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# Using Eye-Tracking and Molecular Modeling to Explore Students' Strategies for Solving Organic Stereochemical Problems

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UNIVERSITY OF NORTHERN COLORADO

Greeley, Colorado

The Graduate School

# USING EYE-TRACKING AND MOLECULAR MODELING TO EXPLORE STUDENTS' STRATEGIES FOR SOLVING ORGANIC STEREOCHEMICAL PROBLEMS

A Dissertation Submitted in Partial Fulfillment
of the Requirements for the Degree of
Doctor of Philosophy

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Department of Chemistry & Biochemistry
Chemical Education Program

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This Dissertation by: Travis Howard Knowles

Entitled: *Using Eye-Tracking and Molecular Modeling To Explore Students' Strategies For Solving Organic Stereochemical Problems*

has been approved as meeting the requirement for the Degree of Doctor of Philosophy in College of Natural and Health Sciences in School of Chemistry, Program of Chemical Education

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# ABSTRACT

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Stereochemistry concepts are often some of the most difficult topics for students to grasp in the organic chemistry curriculum. Several factors may influence students' abilities to solve stereochemistry problems, including their spatial abilities, strategy choice, and ability to use various types of spatial representations. A mixed-method study was conducted to investigate the role that these factors play when novice organic chemistry students solve stereochemistry problems. Eye-tracking methods were used in an attempt to capture cognitive processes of students while solving these problems. Additionally, three-dimensional molecular models and spatial ability measures were used to further analyze and characterize their strategies for solving these problems.

Quantitative eye-tracking data revealed key insights into how organic chemistry students solve stereochemistry problems. Further, qualitative data indicated that strategy choice and representation type impact success on stereochemistry problems. Finally, results showed a significant relationship between spatial ability and performance in a first semester organic chemistry course.

The findings of this study have several implications for how we teach chemistry. First, students who struggle with visuospatial tasks due to their inability to successfully apply holistic mental rotation strategies may benefit when they are taught to use analytic strategies. However, while analytic strategies may help students to arrive at the correct answer on stereochemical problems, they may do little to help students visualize the three-dimensional arrangement of atoms or the spatial relationships between molecules. Additionally, performance on stereochemical problems may be enhanced when students are allowed to use physical models, and when they are encouraged to search for key features of the molecule during the problem-solving process.

# ACKNOWLEDGEMENTS

There are no words to describe how grateful I am to everyone that has helped me throughout this journey. My family has been the single strongest source of support – from the very moment that I embarked upon this journey. I could not have turned this dream into a reality without any of you! From the words of encouragement that you have shared with me and the prayers that you have said on my behalf, it has been good to know that I was not alone during this process.

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# CHAPTER 1

# INTRODUCTION

Organic chemistry is a scientific domain where visuospatial thinking plays a central role, especially for identifying important spatial relationships within molecular structures and understanding their transformations over time (Stieff, Ryu, Dixon, & Hegarty, 2012).Visuospatial thinking occurs when an individual forms a mental image and manipulates it in a principled manner (Mayer, 2005). Anecdotally, the importance of visuospatial thinking within organic chemistry was demonstrated in 1865 when the German organic chemist Friedrich Kekulé had a daydream about a group of atoms moving like a snake and grabbing its own tail (Rothenberg, 1995). It is reported that Kekulé credited his discovery of the ringed structure of benzene, one of the most important compounds involved in the study of organic chemistry today, to his daydream (Wu & Shah, 2004).

Due to the highly visual nature of organic chemistry, it should come as no surprise that undergraduate organic chemistry textbooks are filled with numerous types of visual representations, including drawings of stick structures, space-filling models, Newman projections, Fisher projections and other types of two-dimensional (2-D) molecular representations of three-dimensional (3-D) molecules (Pribyl & Bodner, 1987).

Consequently, organic chemistry students are expected to correctly interpret the structure information shown in these representations (Burrmann & Moore, 2015), and to use them to construct and manipulate three-dimensional mental images (Pribyl & Bodner, 1987). Organic chemistry students are challenged to use their visuospatial thinking when they are solving problems (Stull, Hegarty, Dixon, & Stieff, 2012). For example, when students are asked to predict the reactivity of a molecule, they must not only consider the number and type of atoms that make up a molecule, but also the spatial configuration of these atomic substituents (i.e., functional groups of atoms) (Stull et al., 2012). An illustration of this can be seen with the pair of molecules, maleic acid and fumaric acid (Figure 1-1), which have the same atomic makeup and differ only in the spatial configuration of their atoms (i.e., they are stereoisomers). However, these molecules have distinctly different properties – maleic acid is a harmful toxin, while fumaric acid is a common food additive.

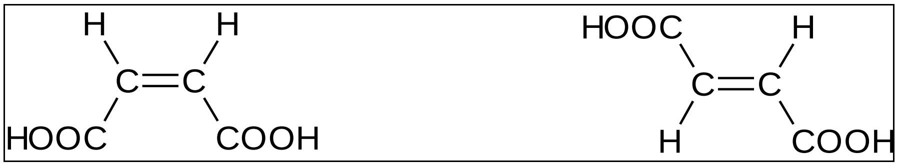


Figure 1-1: A pair of stereoisomers, maleic acid (left) and fumaric acid (right)

## Statement of the Problem

Although visuospatial thinking is important for the study of organic chemistry, many students have difficulty with it, especially in three dimensions (Tuckey, Selvaratnam, & Bradley, 1991). This obstacle ultimately impacts their success on mastery of various chemistry topics (Carter, LaRussa, & Bodner, 1987; Wu & Shah, 2004). *Stereochemistry*, which is concerned with chemistry in three dimensions (Carey, 2008), is a particular area of organic chemistry that may present challenges for students who struggle with visuospatial thinking.

Indeed, topics related to stereochemistry are often some of the most difficult for students to grasp in the organic chemistry curriculum (Richardson, 1989; Varghese, 1996). Barta and Stille (1994) argue that stereochemical concepts are among the first stumbling blocks that students encounter in organic chemistry, and failure to master these concepts can handicap a student throughout an entire course. Furthermore, Varghese (1996) asserts that even after finishing the first semester of an organic chemistry course, students are still unable to determine stereochemical relationships (such as whether two molecules are identical or whether they are non-superimposable mirror images called enantiomers). Furthermore, they are unable to assign the absolute configuration of stereocenters (i.e., chiral centers, atoms that have four nonequivalent atoms or groups attached to them).

## Background

### Stereochemistry Problem Solving

There are several reasons to account for why stereochemistry topics may be especially difficult for many students. The first reason may be due to their inability to visualize and spatially reason in three dimensions (Taagepera et al., 2011), which is strongly related to their level of spatial abilities (Stieff et al., 2012). The construct of *spatial ability* may be defined as the ability to generate, retain, retrieve, and transform well-structured visual images (Lohman, 1979). Indeed, there is often significant variation in students’ ability to visualize and mentally manipulate 3-D structures (O’Brien, 2016). For students with low levels of spatial abilities, topics related to stereochemistry can be especially challenging because they require students to be able to visualize 3-D molecular structures (Popova, Bretz, & Hartley, 2016).

In addition to factors related to spatial ability, the type of spatial representation may also impact a student's ability to solve stereochemistry problems. Chemists use two general types of spatial representations to convey information about molecules. One type is *molecular models* which are physical models that represent the 3-D spatial relations between atoms in a molecule. The other type is 2-D diagrams which use conventions to represent 3-D relations in the two dimensions of the printed page (Stull et al., 2012). Abraham and colleagues (2010) argue that the difficulty some students have when solving stereochemistry problems may be because 3-D molecular structures are shown in textbooks as 2-D objects. Consequently, students must transfer between 3-D mental images of a molecular structure and its 2-D representation. In translating between these representations, students are typically taught to make step-by-step changes until the conversion is complete. However, many students are unable to visualize molecular shapes properly, and hence one or more steps in this process may fail.

Another factor that may impact an organic chemistry student's ability to solve stereochemistry problems is related to their choice of strategies. Research on how individuals complete visuospatial tasks has shown that it is possible to use a variety of strategies to complete them (Hinze et al., 2014). When completing these tasks, such as stereochemical problems, strategies may be broadly classified as holistic (mental manipulation of the stimulus representation) or analytic (using reasoning processes rather than mental manipulation) (Wang, 2017). Some of these strategies impose greater cognitive load on the problem solver than do the others. As a result, the problem solver often selects the strategy that requires the least amount of their cognitive resources (Contreras, Rubio, Peña, & Santacreu, 2010).

## Spatial Ability and Organic Chemistry

Organic chemistry is a spatially complex discipline that places demands on the spatial ability of students who take this course (Stull et al., 2012). The processing of visuospatial information, such as when solving stereochemistry problems, involves the visuospatial working memory (Baddeley, 2006). Such processing of information in visuospatial working memory is influenced by an individual's level of spatial ability (Miyake, Friedman, Rettinger, Shah, & Hegarty, 2001).

Several factors can impact spatial ability: "age, gender, culture, learning opportunities, and the everyday environment" (Ferk, Vrtacnik, Blejec, & Gril, 2003, p. 1229). This means that within an organic chemistry classroom, there will be individual differences in the spatial abilities of students, with the possibility of gender accounting for some of these differences. From the 1930s to the 1970s, research was conducted in an effort to define the major and minor factors of spatial ability, primarily through factor analytical methods (Harle & Towns, 2010). Such studies have led to the identification of five or more separate factors that make up the construct of spatial ability (Carroll, 1993; Wu & Shah, 2004).

While there still remains no consensus as to how many factors comprise the construct of spatial ability (Harle & Towns, 2010), Antonoglou and colleagues (2008) point out that there are several spatial ability factors that have been discussed in chemistry education literature. These include *spatial visualization,* which involves the ability to mentally represent and dynamically manipulate objects; *spatial orientation,* which may be defined as the ability to imagine how a representation will appear from a different perspective; s*patial relations* which is gauged by speed in manipulating relatively simple visual patterns; and *closure flexibility*, which is the ability to apprehend and identify a visual pattern in the presence of distracting stimuli (Antonoglou et al., 2008).

## The Mental Rotations Test

Due to the many factors contributing to spatial ability, psychometric tests of spatial abilities often vary in the underlying skills they are measuring (Wu & Shah, 2004). Consequently, there are currently dozens of published instruments designed to measure the various components of spatial ability.

The most classic cases of visuospatial thinking studied by cognitive psychologists involve *mental rotation* (Hegarty, 2010). Mental rotation involves using spatial visualization to mentally transform or rotate 2-D or 3-D objects (Maeda & Yoon, 2013). An instrument that is widely used to assess this ability is the Mental Rotations Test (MRT, Vandenberg & Kuse, 1978), which is a pencil-and-paper test that requires comparison of 3-D figures (cube constructions) (see Appendix B).

