotation, followed by problems depicting NPs having undergone a simple rotation, and finally problems in which the NP had undergone a complex rotation (Table 2).

Table 1. Repeated measures ANOVA results for Newman Projection Assessment (NPA)

	df	F	η^2
Degree of Rotation	(2, 96)	37.056**	.436
Molecule Conformation	(1, 48)	2.494	.049
Degree of Rotation × Molecule Conformation	(2, 96)	0.389	.008

**$p < 0.001$

Table 2. Marginal means of student scores (percent correct) stratified by degree of Newman projection rotation

	Mean Score (SD)	t-statistic[a] (df = 48)	Cohen's *d*
Direct Newman Projections	73.72 (27.15)	6.160**	0.95
Simple Rotations of Newman Projections	48.47 (25.72)	2.105*	0.27
Complex Rotations of Newman Projections	41.07 (28.30)		

[a] Post-hoc t-statistic comparing mean scores of indicated conditions; *$p < 0.05$; **$p < 0.001$

Frequency statistics showed that in instances where participants did not select the correct response, they most often selected the enantiomer (>25% of tasks involving direct translations; >45% of tasks involving simple or complex rotations of the NP) or C3 diastereomer (~1% of tasks involving direct translation; ~10% of tasks involving simple or complex rotations of the NP) of the Dash-Wedge molecule. This observation is consistent with previous reports in the literature describing student errors when translating between Dash-Wedge and Newman diagrams (Stull *et al.*, 2012).

Taken together, the results we present here demonstrate that although tasks requiring manipulation and mental rotation of NPs are authentic both in the discipline (Newman, 1955) and in instructional contexts (American Chemical Society, 2010), it is clear students struggle at interpreting NP conventions when the three-dimensional depiction of the Newman projection is not as they anticipated (in this case, when the NP is not an exact conformer of the DW diagram). We suspect that this may be the case for two reasons.

First, participants' low performance on tasks requiring indirect translation between the Dash-Wedge and Newman diagrams may be due to the fact that students lack a clear understanding of the structure of the NP (i.e., what it looks like three-dimensionally in space) and/or fail to recognize the dynamic nature of molecules. In their research on Algerian pre-service teachers' knowledge of stereochemistry, Boukhechem et al. (2011) state, for instance, that students possess a "lack of consideration of free rotation around the carbon-carbon bond…many students consider the representations [Newman and Cram] as fixed and simply compare the positions of certain substituents relative to the plane of projection" (p. 341). Bodner and Domin's (2000) review of problem solving in the domain reaffirms this claim, suggesting that although novices tend to be able to recognize multiple representations of the same molecule, their inability to identify or construct initial representations that activate appropriate schema for answering the problem lead them to be unsuccessful at the task at hand.

Secondly, for tasks requiring identification of rotated NPs, additional mental manipulation is necessitated, increasing the level of cognitive demand placed upon the student. A multitude of previous studies have examined the effects of angular disparity on response time and difficulty of rotation tasks, demonstrating a positive, linear correlation between task difficulty and the complexity of rotation (Shepard & Metzler, 1971; Cooper, 1975; Voyer, 1995; Wraga *et al.*, 2003; Stieff, 2007; Wiedenbauer *et al.*, 2007). It is likely that students in our study population are experiencing the same difficulties, particularly as they attempt to simultaneously negotiate chemistry content and perform mental manipulation of the NP presented in the task.

Ultimately, however, we are unable to determine whether it is students' misinterpretation of the physicality and dynamic nature of molecules or their (in)accurate use of mental modeling strategies that leads them to perform more poorly on indirect versus direct translation tasks between Dash-Wedge and Newman diagrams. In either case, it is clear that if we are to ask students to make effective use of these diagrams, for instance in determining the energetic stability of molecules, they must be provided with an opportunity to appropriate and apply representational skills central to accomplishing that goal. We suggest, first and foremost, that this agenda requires targeted instruction on the various types of 2D stereochemical diagrams encountered in the field and the *relationship* between these representations. Such instruction should be supplemented by explicit discussion of imagistic and analytic strategies for solving visuospatial tasks in the domain (Stieff, 2007; Stieff *et al.*, 2010), as well as repeated opportunities for students to engage in applying knowledge in practical contexts (Leone *et al.*, 1993; Voyer, 1995). Ideally, adopting this approach should lessen the chance that students will

simply be conditioned to solve representational translation tasks or utilize representations in singular, discrete ways, instead focusing on the interconnected and dynamic nature of molecules.