In 1971, Shepard and Metzler designed the original MRT to investigate the ability to rotate 2-D or 3-D figures rapidly and accurately. They devised individually administered tasks to measure the speed of response to different amounts of rotation. Subsequently, Vandenberg and Kuse (1978) modified the Shepard-Metzler Mental Rotation Test for group administration by developing a test known as the Mental Rotation Test (MRT) (Linn & Petersen, 1985). Later, Peter and colleagues (1995) took up the task of re-drawing the MRT, stating that the available versions of the MRT at that time had physically deteriorated because only copies of copies were available.

The MRT consists of the presentation of a 3-D target object, followed to the right by four similar objects (Moè, Meneghetti, & Cadinu, 2009) (see Appendix B). In each item, participants must decide which two of these four figures are rotated versions of the target. This task is similar to common stereochemistry tasks, where organic chemistry students are required to recognize whether two molecules with the same connections of atoms but in a different rotational arrangement are identical or whether they are non-superimposable mirror images of each other (enantiomers). “That is, both the traditional psychometric stimuli and stereochemistry tasks require a similarity judgment be made about a pair of represented 3-D objects that have been rotated apart to some degree (Stieff, 2007).

Although the MRT was intended to measure the ability to mentally rotate objects (i.e., holistic strategies), some items may be solved using analytic strategies that do not involve mental rotation (Geiser, Lehmann, & Eid, 2006; Hegarty, 2010). In a study by Hegarty (2010), most of the test subjects used holistic strategies to solve items on the MRT. However, there were also a variety of analytic strategies that could be used to solve items, such as inspecting the relative directions of the different segments of the object, or attempting to count the number of cubes in the different segments of the object (Hegarty, 2010). Furthermore, using latent class analysis of response patterns on the MRT, Geiser and colleagues (2006) found that test subjects could be classified into five subgroups (classes) based on their strategies. These distinctions were justified on the basis of overall performance, speediness of response, and whether it involved spatial or non-spatial strategies (Wang, 2017).

## Problem Solving with Molecular Models

Burrmann and Moore (2015) suggested that one of the reasons many students often struggle with the interpretation of molecular structures, particularly in stereochemical contexts, is due to the fact that most molecules are represented using 2-D structures. Consequently, research has indicated that concrete molecular models can help reduce the problems that students encounter with structural interpretation (Burrmann & Moore, 2015).

While research has shown evidence that student performance involving structural interpretation is improved when 3-D physical models are utilized, they are less commonly used in organic chemistry courses than 2-D representations (Burrmann & Moore, 2015). Reasons for the less frequent use of 3-D models include their construction often being time-consuming and spatially cumbersome, especially when building larger molecules (Burrmann & Moore, 2015).

Molecular models may be advantageous to organic chemistry students in several ways. First, as manipulating models eliminates the need to imagine and maintain a 3-D representation in working memory, students are able to ‘off-load’ cognition (Stull, Gainer, Padalkar, & Hegarty, 2016). Furthermore, molecular models allow the 3-D relations between atoms in a molecule to become directly visible rather than deciphered from the conventions used in 2-D models. Additionally, students are able to easily manipulate and observe the results of manipulations of an external representation as opposed to the mental transformations needed for an internal representation. Stull and colleagues (2016) argue that for these reasons, molecular models reduce the demand on working memory and lower a student's cognitive load. This can allow students to devote more cognitive effort to other parts of the problem-solving process.

## Eye-Tracking and Visual Information

Eye movements can be considered direct and non-biased indicators of attentional allocation, which is one indicator of cognitive activity (Tai, Loehr, & Brigham, 2006). In other words, if there is a way to track someone's eye movements, it is possible to gain some insight as to what they found to be interesting or what drew their attention to a particular area (Duchowski, 2007). Therefore, using an eye tracker, it is possible to detect where someone looked at a moment in time, how long they looked at something, and the path that their eyes followed (Bergstrom & Schall, 2014). The recordings of a person's eye movements obtained with an eye tracker can provide information about a person's overt visual attention (Duchowski, 2007).

In the last two decades, eye tracking technologies have been applied in studies of visual attention and comprehension as well as problem solving (Topczewski, Topczewski, Tang, Kendhammer, & Pienta, 2016). With the ability to track both conscious and unconscious eye movements, eye-tracking methodology provides researchers with valuable insights into the student experience that no other technique can capture (Havanki & VandenPlas, 2014). That is, compared to traditional assessment methods such as examination scores and times to accomplish tasks, eye tracking can provide more subtle and accurate data related to learners' attention and cognitive processing (Tang, Kirk, & Pienta, 2014).

## Theoretical Framework: How is Information Processed from Visual Stimuli?

The *information processing theory* provides an important learning theory regarding how information from visual stimuli is processed by the brain (Newell & Simon, 1972). In this theory, the mind is often compared to a computer, because both computers and humans engage in cognitive processes such as learning, remembering, making decisions and answering questions (Mayer, 1996). Using computer processing as a metaphor, the model describes the flow and processing of information from sensory input, such as visual stimuli, to the storage of this information and behavioral responses related to the information (Dehn, 2011). According to this model, the cognitive processing system is comprised of a set of separate but interconnected information processing subsystems, with memory components constituting the core of the system (Dehn, 2011), including sensory, short-term and long-term memory.

Baddeley and Hitch (1974) developed the idea of a working memory within short-term memory, defining it as ‘a system for the temporary holding and manipulation of information during the performance of a range of cognitive tasks including comprehension, learning, and reasoning.’ Working memory has limited attentional resources, meaning that only a limited number of visual stimuli can be focused on at any given time. Consequently, there must be *selective processing* of information. That is, decisions must be made as to which stimuli are worthy of attention and which stimuli can be safely ignored. With respect to visual stimuli, by moving the eyes, attention can be shifted selectively from one place to another, helping to filter information.

## Significance of the Study

This study adds to the sparse research on the cognitive strategies that organic chemistry students use to solve stereochemistry problems. Over the years, one approach to understanding the cognitive processes involved in problem solving has focused on differences between experts and novices (Bodner & Domin, 2000; Mayer, 1992). In keeping with this tradition, this study highlights differences between ‘expert’ and ‘novice’ problem solvers, in how they process information when solving stereochemistry problems.

Additionally, this study focused on differences between ‘successful’ and ‘unsuccessful’ novice problem solvers on stereochemistry tasks. The assumption was that ‘successful’ problem solvers often share more procedural characteristics with experts, and thus distinguishes them from ‘unsuccessful’ novices (Bodner & Domin, 2000; Smith, 1992). Also, through a better understanding of the strategies that successful students use, information on how to help students who are not successful in these problems is provided.

Furthermore, this study adds to the growing chemical education literature on how eye tracking can be used successfully to gain information about the cognitive processes that occur while chemistry students solve problems. As eye tracking is relatively new to the field of chemical education, this study will further demonstrate the value of this tool to the chemical education community.

## Purpose of the Study

Due to the challenges that many students encounter when solving stereochemical problems, a better understanding of the cognitive processes that occur when students solve such problems is warranted. No other studies have used eye tracking and molecular modeling to capture the cognitive strategies of novice organic chemistry students while they solved stereochemistry problems. Therefore, the purpose of this study was to use a mixed-methods approach to investigate the role that strategy choice, spatial abilities, and spatial representation type (i.e., 2-D or 3-D) played when first semester organic chemistry students solved stereochemistry problems.

## Research Questions

The research questions addressed in this study were:

Q1 Were there significant differences in the observed distribution of solution strategies between male and female novice organic chemistry students when solving problems on the Mental Rotations Test-A (MRT-A)?

Q2 When novice organic chemistry students were solving stereochemical problems, could a) eye-tracking methods and b) molecular modeling serve as tools to reveal their cognitive processes?

Q3 Do the strategies used to solve simple and complex organic stereochemical problems differ a) for expert versus novice stereochemistry problem solvers and b) for successful novice stereochemistry problem solvers versus unsuccessful novice stereochemistry problem solvers?

Q4 Were novice students’ solution strategies for solving mental rotation tasks related to their achievement on the American Chemical Society (ACS) standardized organic chemistry examination?

## Assumptions and Limitations

The researcher acknowledges that several assumptions were needed regarding the data collection, its analysis, and interpretations. First, it was assumed the sample selected for this study was representative of students enrolled in first semester organic chemistry courses at similar institutions of higher education – that is, a middle-sized, public university in the Midwest US. Among the participants who volunteered to be interviewed, it was assumed that their performance was representative of the entire sample of students enrolled in this course.

Also, the researcher assumed that since all students had the same organic chemistry instructor, regardless of their lecture section, any ‘instructor effect’ was nil. The researcher also assumed that the MRT, which is a well-established instrument, was a reliable and valid measure of participants’ spatial abilities when these data were collected. For participants who volunteered to be interviewed, it was assumed that the processes they used reflected the strategies and thought processes that they typically used under normal classroom conditions and during assessments.

The researcher recognizes the following limitations regarding the generalizability of this study’s results. This study looked at students enrolled in a first semester organic chemistry course at one university. Consequently, the findings were not assumed to apply to all universities and colleges that teach organic chemistry. That is, generalizations were restricted to institutions with mean ACT scores similar to those at the institution where data was collected.

In regard to all of the qualitative aspects of this study, the researcher was the primary instrument of analysis and interpretation of the qualitative data, and were therefore subject to any biases held by the researcher. Possible biases included the expectation that students would use different strategies to solve stereochemical problems. Further, there was the expectation that the strategies used by experts would differ from those used by novice organic chemistry students.

# CHAPTER 2

# LITERATURE REVIEW

## The Visuospatial Nature of Stereochemistry Tasks

The concept of stereochemistry involves the connectivity and three-dimensional (3-D) spatial arrangement of atoms within an individual molecule (Stieff, Bateman, & Uttal, 2005). This concept has its origins in the year 1848 in Paris, when Louis Pasteur made a set of observations that eventually led him to make a proposal regarding the optical activity of organic solutions. This has become the foundation of stereochemistry: the optical activity of organic compounds is determined by molecular asymmetry (which results in the existence of non-superimposable mirror image structures called enantiomers) (Wainer, 1993). Specifically, Pasteur found that the mold *Penicillium glaucum* ferments the naturally occurring (+)-tartaric acid but leaves its enantiomer untouched (Eliel, 1964).

Today, stereochemistry concepts have become central to the study of organic chemistry, and chemistry educators have devised several different techniques for teaching these concepts. One common stereochemical task involves comparing two or more molecular representations to determine whether they are the same (identical) molecule or stereoisomers (molecules with identical connectivity, but differ from each other only in the way their atoms are oriented in space) (Stieff, 2013). For example, organic chemistry students may be required to determine the relationship between the two molecules shown in Figure 2-1.

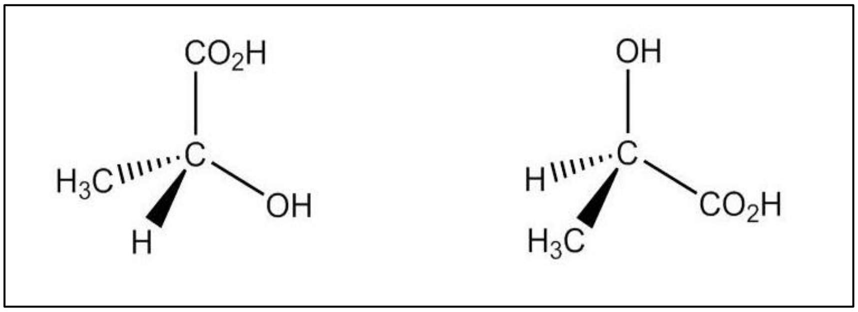


Figure 2-1: Common Stereochemical Comparison Task – Determining the Relationship Between Molecules

The *spatial visualization* factor of spatial ability taps into the skill of mentally manipulating all or part of an object (Tartre, 1990). One component of this spatial ability factor is mental rotation (Tartre, 1990), which may be defined as the ability to mentally manipulate, rotate, twist, or invert objects into different positions (McGee, 1979). As one common strategy for determining the relationship between molecules (such as those in Figure 2-1) involves mental rotation of one of the molecules in an attempt to superimpose it on the other, this is often an important skill when solving stereochemistry problems. If the molecules align perfectly, this allows the problem solver to know that they represent identical structures.

Another common stereochemical task that organic chemistry students encounter is the assignment of absolute configuration (three-dimensional arrangement of atoms or groups at a stereocenter). When solving stereochemistry problems related to absolute configuration, the Cahn-Ingold-Prelog nomenclature system (Cahn, Ingold, & Prelog, 1966) is used. This nomenclature system uses an algorithm to assign the configuration of chiral center(s) within a molecule as *R* (rectus) or *S* (sinister), where the first step for this process requires an assignment of priority sequence to each group about the stereocenter. The sequence is based primarily on the atomic number, where the higher the atomic number of a group, the higher its priority. The viewer then observes and relates the groups on a high to low priority basis, either in a clockwise (denoted as the *R* configuration) or counterclockwise (denoted as the *S* configuration) direction. However, according to the algorithm, the lowest priority group (group with lowest atomic number) that is attached to the chiral center under consideration must be pointing away from the problem solver. That is, if the problem solver is looking at the molecule on paper, the lowest priority group must be going behind the plane of the paper.

"For beginners with little experience in stereochemistry, determining the absolute configuration of chiral molecules can be difficult" (Siloac, 1999, p. 798). Brun and Leblanc (1983) argue that when determining the absolute configuration of a chiral center, the usual textbook method requires students to mentally 'lift out' a molecule from the two-dimensional (2-D) plane, and twist the molecule to look down at the lowest priority group axis, such that this group is behind the chiral center. Brun and Leblanc (1983) go on to state that in order to determine the configuration, one must correctly transfer mentally or with a model, every part of the molecule about the chiral center under consideration. However, many students fail this task because they struggle with spatial visualization (Brun & Leblanc, 1983).

## Spatial Ability and Organic Chemistry Achievement

The capacity to perceive visual images accurately, construct mental representations, and imagine visual information, as well as understand and manipulate the spatial relations among objects have been considered as spatial ability (Khine, 2017).

Spatial ability involves a combination of visual memory, visual imagination, and mental processing of this visuospatial information (Burrmann & Moore, 2013). Researchers have attempted to answer the question of how spatial ability affects students' ability in the learning of chemistry subject material. Indeed, several prior studies have provided correlational evidence that visuospatial abilities are an important component of students' learning in chemistry (Wu & Shah, 2004). For instance, it has been shown that high spatial ability leads to a deeper understanding of the mechanisms underlying most chemical processes (Jackson, Woods, Hyde, & Shaw, 1995).

When looking specifically at how spatial ability impacts performance in organic chemistry, some researchers have shown that spatial abilities are correlated with organic chemistry grades (Turner & Lindsay, 2003). For example, Bodner and McMillen (1986) found that total scores on spatial visualization and closure flexibility tests were significantly correlated with performance on both spatial and non-spatial chemistry problems. More recently, a slight but significant relationship between spatial abilities and organic achievement was discovered using the 2004 American Chemical Society (ACS) organic chemistry exam (Harle & Towns, 2010).

Spatial ability skills are also important for problem solving within organic chemistry. Carter et al. (1987) found that students with high spatial ability appeared to have higher scores on problems that required problem-solving skills rather than rote memory or the simple algorithms. For example, students with high spatial scores did significantly better on questions such as completing a reaction or outlining a multi-step synthesis, and questions which required students to mentally manipulate two-dimensional representations of a molecule (Pribyl & Bodner, 1987). Additionally, it has been shown that students who perform poorly on measures of spatial ability may struggle to extract important spatial information depicted in molecular representations and to execute spatial problem-solving strategies (Stieff et al., 2012).

However, it should be noted that studies have been inconsistent in their findings about the relationship between spatial abilities and its impact on performance in organic chemistry. That is, nonsignificant-to-moderate correlation coefficients have been reported, with results varying by curriculum topic, course, and institution (Turner & Lindsay, 2003). Stieff and colleagues (2012) argue that although some correlation studies have suggested a predictive role for visuospatial ability in organic chemistry, none have reported large correlations between achievement and visuospatial ability, and few studies have controlled for the possibility that the observed correlations may reflect common variance with general intelligence. Stieff and colleagues (2012) go on to state that significant correlations between visuospatial ability and chemistry achievement are actually often relatively low, and that no true experiments have been conducted to determine the predictive validity of visuospatial ability for chemistry achievement.

## Gender Differences in Organic Chemistry Due to Spatial Ability

Many chemistry instructors may make the assumption that students come into the classroom possessing the spatial abilities necessary to be successful in the course. However, not all students are equally equipped to perform tasks of spatial ability. One important difference in the spatial abilities of students is due to gender. For example, one component of spatial ability, the ability to mentally rotate an object, has been found to “produce one of the largest gender differences in cognitive literature” (Parsons et al., 2004, p. 555). Starting with the seminal work of Maccoby and Jacklin (1974), “gender-related differences on spatial test scores have been widely reported and acknowledged" (Saccuzzo, Craig, Johnson, & Larson, 1996, p. 599).

Generally speaking, males outperform females on tests of spatial ability. Although differences in spatial ability may be small, they occur with great regularity and should not be ignored (Saccuzzo et al., 1996). Research has shown that the magnitude of gender differences depends on the type of spatial task, with the largest differences found in tasks involving 3-D rotation (Halpern & Collaer, 2005; Harle & Towns, 2010; Sorby, 2009). There are numerous explanations about the origin of these differences, but there is little agreement among researchers as to the developmental or physiological origins (Harle & Towns, 2010).

Lawton (2010) summarized several explanations based on the literature that account for gender differences in spatial abilities. These include biological factors such as hormonal influences, differences in the way the brain is organized in females as compared with males, or evolution of this skill over time. There may also be experiential and societal factors, such as differences in the experiences of males and females that promote the development of spatial skills, socio-cultural differences which may promote spatial skills in one gender more than the other, or stereotype threat which means the disruption in performance due to awareness of negative stereotypes concerning the aptitude of members of one's group.

Although the literature has shown differences in spatial abilities due to gender, Stieff and colleagues (2012) report that despite repeated efforts by the chemistry education research community, evidence to substantiate the predictive role of gender differences in visuospatial ability on chemistry achievement remains outstanding.

Furthermore, studies exploring the relationship between visuospatial ability, sex, and chemistry achievement have produced conflicting results (Stieff et al., 2012). That is, while some early correlation studies have suggested that gender differences in spatial ability might account for differences in the performance of chemistry students, more targeted experimental approaches have been unable to find consistent relationships between gender, spatial ability, and achievement in chemistry. Stieff and colleagues (2012) argue that these inconsistencies may be due to differences in the dependent measures used among the studies (such as exam subscales versus course grade) or the wide variety of spatial ability measures employed.

## Training to Improve Spatial Ability

Although some researchers question training effects, many more researchers advocate the use of training to improve spatial ability (Bosco, Longoni, & Vecchi, 2004; Harle & Towns, 2010; Sorby, 2009; Uttal, Meadow, et al., 2013). Researchers remain divided on whether or not spatial ability is an innate ability rather than a trainable skill. That is, some researchers feel that spatial abilities are innate from birth and thus cannot be taught (Barnea & Dori, 1999). Despite this controversy, much of the literature shows that spatial ability develops over a person’s lifetime, and that interventions can improve spatial ability (Harle & Towns, 2010). After a review of the existing evidence for the effectiveness of spatial training in STEM fields, Stieff and Uttal (2015) came to the conclusion that spatial training offers one of the many promising avenues for increasing student success in STEM fields; however, most of the quasi-experimental studies that have attempted to show the effectiveness of spatial training have suffered from serious threats to internal validity, which compromises the interpretation of the findings (Stieff & Uttal, 2015).

There are several research studies which have found that spatial ability can be improved through training or practice on visuospatial tasks. Hegarty (2010) provides examples of studies which have shown that performance on tests of spatial ability and tasks such as mental rotation can be improved with practice, instruction and even by playing video games. Furthermore, the malleability of spatial skills was demonstrated in a meta-analysis including over 200 studies which showed that spatial training led to an average improvement of 0.47 standard deviations in spatial ability measures (Stieff & Uttal, 2015; Uttal, Meadow, et al., 2013; Uttal, Miller, & Newcombe, 2013). Additionally, in studies examining the durability of training effects, it was found in some cases that these effects lasted for months and transferred to tasks that differed at least moderately from training tasks (Uttal, Miller, et al., 2013).

Similarly, it was shown that students who received training on visualization skills had significantly higher scores on questions that required the use of 3-D models in a retention test (Wu & Shah, 2004). Additionally, the results of a study conducted by Sorby (2009) found that it is possible for the spatial skills of students to be improved. In this study, first-year engineering students with weak 3-D visualization skills were identified through administering the 30-item Purdue Spatial Visualization Test of Rotations. Students who received a score of 60% or less on this test were encouraged to enroll in a spatial skills course, which was aimed at improving students’ 3-D skills. Through this course, consistent and large gains were seen in participants of the course. Longitudinal studies also showed that students who initially exhibited poor spatial skills and who participated in the spatial skills development course earned higher grades in a number of introductory engineering, mathematics, and science courses as compared to students with weak spatial skills who did not participate in the spatial skills course. Furthermore, there was a higher retention rate in these STEM courses for students who participated in the spatial skills training, especially women, in comparison to similar students who did not participate in the training.

## Strategy Preferences for Spatial Problem Solving

Spatial ability tests are often presumed to elicit strategies that involve the generation and manipulation of mental images. However, research has shown that when completing tests of spatial ability, different individuals use different strategies in solving the same test items (Glück, Machat, Jirasko, & Rollett, 2001; Harle & Towns, 2010). For example, Just and Carpenter (1985) describe three different strategies that could be used to perform cube comparison tasks, including a mental rotating strategy, a perspective-change strategy, and an orientation-free (nonmanipulative) strategy. In another study, Kyllonen, Lohman, and Snow (1984) discovered that participants sometimes solved complex spatial problems using analytic strategies without imagining a sequence of transformations to the figure (Chen & Yang, 2014). Furthermore, in a more recent study conducted by Hegarty (2010) involving the Paper Folding Test (Ekstrom, French, Harman, & Dermen, 1976), intended to measure spatial visualization abilities, while most participants indicated that they had used mental imagery strategies such as visualizing the folding of the paper and noting where the holes would be, some participants instead used analytic or rule-based strategies such as counting the number of folds of paper that were punched through to determine how many holes there should be.