Student Performance on the FPA is influenced by the Conformation of the Dash-Wedge Diagram and Orientation of Substituents on the C2 Carbon

In order to next assess student performance on Dash-Wedge to Fischer translation tasks, a 2x2x2 RM ANOVA was performed. Question Type (multiple choice vs. open-ended), Dash-Wedge Molecular Conformation (staggered vs. eclipsed), and Orientation of the C2 Y-template (upright vs. inverted) of the DW diagram served as within-subject variables in this analysis.

Results revealed a main effect both for DW molecular conformation and C2 Y-template orientation, as well as an interaction effect between these two variables (Table 3). *A posteriori* pairwise comparisons with Bonferroni correction indicated that participants performed significantly better on tasks depicting DW diagrams in an eclipsed conformation, with greater levels of accuracy observed for eclipsed tasks that also presented the C2 Y-template in an inverted orientation (Table 4; Figure 5c).

Table 3. Repeated measures ANOVA results for Fischer Projection Assessment (FPA)

	F (1,43)	η^2
Question Type	0.898	.020
C2 Y-template	23.112**	.350
Molecule Conformation	378.052**	.898
Question Type × C2 Y-template	1.811	.040
Question Type × Molecule Conformation	0.123	.003
C2 Y-template × Molecule Conformation	18.373**	.299
Question Type × C2 Y-template × Molecule Conformation	1.811	.040

**$p < 0.001$

Table 4. Differences in participant scores (percent correct) stratified by Fischer projection question conditions

	Mean Score (SD)	t-statistic[a] (df = 43)	Cohen's *d*
Eclipsed, Inverted C2 Y-template	67.05 (33.14)		
		4.57**	1.27
Eclipsed, Upright C2 Y-template	26.14 (31.42)		
		4.96 **	1.02
Staggered, Inverted C2 Y-template	2.84 (8.03)		
		1.00	0.16
Staggered, Upright C2 Y-template	1.70 (6.37)		

[a] Post-hoc t-statistics comparing mean scores indicated; ** $p < 0.001$

A closer examination of participants' top responses stratified by DW molecular conformation and C2 Y-template orientation provides further detail regarding the above observation (Table 5). For eclipsed molecules with an inverted C2 Y-template, the correct answer choice was chosen or drawn most often (67.05%), while the enantiomer was chosen or drawn most often for eclipsed molecules with an upright C2 Y-template (64.20%). The FP of the C3 diastereomer was chosen or depicted most frequently for staggered molecules with an inverted C2 Y-template (63.64%), whereas the C2 diastereomer was chosen or depicted most frequently for staggered molecules with an upright C2 Y-template (64.20%).

Table 5. Comparison of top answer choices on Fischer projection items

Molecule Conformation, C2 Y-template & Top Answer Choices[a]	Mean % of Answers (SD)	t-statistic (df = 43) Comparing First and Second Answer Choices	t-statistic (df = 43) Comparing First and Correct Answer Choices
Eclipsed, Inverted Y			
Correct	67.05 (33.14)	4.27**	
Enantiomer	26.70 (31.16)		
Eclipsed, Upright Y			
Enantiomer	64.20 (37.12)	3.83**	
Correct	26.14 (31.42)		
Staggered, Inverted Y			
C3 Diastereomer	63.64 (32.10)		
C2 Diastereomer	25.57 (28.27)	4.40**	11.22**
Correct	2.84 (8.03)		
Eclipsed, Upright Y			
C2 Diastereomer	64.20 (33.41)		
C3 Diastereomer	24.43 (30.26)	4.37**	11.66**
Correct	1.70 (6.37)		

[a] The percent of correct answer choices has been included for comparison; **p<.001; Cohen's *d* values were greater than 1.10 for all comparisons.