The most commonly reported strategy distinction reported in the literature for mental rotation uses a dichotomous classification system (Wang, 2017). These two broad classes of solution strategies for mental rotation tasks are referred to as holistic or analytic. Holistic strategies involve rotating the stimulus representation as a whole (Janssen & Geiser, 2010), and may be broken down further into two more subcategories. The first is to imagine objects move along their central axes (endorsing the allocentric frame of reference). The next type of holistic strategy is imagining a shift in perspective from which the object is viewed (endorsing the egocentric frame of reference) (Schultz, 1991; Wang, 2017)

However, Wang (2017) states that defining analytic strategies is not as straight forward. Some have argued that they are essentially non-spatial in nature (Geiser et al., 2006; Lohman & Kyllonen, 1983), involving the identification of key features of an object and notation of their presence, absence, or change (Schultz, 1991). That is, analytic strategies involve reasoning rather than mental manipulation of objects (Geiser et al., 2006). This is in keeping with other studies the field of chemistry which have applied this definition of analytic strategies (Stieff, 2007; Stieff & Raje, 2010), and for the purposes of this dissertation study, this definition of analytic strategies will be also be applied. However, it should be noted that other researchers have suggested that an analytic strategy is less efficient type of spatial strategy in that segments of, rather than the whole object, is rotated at a time (Wang, 2017). In this context, analytic strategies are sometimes labeled as ‘piecemeal’ strategies (Heil & Jansen-Osmann, 2008; Wang, 2017).

Since subjects may use different strategies on a test of spatial ability, this switching of approaches complicates the interpretation of scores on spatial ability tests, because the validity of the test hinges on the assumption that all subjects solve the tasks using the same strategy (Harle & Towns, 2010). As it is possible to solve some items on tests of spatial ability without using the ability it was designed to measure, this may impact the instrument validity (it does not measure what it is intended to measure), thus rendering the instrument invalid (Harle & Towns, 2010).

Furthermore, these different strategies for solving a particular visuospatial task can play a significant role in performance of the task. According to Dror, Schmitz-Williams, and Smith (2005), holistic strategies are more robust because they are relatively less dependent upon or affected by the images. However, with increasing task difficulty, holistic strategies may become less desirable and the frequency of analytic strategies increases. According to Gluck and Fitting (2003), most people can solve easy tasks by holistic strategies, whereas with more complex spatial information or more complex stimulus manipulations, strategies shift towards being more analytic.

A study by Contreras and colleagues (2010) found that while many participants maintain a particular type of strategy throughout a spatial ability assessment, individuals may switch to a more efficient strategy, depending on the problem type. According to Dror (2005), some types of visual stimuli lend themselves to more analytic processing, while others lend themselves to more holistic mental rotation strategies. More complex stimuli are often more difficult to mentally rotated in a holistic fashion. Furthermore, some stimuli possess visual characteristics that make them either more appropriate for analytic or for holistic visual mental rotation.  Gluck and Fitting (2003) proposed that individuals often use more than one strategy to solve a task, for example, to double-check a solution. In fact, Hegarty (2010) argues that one important component of spatial ability is flexibility in strategy choice between visualization and a more analytic thinking process. That is, individuals with a high spatial level can readily switch between a more holistic visualization strategy and an analytic strategy. Hegarty (2010) suggested that spatial visualization is an effortful process, and that the best spatial thinkers are those who are able to “augment visualization with more analytic strategies, and use these analytic strategies when they can, so that they visualize only the information that they need to represent and transform in order to solve a problem” (p. 281).

## Strategies on the Mental Rotations Test

Noting that prior research on spatial ability tests showed that different test items are often prone to different solution strategies, Geiser and colleagues (2006) were concerned that the same was true for the MRT:

> It is interesting that, in spite of its widespread use, there is relatively little information available concerning the item properties of the MRT. Currently, we know of no detailed MRT item analysis. Therefore, it is not entirely clear whether all items of the test measure mental rotation appropriately.

Consequently, the researchers set out to investigate the different strategies that could be used to solve items on the MRT, and in doing so attempted to separate the “rotators” (participants that used holistic strategies), from the “nonrotators” (participants that used analytic strategies to solve these items). To accomplish this, the researchers used a statistical method called Latent Class Analysis (LCA) with a large sample (N = 1,695) to classify participants into subgroups (latent classes) based on their strategies for solving items on the MRT. Within each subgroup, participants are assumed to have identical patterns of solution probabilities, that is, the solution probability of a given item is the same for all individuals belonging to the same subgroup.

The results showed that five subgroups (latent classes) could be distinguished, with three of these groups differing mainly in the number of items reached, and one group showing low performance overall. The final group was the analytic strategy group, whose members had high solution probabilities on items where the distractors were different in shape from the target figure. A summary of the groups is shown in Table 2-1.

Table 2-1

*Strategy Group Descriptions on the Mental Rotations Test (Geiser et al., 2006)*

| Group | Description |
|---|---|
| 1: Poor rotators | Low solution probabilities for all items |
| 2: Analytic | High solution probabilities for items where distractors were different in shape from target |
| 3: Moderate rotators | High solution probabilities for the first 8 items |
| 4: Slow rotators | High solution probabilities for the first 4 items |
| 5: Fast rotators | High solution probabilities for all items |

## Strategies for Solving Stereochemistry Problems

Stereochemistry is one of the most difficult concepts of chemistry for students (Burrmann & Moore, 2013; Luján-Upton, 2001). One reason for student difficulties with stereochemistry concepts is that they lack the spatial intelligence necessary for proper comprehension of stereochemical concepts (Burrmann & Moore, 2013). For students who may struggle with thinking in three dimensions, stereochemistry may be especially difficult due to necessity of visualizing three-dimensional molecules mentally and representing them on a two-dimensional surface (Varghese, 1996). Consequently, students with higher spatial abilities have been shown to have higher achievement in learning stereochemistry concepts (Abraham et al., 2010).

However, Stieff and colleagues (2014) concluded that achievement on organic chemistry spatial problems was dependent not only on spatial ability but also on the strategy choice made by students to solve spatial problems. Just as there are various strategies – holistic or analytic – for solving problems involving non-chemical objects (such as on the MRT), such strategies also exist for solving stereochemistry problems. For example, in a study conducted by Stieff (2007) where subjects were required to determine the relationship between two molecules, although it was hypothesized that the subjects would mentally rotate one molecule into the other to make an identity judgment, it was found that some subjects first searched for symmetry planes or chiral centers to make a judgment before attempting to use mental rotation. If a symmetry plane was present, some subjects were able to immediately determine an identity relationship without employing a mental rotation strategy. Furthermore, when determining the absolute configuration, if the lowest priority group is not pointed away from the problem solver (as the Cahn-Ingold-Prelog rules dictate), the problem solver has several options for proceeding. The problem solver may attempt to holistic mental rotation strategies the molecule to reposition so that it is oriented in the proper way, or the problem solver may mentally reposition themselves (imagine looking at the molecule from a different perspective). However, Brun and Leblanc (1983) describe a more analytic method to determine the configuration, which allows the problem solver to circumvent any type of mental repositioning (either the molecule or themselves). That is, the configuration is determined using the molecule as presented, however, the observed configuration is reversed.

Hegarty, Stieff, and Dixon (2013) investigated the use of holistic strategies and analytic strategies at various points during an organic chemistry course. It was found that with increasing expertise, there was a switch from holistic strategies to more frequent use of analytic strategies in the form of rule-based reasoning across a wide range of organic chemistry problems, including predicting reaction products, translating between different molecular representations, and determining the mechanisms underlying chemical reactions. That is, both experts and novices use analytic strategies to solve these types of problems; however, it appears that experts use these strategies more frequently and consistently than novices. Furthermore, students tended to use holistic rotation strategies immediately after the relevant material was covered during lecture; however, they appeared to switch to more analytic strategies near the end of the semester.

In another study, Stieff (2013) compared two strategies (holistic and analytic) for making stereochemical comparisons, and he found that briefly training students to use an analytic strategy can improve achievement more effectively than training in the holistic strategy. It was observed that regardless of gender, students who used the analytic strategy were more likely to answer the problems correctly. However, it should be noted that even though this instruction to use the analytic strategy improved performance on the task, it also significantly increased the amount of time required to solve each task. Thus, there may be trade-offs between success on a stereochemical task and the time required to complete it. This is consistent with findings by Hirnstein and colleagues (2009) in the field of psychology who assert that solving mental rotation tasks using analytic strategies takes more time and therefore often leads to poorer performance on tasks which include time restrictions.

## Visuospatial Tasks and Working Memory

Working memory may be defined as the aspect of cognition relating to the maintenance of task-relevant information during the performance of a cognitive task (Miyake & Shah, 1999). Baddeley and Hitch (1994) proposed that working memory within short term memory is comprised of several components, including a visuospatial sketchpad, a phonological loop, and a central executive component that controls the other two subsystems. Processes such as generating, manipulating, and interpreting visual or spatial images occur in the visuospatial sketchpad, whereas verbal processes such as the rehearsal of words occurs within the verbal phonological loop (Kozhevnikov, Motes, & Hegarty, 2007).

An individual’s working memory is limited in size to containing about five to seven bits of information (Miller, 1956) and is generally considered to be fixed (Baddeley & Hitch, 1994). Thus, completing spatial tasks of varying levels of difficulty imposes different amounts of ‘cognitive load’ on an individual’s mental processing systems. *Cognitive load* may be described as the amount of information that performing a particular task imposes on the cognitive system of an individual (Paas, Tuovinen, Tabbers, & Van Gerven, 2003). That is, solving visuospatial tasks at higher levels of difficulty make more demands on the working memory of an individual than solving problems at lower levels of difficulty. Thus, solving more complex stereochemistry tasks impose greater amounts of cognitive load.

The visuospatial sketchpad of working memory is responsible for the short-term storage of visual and spatial information (Dehn, 2011), such as when organic chemistry students solve stereochemistry problems. However, Dehn (2011) argues that the maintenance and manipulation of visual images is highly demanding of working memory resources, probably beyond the capacity of the visuospatial sketchpad itself. Consequently, working memory's central executive must also be involved whenever internally generated visual images are being consciously generated and manipulated (Pearson, Logie, & Gilhooly, 1999). Furthermore, the phonological loop may also lend some assistance during image processing by attaching labels to the shapes involved.

However, even with this extra assistance, there are some instances when the number of elements of information that need to be processed simultaneously could exceed the available capacity of working memory (Kalyuga, Renkl, & Paas, 2010). *Cognitive overload* refers to cases when the information in a problem exceeds the limited capacity of working memory during problem solving (Mayer & Moreno, 2003). Thus, if the amount of information in a visuospatial task exceeds an individual's working memory, then the individual will be unlikely to solve this task.