It is interesting to note that each of these top responses would result from a simple, albeit potentially fallible, "flattening" of the DW diagram. As discussed above, participants repeatedly constructed or selected FPs of both the C2 and C3 diastereomers when shown staggered DW molecules. Such diastereomers are created when staggered molecules are flattened onto the FP template without regard for the stereochemical properties of the Fischer projection, as is illustrated in Figure 5a & b, respectively. As previous research confirms that similar "flattening" strategies have been employed by students outside of our sample (Boukhechem *et al.*, 2011) – an

observation that has been attributed to those individuals failing to remember that the FP must be in an eclipsed conformation – we believe that this misconception exists strongly among students enrolled in introductory Organic Chemistry courses both nationwide and globally.

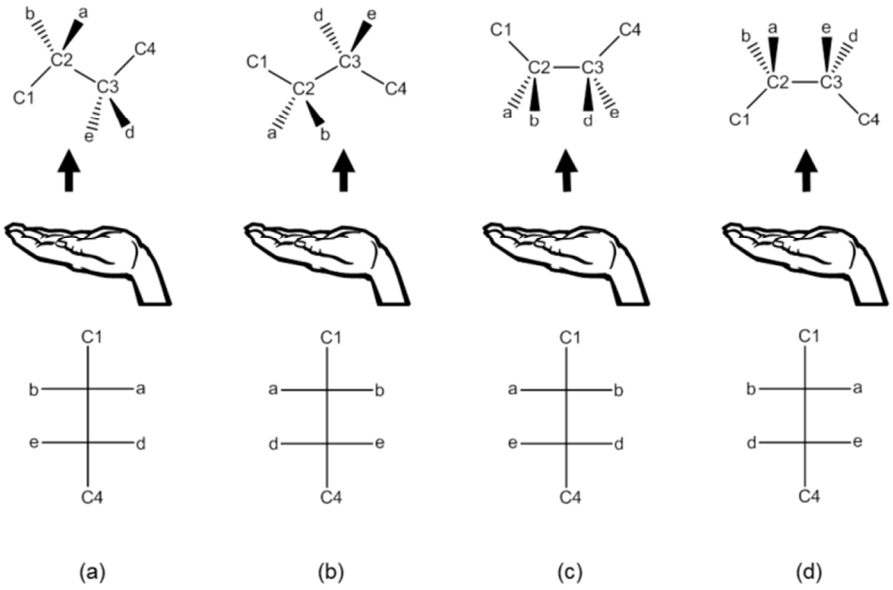

Figure 5. The same DW molecule with different conformations and C2 Y-templates is shown being flattened from below. Below each hand is the resulting Fischer projection. Flattening of the staggered molecule with an upright C2 Y-template produces the Fischer projection of the C2 diastereomer (a), and flattening of the staggered molecule with an inverted C2 Y-template produces the Fischer projection of the C3 diastereomer (b). Only the eclipsed molecule with an inverted C2 Y-template produces the true Fischer projection when flattened from below (c). Flattening from below of the eclipsed molecule with an upright C2 Y-template produces the Fischer projection of the molecule's enantiomer (d).

Furthermore, our analyses suggest that the observer consistently positions him- or herself "below" the Dash-Wedge diagram prior to employing the flattening technique. When shown eclipsed DW molecules with an upright C2 Y-template, for instance, participants in our study overwhelmingly generated or selected FPs corresponding to the molecule's enantiomer. In order for this to occur, the observer must be lying below the molecule with the substituents pointing away from him (Figure 5d) rather than above the molecule with the substituents pointing toward him, as would be the proper perspective to adopt.