The strategy an individual uses to complete a visuospatial task may impact the demands placed on working memory. For example, the use of holistic strategies may place high demands on visuospatial working memory (Shah & Miyake, 1996). The completion of mental rotation tasks of objects requires that the individual be able to maintain an active representation of all the parts, and the interrelation of these parts, while simultaneously rotating the image in the mind. This feat of storing the constituent parts of an object in memory, while simultaneously processing the object, is directly related to the working memory of an individual (Kaufman, 2007).

A number of studies have shown that working memory and spatial ability are closely related across the lifespan (Wang, 2017), and spatial ability tests, to some degree, measure differences in visuospatial working memory capacity (Kozhevnikov et al., 2007). It has been suggested that an individual's performance on a test of spatial ability may "reflect simultaneous processing and storage demands required to maintain and transform spatial images within the limits of visuospatial working memory resources" (Kozhevnikov et al., 2007, p. 550). Therefore, differences in spatial working memory when solving stereochemistry problems may account for some of the individual differences in spatial abilities.

## Problem Solving, Knowledge Organization and Expertise

"Efforts to understand the cognitive processes involved in problem solving have been underway for at least 100 years. One approach has focused on differences between 'expert' and 'novice' problem solvers" (Bodner & Domin, 2000, p. 26). As expertise in a particular area develops, this can have a dramatic impact on the cognitive load associated with activities, such as problem solving, related to that area of expertise (Cranford, Tiettmeyer, Chuprinko, Jordan, & Grove, 2014). Expertise is characterized by an increase in the knowledge base, which can dramatically decrease the cognitive load of an activity (Cranford et al., 2014). Furthermore, research has shown that experts differ from novices in several key ways, including how they organize their knowledge and use this knowledge to solve problems and understand the world around them (Kozma & Russell, 1997).

Experts do not have better memory capacities or superior cognitive skills, but instead some studies have shown that the two most important differences between experts and novices concerned the way in which knowledge is organized in memory and the strategies that are used in problem solving (Mayer, 1992). The knowledge of experts consists of a large number of interconnected elements that are stored and recalled as extended, coherent ‘chunks’ of information organized around underlying principles in the domain (Kozma & Russell, 1997). These highly organized structures in which knowledge is stored are called schemas, where each piece of information is connected in multiple ways to additional pieces of information within the schema, and most likely to other schemas in long-term memory (Chi, Feltovich, & Glaser, 1981).

On the other hand, novices tend to store information in more isolated pieces, and their schemas show fewer interconnections. For example, when looking at molecule, a novice may see individual atoms, the individual bonds between these atoms and individual electron pairs (Cranford et al., 2014; Johnstone, 1983). When viewing a molecular representation in this way, the total cognitive load associated with the representation may be quite high (Cranford et al., 2014). Consequently, this leaves little free working memory capacity for other aspects of the problem-solving process, such as the actual manipulation and use of the representation (Cranford et al., 2014). As molecules must frequently be manipulated when solving stereochemistry problems, this may result in cognitive overload. On the other hand, an expert organic chemist may view a molecule and perceive atoms, bonds and electrons as belonging to larger ‘chunks’ such as functional groups (Cranford et al., 2014). As a result, the overall load associated with using the representation is substantially decreased, allowing for more of the working memory capacity to be devoted to other aspects of the problem-solving process (Cranford et al., 2014).

Indeed, one advantage of organizing information in this way is that although they may contain huge amounts of information, each schema may be processed as a single unit in working memory – regardless of the size, complexity and sophistication of the elements of which the schema is comprised (Kirschner, 2002). Furthermore, by organizing multiple elements of information as chunks of single elements in cognitive schemas, after they have been worked with sufficiently, these schemas start to operate under automatic rather than controlled processing (Kalyuga, Ayres, Chandler, & Sweller, 2003). The automatic processing of schemas can bypass working memory during mental processing, thereby circumventing the limitations of working (Paas et al., 2003). This then allows problem solving to proceed with minimal effort.

Kozma and Russell (1997) assert that another key difference between experts and novices is that experts can use these schemas to perceive and recognize underlying patterns and principles during problem solving. Consequently, experts ‘see’ a problem in a different way than novices do. Furthermore, Kozma and Russell (1997) state that experts are able to use these principles to build a mental representation, or mental model, which they can use to test and select potential problem solutions.

Yet another hallmark of expertise in problem-solving domains is the development of flexible knowledge, where learners know multiple strategies and apply them adaptively to a range of situations (Star & Rittle-Johnson, 2008). A flexible problem solver is one who has knowledge of multiple solution procedures. and has the capacity to invent or create new procedures for solving unfamiliar problems or when seeking an optimal solution for familiar problems (Star & Seifert, 2006). That is, a flexible problem solver has more expertise in the domain and thus has a greater range of problem-solving strategies from which to choose (Star & Seifert, 2006). On the other hand, an inflexible solver must rely on a small set of procedures, because this is all that he or she knows how to do (Star & Seifert, 2006). Consequently, more knowledgeable learners (such as experts) are able to select more sophisticated strategies and execute these strategies more effectively than learners with lower levels of prior knowledge (novices) (Lazonder, Wilhelm, & Hagemans, 2008). Furthermore, flexibility involves knowledge of strategy efficiency. Flexible problem solvers know which strategies are more efficient than others under particular circumstances. Knowledge of strategy efficiency is a fundamental characteristic of problem-solving expertise and is also a prevalent mechanism underlying learning (Star & Rittle-Johnson, 2008).

## Eye-Tracking Methodology

Just and Carpenter (1976) stated that the rapid mental operations of the brain can be revealed by an analysis of the eye fixations during a task involving visual input. Therefore, eye tracking can be used to help understand the cognitive processes that occur during problem-solving tasks. Eye tracking makes use of two underlying assumptions. The first is the immediacy assumption, which posits that the viewer begins immediately interpreting the information that is viewed before the eye moves to the next point of fixation (Just & Carpenter, 1980). The other assumption is the eye-mind hypothesis, which states that what a person is looking at is typically associated with what they are currently thinking about or attending to (Just & Carpenter, 1980). That is, when individuals are free to move their eyes anywhere in a visual scene or display, the location of their current gaze is a good indication of where they are focusing their attention (Rayner, 1998; Stieff, Hegarty, & Deslongchamps, 2011). Consequently, eye movements can be used to provide insights about what information is being processed cognitively by the individual.

As eye tracking is concerned with eye movements, it is important to understand how the eyes move. The eyes do not move across objects or visual stimuli in one smooth and panning way. Instead, they move in a series of very short rest periods and spurts between these rests (Nielsen & Pernice, 2010). The rests are known as *fixations*, which can be defined as when the eyes focus on a certain point for a period of time usually lasting between 250 and 300 milliseconds (Williamson, Hegarty, Deslongchamps, Williamson III, & Shultz, 2013). It is during fixations that the brain interprets visual information that has been received by the eyes. The spurts are known as *saccades*, which can be defined as the rapid eye movements between fixations. During saccades, no new visual information is taken in by the eyes (Nielsen & Pernice, 2010). When using eye-tracking software to analyze the data, fixations are typically represented by dots with larger dots indicating a longer fixation time. Saccades are indicated by lines between these dots (Nielsen & Pernice, 2010). Another option for visualizing fixations of participants are heatmaps. Heatmaps aggregate fixation data and overlay the information on top of the stimulus image, using different color to show ‘hot spots’ (regions where many fixations were made) and ‘cool spots’ (regions where relatively few fixations were made) (Havanki & VandenPlas, 2014).

After collecting eye movement data, researchers are often interested in asking questions about the specific regions of a visual stimulus rather than its entirety (Tang & Pienta, 2012). Eye-tracking software allows the researcher to select or define these regions. Such defined regions are called *Areas of Interest*, commonly abbreviated as AOIs. AOIs allow the researcher to determine if participants look where it is expected that they would (i.e., relevant information) and to assess the properties of their eye movements in these areas. Defining AOIs allows different eye-tracking metrics (or measures) to be computed. In eye-tracking research, fixation duration is likely the most-frequently reported eye-tracking metric, and other common measures include fixation count and visit count (Tang et al., 2016).

## Eye-Tracking and Chemistry Problem Solving

Eye tracking provides an online measure of where participants look as they process material, which may provide clues as to the visual features and content that were important during the problem-solving process (Hinze et al., 2013). Consequently, eye-tracking methodology can provide meaningful information about cognitive activity that occurs during problem solving (Tang et al., 2014).

According to Grant and Spivey (2003), an individual’s overt visual attention during problem solving, as measured by eye movements, has been used in numerous studies to reveal critical aspects of the problem-solving process. For example, eye-tracking studies have shown that successful problem solvers spend a greater proportion of their time focusing on the relevant features within a problem, while problem solvers that are less successful spend more time on irrelevant information (Tsai, Hou, Lai, Liu, & Yang, 2012). Furthermore, previous studies have shown that eye movement patterns differ for experts as compared with novices when they read and/or attempt to solve problems (Topczewski et al., 2016).

Eye tracking has also been used in several studies within the field of chemistry to investigate the cognitive processes that occur while solving problems (Havanki & VandenPlas, 2014). For instance, a study conducted by Tang and Pienta (2012) used eye tracking to investigate the cognitive processes that occurred while chemistry students solved problems related to gas laws, and found that students who performed better at solving the gas law problems showed different eye movement patterns from lower performing students. In another study, Tang et al. (2014) used eye tracking to investigate students' cognitive processes while solving stoichiometry problems. This study also found that eye fixation durations were different between novice students at different levels of success when they solved chemistry word problems. Cullipher and Sevian (2015) attempted to use eye tracking to examine how students look at an infrared (IR) spectra of various substances and relate the molecular structures of these substances to their respective IR spectra. The researchers concluded that analyzing the sequences of fixations of students can provide useful information about what students are thinking when relating molecular structures to spectroscopic responses. In a more recent study, Topczewski et al. (2016) used eye tracking to investigate aspects of proton NMR spectra that organic chemistry experts and novice students considered while matching organic structure with a provided spectrum. Significant differences were found for eye movement patterns between the expert and novice groups, as well as between novices who performed well on the task and those who did not.

Eye tracking has also been used within the field of chemistry education to investigate how students use various types of molecular representations to solve problems In one such study, Williamson et al. (2013) used eye tracking to explore how organic chemistry students used ball-and-stick versus electrostatic potential maps to answer questions about organic molecules. The researchers concluded that eye tracking is an effective technology to understand how organic chemistry students use multiple representations when answering questions about molecules. Furthermore, Stieff and colleagues (2011) used eye tracking to examine how students allocate their attention to different locations of a multi-representational display. One of their major findings was that students can use diverse representation types to answer questions.