Students' positioning below the DW diagram is likewise evident in tasks where the initial representation is staggered. In this case, we can determine the viewing perspective used by the participant through investigation of the location of the diastereomer error made – that is, if the error occurred at the C2 or C3 carbon center. In our sample, participants created or selected FPs of the C2 diastereomer most often when shown staggered molecules with an upright C2 Y-template, and they generated or chose FPs of the C3 diastereomer most often when shown staggered molecules with an inverted C3 Y-template. In both situations, the diastereomer error

occurs at the carbon center on which substituents point to the top of the molecule and the carbon center where substituents point below the molecule is projected correctly on the FP (Figure 5a & b), suggesting alignment of participants' viewing perspective below the molecule.

Together, the inappropriate combination of representational skills utilized by students when translating between DW and FP diagrams is indicative that students do not appreciate the conventions represented by the horizontal and vertical lines in the Fischer projection. Although the eclipsed nature of the FP is discussed in class, and though textbooks note that in the Fischer projection the "horizontal lines…emerge from the page, toward the observer, and the vertical bonds… recede behind the page, away from the observer" (Loudon, 2008; p. 1169), it is likely that participants tend either to see the DW molecule as static (and, therefore, unable to rotate from a staggered to an eclipsed conformation) or else are unsure which perspective to adopt when translating between DWs and FPs. This is, perhaps, not entirely surprising, as the conventions of the Fischer projection are distinctly unique in comparison to the DW and NP (Loudon, 2008). The fact that the difference in student performance on multiple-choice versus open-ended items was not statistically significant ($F(1,43) = 0.898$, $p = 0.349$) despite the limited number of potential answers on the former set of tasks only serves to highlight the strong degree of difficulty students have in understanding the conventions of the FP.

At the extreme, previous research has called into question the value of teaching Fischer projections alongside the Dash-Wedge and Newman diagrams, if at all (Bentley, 1997). In some cases, textbooks mirror this perception, placing Fischer projections in a separate unit on carbohydrate chemistry rather than in the section devoted to 2D molecular representations and stereochemistry (Kumi *et al.*, 2013). Given Fischer's original rationale for developing the diagram (Loudon, 2008), this is not unexpected; however, we believe presenting the FP as disconnected from the DW and NP inflates the likelihood that students will come to see these three representations as being unrelated, at least to some degree. Furthermore, if students are expected to make *use* of the Fischer projection, for instance on in-class assessments or standardized exams (American Chemical Society, 2010), it is essential that attention be placed on promoting students' understanding of the conventions of the FP.

Conclusions and Implications for Instruction

In this paper, we examined the impact 2D diagrammatic conventions had on students' ability to translate from a Dash-Wedge diagram to either a Newman projection or Fischer projection. Specifically, we showed that participants in our study exhibited difficulty in translating from a DW to NP when the Newman projection had undergone increasing degrees of rotation, with the greatest level of accuracy observed when the NP was depicted as an exact conformer of the original Dash-Wedge molecule, followed by NPs that had undergone simple rotation, and then NPs that had undergone complex rotation. It is likely that these data resulted from students' lack of or incomplete understanding of the dynamic nature of molecules, as well as difficulty employing mental rotation techniques to translate between different representations of the DW and NP diagrams.

As further evidence of this latter claim, we have demonstrated that students' ability to successfully translate between DW and FP diagrams is impeded when the Dash-Wedge molecule is not depicted in an eclipsed conformation with the C2 Y-template of the DW oriented in an inverted position. Based upon previous empirical evidence in the literature (Boukhechem *et al.*,

2011; Olimpo, 2013), we believe that this inaccuracy emerges as a result of students simply "flattening" the DW diagram onto the skeletal structure of the FP without regard for the spatial arrangement of substituents on either representation. From a comparative standpoint, employment of this technique is reflective of the same trend observed for the NP data discussed above – namely, that as the cognitive demand placed upon the student increases (i.e., as they are asked to increasingly grapple both with chemistry content and mental manipulation of diagrams), the complexity of the task, as perceived by the student, likewise increases as does the chances the student will respond incorrectly to the prompt. We discuss the implications of cognitive demand on student learning in further detail momentarily.