## Eye-Tracking and Spatial Problem Solving

As stereochemistry problems encountered in organic chemistry courses require students to use their spatial abilities, the researcher conducted a careful review of the literature on prior eye-tracking studies that have been used to analyze how participants solve visuospatial tasks. For example, eye-tracking studies conducted by Just and Carpenter (1976) required participants to solve problems related to Shepard-Metzler rotated figures (Shepard & Metzler, 1971). The main difference between these Shepard-Metzler tasks and the Vandenberg and Kuse MRT is the number of alternatives. Through the results of this study, Just and Carpenter (1976) concluded that there were three distinct stages in the processing of these problems. These stages included search, transformation and comparison, and confirmation. In the *search step*, the participant searches for a segment corresponding to the target that can be potentially transformed into each other. During the *transformation and comparison step*, the two corresponding segments are rotated into each other. This is done until the internal representations of the two segments are sufficiently congruent in orientation. The final *confirmation step* involves checking whether the rotation that brought the two segments into congruence will also bring other portions of the two figures into congruence.

Shiina, Saito, and Suzuki (1997) also used eye tracking to analyze the performance of experts and novices in Shepard-Metzler mental rotation tasks. Eye-tracking data along with verbal protocols allowed them to classify the problem-solving process into three different strategies, including mental rotation, detecting structural features and matching encoded descriptions. Shiina and colleagues (1997) assert that the results obtained from this study provided some indication about how visual information is internally manipulated.

In yet another study, Martini and colleagues (2011) used eye tracking to investigate Shepard-Metzler mental rotation tasks. Martini and colleagues (2011) found that the number of fixations is higher between two mirrored objects (non-rotatable) than nonmirrored (rotatable) objects, when determining if they can be rotated into congruence. Martini and colleagues (2011) assert that one possible reason for this is that the phases of search, rotation, and confirmation when completing rotation tasks must be completed several times when corresponding parts cannot be brought into conformity, such as in the case for two mirrored objects. Since transitions (fixation switches) can be seen as a 'refresh rate' within the visuospatial working memory, more transitions must be made in order to keep up the fading object representation within the working memory when attempting to bring two mirrored objects into congruence.

Additionally, Chen and Yang (2014) attempted to use eye tracking to better understand visual attention and strategies when participants solve items from the Purdue Visualization of Rotations Test (PVRT; Bodner & Guay, 1997) . One of the key findings of this study was that performance on the PVRT was correlated with eye movement patterns.

## Molecular Models and Stereochemistry Problems

In 1874, Jacobus Henricus van't Hoff laid the foundations for stereochemistry with a publication in which he openly suggested that molecules were real physical entities with a three-dimensional structure (Van der Spek, 2006). To help him visualize this new spatial concept, he not only used illustrations but also made small cardboard molecular models. More than once, van’t Hoff referred to the fact that his models had played an important role in the development of his stereochemistry theory (Van der Spek, 2006). Based on the historical significance of physical models to the development of stereochemistry, it is interesting to look at the role that such models can play in the study of stereochemistry in modern times.

O’Brien (2016) asserts that “molecular models, either real or virtual, are an extremely useful tool in aiding students’ understanding of stereochemical concepts” (p.1663). Furthermore, Abraham and colleagues (2010) state that textbooks often encourage students to use three-dimensional models along with 2-D drawings, and view the suggestion that students use physical models to help them learn stereochemistry as being a ‘sound tactic.’ Abraham and colleagues (2010) conducted a study that sought to investigate the relative effectiveness of various kinds of molecular representations on students’ understanding of stereochemistry concepts. While they found computer visualization software to be the most effective of the representation types looked at in their study, they argue that handheld models can also help students learn difficult stereochemistry concepts. This may be especially true in organic chemistry classrooms that have no access to computer visualization software.

Furthermore, in a study with 102 organic chemistry students, Kuo and colleagues (2004) discovered a relationship between the abstractness of a representation and performance on a test of stereochemistry. In this particular study, students were required to solve stereochemistry problems using representations of increasing abstraction:

physical models, computer-generated rotatable models, three-dimensional (dashed-wedge) paper structures, or two-dimensional (Fischer or Haworth) projections. Results from this study revealed that overall, scores on the test items were actually highest for the physical models and lower for the more abstract representations (Akaygun & Jones, 2013).

Stull and colleagues (2012) argue that there are several advantages of physical models. One of these advantages is that “a model can represent the three-dimensional structure externally, so that the conventions of a diagram (for depicting the 3-D structure of the molecule in the 2 dimensions of the page) do not have to be maintained in working memory” (p. 408). Furthermore, even simply viewing a model may be beneficial. However, if the problem requires manipulation of the molecule that is represented by the physical model (which is often common when solving stereochemistry problems), one can physically rotate the model and observe the results rather than mentally rotating, or changing one’s perspective of an internal representation to observe the results. Stull and colleagues (2012) refer to this as a complementary action (Kirsh, 1995), which may be described as an action performed in the world as a substitute for a mental process.

## Gestures While Solving Visuospatial Problems

“Gestures are pervasive in human meaning-making and an increasing amount of attention has been paid to examining their role in education over the last two decades” (Chue et al., 2015, p. 2). Furthermore, according to Hegarty, Mayer, Kriz, and Keehner (2005), there is mounting evidence that gestures reflect people’s internal representations while they reason and solve problems. Gestures can be defined as complex motor movements that occur in three-dimensional space, providing learners with the ability to represent dynamic, spatial-relational information with the hands (Stieff, Lira, & Scopelitis, 2016).

Gestures are produced in space and could emerge from visuospatial thinking (Goldin-Meadow, 2014). Chemistry students often use gestures and their bodies when sharing and exploring ideas with others, providing productive resources for imagining the submicroscopic, three-dimensional, and dynamic phenomena of chemistry (Flood et al., 2014). For example, students frequently produce gestures while solving spatially complex problems (Stieff et al., 2016), such as those typically encountered in the area of stereochemistry.

Gestures appear to play an important role in the processing of visuospatial information (Pouw, De Nooijer, Van Gog, Zwaan, & Paas, 2014). For example, in a study by Hegarty and colleagues (2005), participants were asked to think aloud while solving mental animation problems. It was found that participants gestured on more than 90% of problems, allowing them to express information about the component motions. In another study by Alibali and colleagues (2011), it was found that whether participants were allowed to gesture or not actually impacted strategy choice for solving a problem requiring the prediction of gear movement. That is, participants who were allowed to gesture used a visualization strategy, while those who were not allowed to gesture used an analytic strategy. Furthermore, it has been shown that gestures help individuals perform visuospatial tasks such as mental rotation (Jamalian, Giardino, & Tversky, 2013).

Hegarty et al. (2005) assert that there are at least two ways in which gestures might be functional in solving spatial problems. The first of these reasons is that the hand can be used to represent an object that must be mentally transformed, such that moving the hand reveals something about the motion or its result. As an example of this, Hegarty and colleagues (2005) described a study by Emmorey and Casey (2002) where participants solved a puzzle that involved imagining moving an L-shaped block. In the study, participants made an L-shape with their hands and moved their hands to consider possible positions of the block. A further example provided by Hegarty and colleagues, was a study by Schwartz and Black (1996) which investigated how subjects solved a problem where they were required to imagine how interlocking gears would move. It was found that some participants used their hands to represent the gears, interlocked their fingers, and observed that when one hand moved clockwise the other had to move counterclockwise. Hegarty and colleagues (2005) go on to state that in these situations, subjects were able to use their hands to represent objects that could not be physically moved while solving the problem.

Yet another way that Hegarty and colleagues (2005) argue that gestures may be beneficial while solving spatial problems, is that they can allow information to be offloaded onto the motor system and consequently help to free up working memory resources for other aspects of the problem-solving process. When solving visuospatial tasks that require the internal maintenance of information, this may compete with processing demands of completing the task. However, an individual may use gestures to maintain some of this information, thus freeing up space in working memory. For example, Hegarty and colleagues (2005) describes an individual making clockwise motions when solving a problem related to a gear system, to keep track within working memory of the way that the certain gears move during the problem-solving process.

## Concluding Paragraphs

While there appears to be several eye-tracking studies related to how students solve problems from spatial ability instruments, to the researcher’s knowledge there appears to be no studies at present conducted in the domain of organic chemistry that used eye tracking to solve stereochemical problems. These problems appear to be major stumbling blocks for many organic chemistry students. Therefore, this dissertation study is important because it can be used to gain a better understanding of the cognitive processes involved when students are solving stereochemical problems. This study used both eye-tracking and molecular modeling to assess student cognitive processes while they solved organic stereochemical problems.

In this chapter, some of the literature related to stereochemistry, spatial abilities, representation types, and eye-tracking methods were presented. It provided the theoretical and research background on how eye-tracking methods can be used to assess the cognitive strategies which organic chemistry students used when solving stereochemical problems. In the next chapter, the methodology used to conduct this dissertation study will be described.

# CHAPTER 3

# METHODOLOGY

## Overview

This study used mixed methods (quantitative and qualitative) to analyze and characterize the strategies that students use when solving organic stereochemistry problems. It consisted of two stages: the first stage utilized a spatial instrument designed to gauge student's initial spatial ability, specifically their ability to mentally rotate an object. In the second stage of the study, quantitative data were collected using eye-tracking methodologies while participants solved stereochemistry problems involving two-dimensional representations (i.e., molecular representations). Furthermore, phenomenography (Marton, 1986) was used as the qualitative strategy of inquiry to investigate the experiences of organic chemistry students when solving stereochemistry problems, involving both two-dimensional representations and three-dimensional models (i.e., ball-and-stick models). While this chapter outlines the methodology to be used in collecting the data, Chapter 4 presents the data collected from this dissertation study. Chapter 5 presents the discussion of the results in relation to the research questions and previous published findings.

## Participants

Participants for this study were selected from two sections of first semester organic chemistry courses at a university classified as a medium-sized R2 doctoral research university, located in the mid-western United States. During the Fall 2016 semester, these two sections were taught by the same instructor. The instructor received her PhD in organic chemistry, and had two years of experience teaching chemistry courses. However, this was her first semester to teach organic chemistry.

Demographic data collected from these students revealed that most were majoring in Biology, Sports and Exercise Science, and Chemistry (in that order). The pre-requisite for this course is the successful completion of two semesters of general chemistry for science majors, where the typical mean on the 70-question American Chemical Society (ACS) final examination is 34 (42 percentile) for the first-semester course and 32 (39 percentile) for the second-semester course.

In the first stage of the study, the MRT (Mental Rotations Test) was administered to 137 (48 male, 89 female) students enrolled in the first semester organic chemistry course. In the second phase of the study, 28 participants were interviewed during individual interview sessions. Of these participants, there were 15 (5 male, 10 female) novice organic chemistry students, and 13 ‘experts’ who were chemistry faculty members in the Department of Chemistry and Biochemistry and chemistry graduate students (pursuing masters or doctorate degrees) at the same institution.  For the latter group, the higher scores of ten of these thirteen participants (>80% accuracy) allowed them to be classified as experts on the topic of stereochemistry.