The important question that arises from these analyses, then, is *How do we help students visualize the relationship between multiple representations of the same molecule, particularly when the conventions of these diagrams are varied in nature?* Unfortunately, traditional lectures in Organic Chemistry do not, and perhaps cannot, devote extensive time to explicit discussion of these diagrams nor the mechanisms by which one translates between representations (Grove & Lowery-Bretz, 2012). However, instructors must remain aware of the difficulties students possess in applying representational skills, such as the ability to interpret the conventions of common 2D diagrams, manipulate these diagrams, and translate from one representation to another. From a pedagogical standpoint, we argue that classroom instruction should therefore include examples of molecules depicted in various conformations and offer students extensive opportunities to practice working with each of these representations of a molecule such that they gain a better understanding of the relationship between diagrams.

In their review of spatial ability in the context of chemistry, Harle and Towns (2010) provide several direct recommendations that mirror this goal. Specifically, these suggestions include:

- Explicit articulation of diagrammatic conventions and three-dimensional cues, with "students [being] required to construct and describe 2-D representations that are encoded with 3-D cues such as wedge-dash notation…" (p. 357).
- Continued instruction on molecular representations across lecture, laboratory, and recitation contexts
- Repeated teaching of domain-specific visualization skills, including both imagistic and analytic problem-solving approaches (see Stieff & Raje, 2010 for a description of such strategies)
- Providing extensive resources for students to practice spatial ability skills and achieve mastery of the material

Though imperative to promoting students' development of representational competence in the domain, we contend that these time-on-task recommendations do not fully address the heart of the issue – visuospatial tasks are inherently easier for some students and harder for others.

Indeed, while students' level of spatial ability has been repeatedly shown to mediate performance on visuospatial assessments in the discipline (Harle and Towns, 2010; Stieff, 2007; Stieff & Raje, 2010), it is likewise feasible that the added requirement of simultaneously needing to access chemistry knowledge to solve such tasks increases cognitive load to the extent that novices are unable to effectively interpret and make use of multiple representations when problem-solving. In her review of the use of visual representations in scientific fields, Cook (2006) argues that this augmented cognitive demand stems from the fact that students often lack

extensive prior general knowledge in the field, as well as the specific skills required to make meaning of multiple representations at a non-superficial level. To more effectively promote student understanding of scientific representations, Cook suggests that "multiple representations of information using the same modality, or multiple representations of information in visual and verbal modes, must be physically and/or temporally integrated so that students may extract information out of all of the representations" (p. 1085). She continues by noting that increased instructional guidance and use of instructional design practices that reduce students' cognitive load are likely to benefit individuals of all levels of experience across scientific domains.

Much like Harle and Towns (2010) and Cook (2006), we agree that attending both to novices' prior knowledge in the domain as well as pedagogical strategies employed in the Organic Chemistry classroom is necessary for improving students' representational competence in the discipline. Scaffolding students' understanding of complex, representationally-heavy topics in the field and providing them with the analytical and visuospatial tools (Stieff *et al.*, 2010) to make sense of these representations is critical. Though not an explicit focus of the research presented here, ongoing work from our own group and others also suggests that concrete and virtual models may present one suitable avenue through which to promote students' understanding of 2D molecular visualizations, particularly when coupled with extensive opportunities for novices to make use of these manipulatives in practical settings (Stull *et al.*, 2012; Olimpo, 2013; Stull *et al.*, 2013).

Collectively, the above recommendations are of particular importance given that textbooks and other forms of media in the discipline often perpetuate students' misconceptions about diagrams (Kumi *et al.*, 2013). While we do not claim to provide an exhaustive list of remedies, it is our assertion that more definitive attention to how students are interpreting and manipulating diagrams, particularly with regard to diagrammatic conventions, is imperative for augmenting students' overall representational competence in the domain.

Acknowledgements

We would like to acknowledge Doug Findeisen and Felicia Bartlett for their research assistance. We thank Drs. Mike Stieff and Mary Hegarty for their valuable input into the research design of the study, support of this project, and reviews of early versions of this manuscript. This research was supported by the National Science Foundation grants DRL-0723313 and DRL-1008505.