Table 3-1

*Demographic Information for Novice Participants*

| Participant Pseudonym | Age in Years | Gender | College Status | Description |
|---|---|---|---|---|
| Brian | 19 | Male | Sophomore | Chemistry major with emphasis in pre-health<br>Interested in pursuing a career in pharmacology |
| Ruthie | 20 | Female | Sophomore | Biology pre-med major<br>Interested in becoming an orthopedic surgeon |
| Ernestine | 35 | Female | Junior | Chemistry major with emphasis in industry<br>Non-traditional student |
| Pamela | 19 | Female | Sophomore | Forensic chemistry major<br>Interested in pursuing career in forensics |
| Howard | 28 | Male | Senior | Biomedical pre-health major<br>Interested in pursuing a career in pharmacology |
| Vanessa | 19 | Female | Sophomore | Biology pre-health major<br>Interested in pursuing a career in dentistry |
| Davina | 19 | Female | Sophomore | Biology major<br>Interested in becoming a medical doctor |
| Eve | 20 | Female | Sophomore | Biology – wildlife emphasis major |
| Alicia | 19 | Female | Junior | Psychology pre-med major<br>Interested in becoming a general surgeon |
| David | 20 | Male | Sophomore | Chemistry and biology pre-med major |
| Kimberly | 20 | Female | Junior | Biology pre-health major |
| Cherie | 19 | Female | Sophomore | Chemistry pre-med major<br>Interested in becoming dermatologist |
| Crystal | 19 | Female | Sophomore | Biology pre-med major |
| Donald | 23 | Male | Sophomore | Geographical Information Sciences/Systems pre-med major |
| Michael | 27 | Male | Senior | Sports and exercise science major<br>Interested in becoming physician assistant<br>Airforce for 4 years |

## Spatial Ability Instrument

This study used the MRT that was originally developed by Vandenberg and Kuse (1978), and then redrawn by Peters et al. (1995) (see Appendix B) as an assessment of participants' spatial abilities. There are currently several versions of the instrument available, however in this study, Version A (MRT-A) was administered to all participants.

The MRT is comprised of 24 items, administered in two sets (subscales) of 12 items. When completing this instrument, participants are asked to compare two-dimensional drawings of three-dimensional "block" figures (see Appendix B for examples). These figures were adapted by Vandenberg and Kuse from similar figures used by Shepard and Metzler (Caissie, Vigneau, & Bors, 2009). Vandenberg and Kuse (1978) reported an internal consistency (Kuder-Richardson 20 = 0.88), a test-retest reliability (0.83), and correlations with other measures indicated strong association with tests of spatial visualization.

Each item contains five of these three dimensional representations – a target figure on the left and four figures on the right. In each item, there are two figures on the right which are rotated versions of the target figure, and two figures which cannot be made to match the target figure. The participant is tasked with determining which of the two figures on the right are rotated versions of the target figure.

During the first week of classes, the researcher explained the MRT instructions to the organic chemistry sections and administered the instrument to the participants. The recommended time limit (Peters et al., 1995) of three minutes per subtest were strictly adhered to when it was administered, as performance on the MRT has been shown to be dependent upon the amount of time that students have to perform these mental rotation tasks (Resnick, 1993; Voyer, Rodgers, & McCormick, 2004)

There are several methods for scoring the MRT, however, the strict scoring method for the MRT as recommended by the authors of the instrument was used. Specifically, a participant received credit for an item only if they had marked both correct answers on the test sheet. They did not receive credit for an item if only one of the correct answers was marked. Furthermore, items that were not reached by the participant due to time constraints, were also scored as incorrect. Based on this scoring method, the maximum possible score was 24 if they answered all items correctly. The rationale for using this scoring method was that it minimizes the probability of participants receiving credit for an item by simply guessing – only $p$ = .17 (Geiser et al., 2006).

## Data Collection

This study utilized convenience sampling methods (Graham & Ian, 2014). Before data collection commenced, the researcher obtained approval to conduct this research study from the university’s Institutional Review Board (IRB), which allowed research with human subjects (see Appendix A). Data was collected from both quantitative and qualitative sources.

### Quantitative Data

**Spatial ability instrument.** Prior to the start of the Fall semester, the researcher obtained IRB approval and permission from the organic chemistry instructor to conduct the first stage of the study. During the first week of classes the researcher administered the MRT to students who consented to participate in the study. Specifically, they had read and signed the document approved by the Institutional

Review Board (IRB), which describes the purpose and conduct of the study (see Appendix A). Any students who did not sign this document were excluded from the study, and identities of participants and non-participants were not shared with the course instructor. During data collection for this stage of the study, participants were briefed about the second part of the study and asked to indicate whether they would be willing to participate in this interview stage.

**Eye-tracking.** Immediately after the course examination in which stereochemistry content (similar to problems used in the study) first appeared, an email was sent to students who had expressed an initial interest in participating in the second part of the study. These students were reminded about the purpose and scope of the study in this email, and a time was agreed upon for an individual meeting. These sessions were conducted in a small, sound-proof room, that housed the eye-tracker system. These sessions lasted about 30 minutes and participants were compensated with a $15.00 gift card for their participation.

After demographic information was collected from a participant, they were asked to sit in front of a 17-inch computer monitor, which was connected to the Tobii T120 eye-tracker computer and its software. The Tobii T120 eye-tracking system used during the study provided a sample frame-rate of 120 Hz (meaning 120 gaze points were collected per second for each eye). Most modern eye trackers, such as the Tobii T120, rely on a method called corneal reflection to detect and track the location of the eye as it moves. Corneal reflection uses a light source to illuminate the eye, which then causes a reflection that is detected by a high-resolution camera. The image captured by the camera is then used to identify the reflection of the light source on the cornea. Advanced image processing algorithms are then used to establish the point of gaze related to the eye and the stimuli (Bergstrom & Schall, 2014).

During the eye-tracking session, the table mounted eye-tracker does not provide participants with any visible indicator about their eye movements on the screen, as this might be distracting to them. Furthermore, in comparison to the head-mounted eye tracker which restricts head movements, this table mounted eye tracker allows participants to move their head freely and to behave naturally as they would in front of any other computer screen.

Prior to starting the eye-tracking tasks, the researcher ensured that the participant was seated at a distance of approximately 60-70 cm from the monitor. The eye-tracking system was then calibrated with a five-point moving calibration for each participant. Specifically, each participant was asked to follow a red dot moving across the screen with their eyes and pausing at one of five fixed points. The calibration process took about 60 seconds, and once calibrated allowed for accuracy to be provided within an error of less than 0.5 cm between the measured and intended gaze points (Tobii Technology, 2016).

After calibration, the first screen displayed to participants contained general instructions. Participants were instructed to verbalize their responses so that the researcher could record their answers. After the researcher verified that the participant understood the general instructions, the participant was given unlimited time to solve a practice problem (Figure 3-1) for the first type of task – determining whether two organic molecules were identical or enantiomers. The purpose of this practice problem was to ensure that the participant fully understood the procedure and allowed the researcher to answer any of his/her questions about the task. After solving the practice problem, participants were informed that they would be given a maximum of 60 seconds to answer each problem, after which time the screen would automatically advance. If they provided an answer before the 60 seconds had expired, the researcher pressed a key on the keyboard to advance the screen. If they did not provide an answer before time expired, the screen was automatically advanced.

For the first set of problems, Items R1 through R6 (see Appendix C), participants were required to determine the relationship between two molecules – that is whether they were identical images (could be rotated and brought into congruence) or enantiomers (non-superimposable mirror images that could not be rotated and brought into congruence). There were six of these questions and their order was randomized to reduce any effect on performance of due item order (Schroeder, Murphy, & Holme, 2012; Williamson et al., 2013).

The next set of problems, Items C1 to C5 (see Appendix D) required students to identify any chiral centers within the displayed molecule and to determine the R/S configuration for any chiral centers that they identified. Each participant was again asked to solve a practice problem, shown in Figure 3-2 as a sample item. The order of these problems was again randomized to reduce any effect on performance due to item order.

**Molecular modeling.** In the next part of the interview session, students were again asked questions about chiral carbons within in organic molecules, which was a similar task to the last set of questions in the eye-tracking session. However, this time they were given a ball-and-stick model of the organic molecules. Their first task was to identify any chiral centers within 2-butanol (see Appendix E). If they correctly determined that the molecule contained a chiral center, then they were asked to assign the configuration of each chiral center using the R-S nomenclature system based on the CIP rules (Cahn et al., 1966). Next, they were given a more complex organic molecule (1,3,5-tribromocyclohex-1-ene) that contained multiple chiral centers (see Appendix E).

**2010 American chemical society organic chemistry examination**. At the end of the semester, the 2010 version of the ACS Organic Chemistry Examination was administered as the final exam. As this is a standardized examination, students' scores on this exam were used as the measure of achievement in the course. The national mean for this version of the ACS exam was 39.39 out of 70 questions, and the standard deviation was 11.74.

For this research question, items on the 2010 ACS examination were divided into two categories – questions that required a knowledge of stereochemistry concepts and questions that were not related to stereochemistry. The researcher investigated whether strategy classification on the MRT influenced total scores on these two categories of questions.

## Qualitative Data

Qualitative research methods were utilized in this study to acquire detailed descriptions directly from the participants. Qualitative research methods can be used in an effort to uncover the meanings that individuals assign to their experiences (Creswell, 2012). Specifically, phenomenography (Marton, 1986) was chosen as the qualitative approach to answer questions about the different ways that organic chemistry students experience the phenomena of solving stereochemistry problems. Phenomenography is an empirical, qualitative research methodology used to explore thinking and learning from the perspective of the learner (Lyle & Robinson, 2002). Through this research, it is possible to identify, interpret, systematize, and describe the diverse ways in which individuals experience phenomena (Ebenezer & Erickson, 1996). As there are only a limited number of “qualitatively different ways” in which different people experience a certain phenomenon, the aim of phenomenography is simply to identify the different possible conceptions that individuals have a for a given phenomenon (Orgill, 2007). Since it was expected that participants would not approach stereochemistry problem-solving tasks in the same way, but would do so in only a limited number of ways which could be described and interpreted, phenomenography was considered an appropriate qualitative strategy for this study (Bhattacharyya & Bodner, 2005).

**Interviews.** The primary source of data was semi-structured interviews that were audio-taped. For this study, specific questions were prepared but any unexpected lines of reasoning were also followed. These interview sessions involved solving 2-D problems on the eye tracker followed by 3-D problems (i.e., molecular models).

During the eye-tracking portion of the interview, retrospective think-aloud protocols (Boren & Ramey, 2000; Ericsson & Simon, 1980) in which participants work in silence and verbalize their thoughts afterwards, were used to collect information from participants about their approaches for solving stereochemistry problems in two dimensions. That is, after solving each stereochemistry problem on the eye tracker, the next screen that participants saw was a duplicate of the previous problem. It was at this point that participants were prompted to describe their approaches for solving the problem. This method is preferred over the alternative method – the concurrent think-aloud – in which the participant simultaneously verbalizes what they are thinking and doing while performing the task. Hyrskykari, Ovaska, Majaranta, Räihä, and Lehtinen

(2008) described a major disadvantage of this method because it poses as an unreasonable cognitive demand on the participant. That is, they may be unable to think aloud while performing a cognitively demanding task. Also, their task performance can be adversely affected because either their normal behavior is slowed down or their sequence of steps is changed when they are trying to execute the task while verbalizing it.