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Appendix A. Sample items on the Fischer Projection Assessment

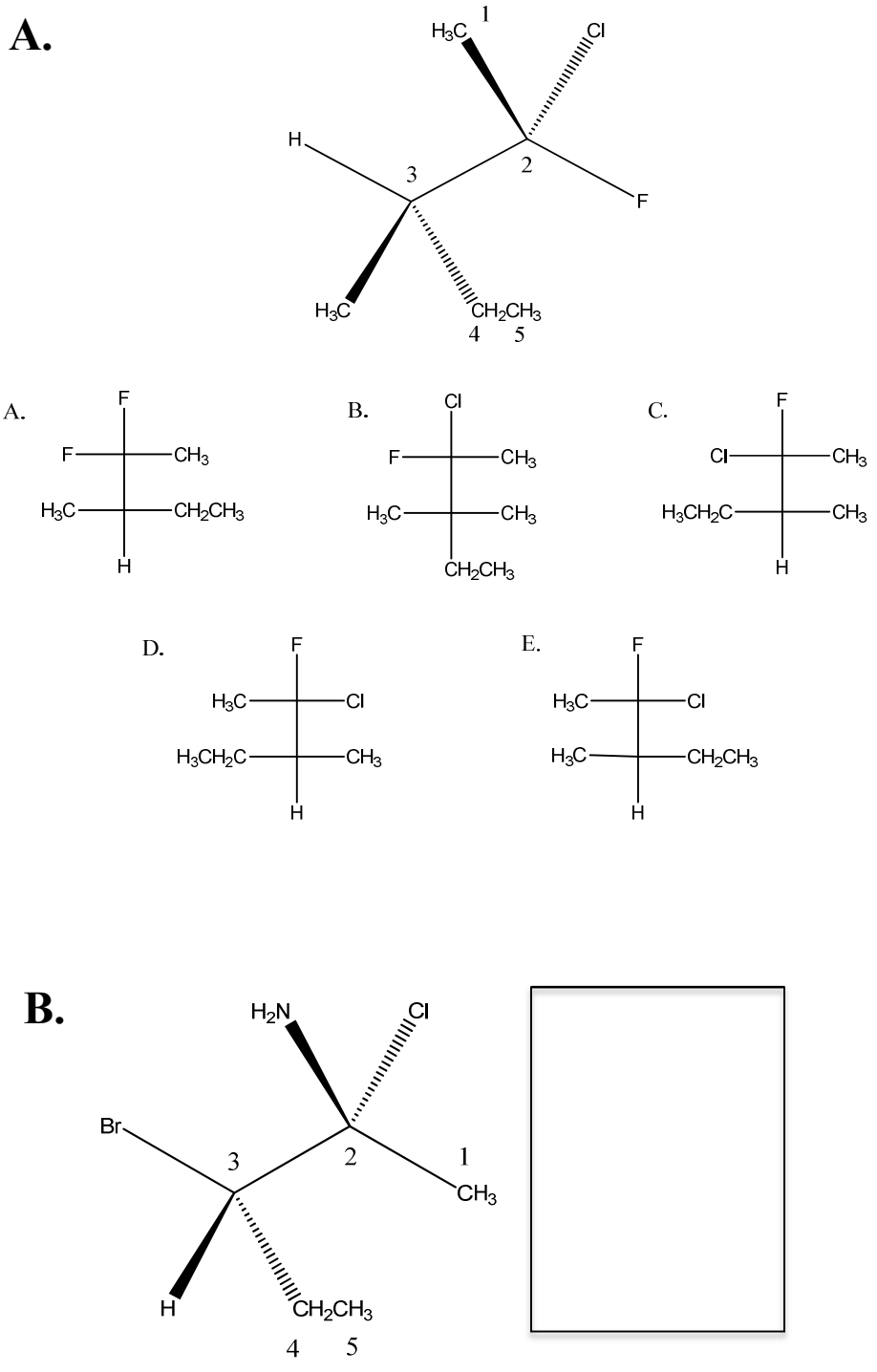

Figure S1. Examples of a close-ended (A) and open-ended (B) item on the FPA.