After completing the stereochemistry problems presented in two dimensions, participants were asked to describe their approaches to solving stereochemistry problems involving a molecular model. This helped to provide further information about key differences in the approaches of students when solving these stereochemistry problems with different types of representations.

**Field notes.** Key observations, in the form of field notes written during the interviews or immediately after the interview, served as an additional source of data. These field notes included observations such as gestures made by participants during problem solving and behaviors such as the repositioning of molecular models. In cases where factors such as gestures or physical manipulation of models seemed to play a role in helping the participant observations to answer the item, the researcher inquired about these observations.

## Data Analysis

### Quantitative Analysis

**Research question one.** After administering the MRT, scores were calculated for all 137 participants. Latent class analysis (LCA) was then used to classify participants into subgroups (classes) based on their solution strategies for solving items on the MRT. Geiser and colleagues (2006) suggested a five class (subgroup) model for solution strategies on the MRT. Following the procedures outlined by Geiser and colleagues, participants were assigned to one of five strategy subgroups. In this study, the computer program Mplus 7.31 (Muthén & Muthén, 2004) was used to assign participants to each subgroup. As the procedures for assigning participants to each subgroup were the same as those outlined by Geiser and colleagues, similar distributions of students were expected in each group. These expected distributions are presented in Table 3-2.

To determine whether the distribution of observed strategy groups (G1 to G5) on the MRT-A differed significantly ($p < 0.05$) from the expected distribution of these strategies as published by Geiser and colleagues (see Table 3-2), a chi square goodness-of-fit test was used. If there was no significant difference, then it would be concluded that the grouping of organic students was similar to the expected distribution as found in the cited research study. Furthermore, a chi square test of proportions was used to determine if there were significant gender differences, $p < 0.05$, in the observed distribution of strategies. If there was no significant difference, then it would be concluded that males and females are equally distributed across the strategy groups.

Table 3-2

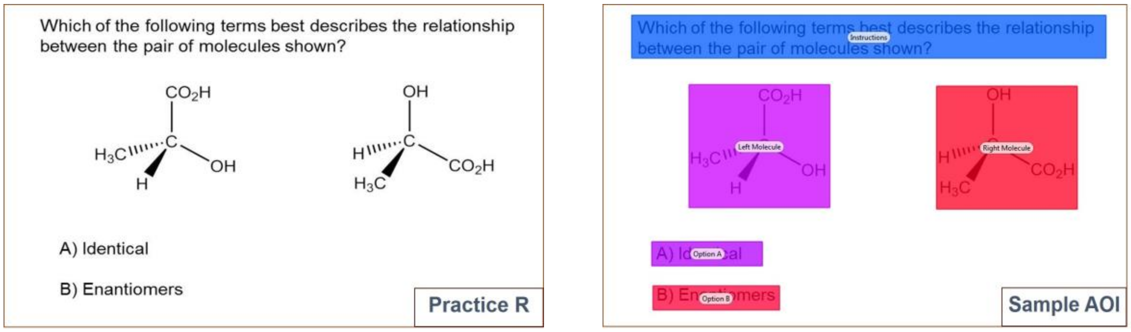
*Expected distributions of students on the Mental Rotations Test-A*

| | Expected Distributions | | | Expected number of participants in each group | | |
|---|---|---|---|---|---|---|
| Group | % Students | % Females | % Males | Students | Females | Males |
| G1: Weak rotators | 25 | 36 | 14 | 34 | 32 | 7 |
| G2: Analytic nonrotators | 15 | 17 | 14 | 20 | 15 | 7 |
| G3: Moderate rotators | 26 | 20 | 33 | 35 | 18 | 16 |
| G4: Slow rotators | 19 | 22 | 15 | 26 | 19 | 7 |
| G5: Fast rotators | 15 | 6 | 24 | 22 | 5 | 11 |
| Total | 100 | 100 | 100 | 137 | 89 | 48 |

**Research question two.** A common method of analyzing eye-tracking data is to identify areas of interest (AOIs), which may be defined as regions in the stimulus that the researcher is interested in gathering data about. Eye-tracking software allows the researcher to define areas of interest (AOIs), and can be used to help researchers answer questions such as whether participants looked in expected regions of the stimuli and allows eye movement patterns in these regions to be characterized.

To analyze eye movement patterns made by participants in this study while solving stereochemistry problems, AOIs were defined for each item. Sample AOIs for the practice problem of each problem type (relationship and configuration items) are provided in Figure 3-1 and Figure 3-2.

Defining these areas allows fixations to be mapped onto the AOIs and allows for the computation of eye-tracking metrics including the number of fixations (measures the number of times the participant makes a fixation on an AOI), fixation duration (measures the duration of each individual fixation within an AOI), and total fixation duration (measures the sum of the duration for all fixations within an AOI).


Which of the following terms best describes the relationship between the pair of molecules shown?

A) Identical

B) Enantiomers

Figure 3-1: Practice Problem and Sample Area of Interest (AOI) for Relationship Problem Type

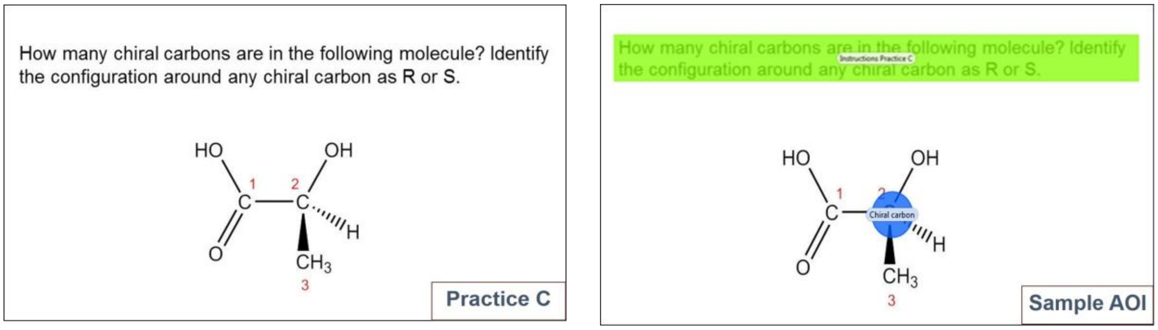
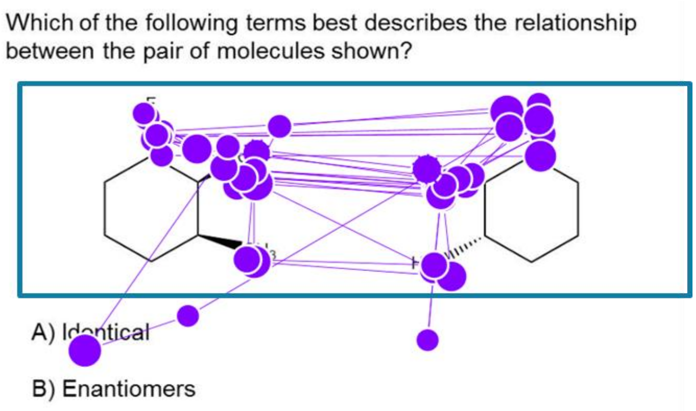

How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

Figure 3-2: Practice Problem and Sample Area of Interest (AOI) for Absolute Configuration Problem Type

Comparative statistics (such as t-tests and ANOVA) can then be performed on these metrics. In order to assess differences in eye-movement patterns between novices, success on each item was used as a basis for statistical comparison between eye-tracking metrics (eye-tracking metrics for successful novices were compared to eye-tracking metrics for unsuccessful novices) Additionally, differences in eye-movement patterns between experts and novices were assessed using statistical comparisons made on eye-tracking metrics for these groups.

For items where participants were asked to determine the relationship (identical or enantiomers) between the displayed molecules, each molecule was defined as an AOI. The number of transitions (fixation switches) *between* the two molecule AOIs were calculated (Figure 3-3). A transition was coded whenever a fixation in one AOI was preceded by a fixation in the other AOI. Movement to or from areas outside of the two molecule AOIs did not count as transitions.



Which of the following terms best describes the relationship between the pair of molecules shown?

A) Identical

B) Enantiomers

Figure 3-3: Transitions Between Molecules

For Items C1 to C5 where participants were required to identify any chiral centers and the absolute configuration around these chiral centers, key features of the molecule that the researcher deemed important for solving the items correctly were defined as AOIs (see Figure 3-2). Eye-tracking metrics were then computed for each of the AOIs using the Tobii Studio software.

**Research question four.** Items on the 2010 version of the ACS first-term organic chemistry examination were categorized as either related to stereochemistry or not related to stereochemistry. To ensure that items that had been categorized appropriately, the researcher enlisted the help of an organic chemistry instructor at the institution where the study was conducted. Initially, there was >80% agreement after the researcher and instructor independently categorized the items. However, after some discussion, there was 100% agreement about the items that belonged to each category.

In addition to total raw score on the ACS exam, both stereochemistry and non-stereochemistry sub-scores were calculated as performance measures for each participant. One-way MANOVA were used as the statistic to determine whether there were any significant differences, $p < 0.05$, among the strategy groups, G1 to G5, on the dependent variables (stereochemistry and non-stereochemistry sub-scores) as determined by the first semester ACS organic chemistry examination, Version 2010. However, it should be noted that the organic chemistry instructor made an error by giving the wrong exam to one of the organic chemistry sections, making their scores unsuitable for use in this study. That is, the instructor gave the full-term organic chemistry exam to one of the sections. Consequently, scores of participants from only one of the sections (roughly half of the total number of participants) were used for this research question.

## Qualitative Analysis

**Research question three.** The main results of phenomenographic research are the development of qualitatively distinct categories that describe the ways in which different individuals experience a phenomenon (Orgill, 2007). In this case, these categories were based on how organic chemistry students approach solving stereochemistry problems. To achieve this, the interviews were transcribed verbatim from the audio recordings to ensure all data were accounted for. The researcher then immersed himself in the sources of data (interview transcripts and field notes) by carefully and repeatedly examining the data for emergent themes. During this process, the researcher developed categories that described different approaches of novice organic chemistry students when they solved stereochemistry problems. Furthermore, to provide data for comparative purposes, expert chemists' approaches to solving stereochemistry problems were analyzed.

# Pilot Study Results

A pilot study was conducted during the 2015 Fall Semester, with the primary purpose of this study being to allow the researcher to become familiar with using the eye-tracker. Additionally, basic qualitative interviews were conducted to investigate novice organic chemistry students' abilities to use three-dimensional molecular models to determine the absolute configuration of the molecules found in Appendix E. The following paragraphs summarize the major findings from the pilot study:

First, the participants in this pilot study overwhelmingly stated that they had trouble using molecular models to assign R or S configuration. It was interesting that 7 of the 9 participants (78%) made comments that reflected their challenges with using models to assign R or S configuration. For example, Trevin verbalized the following:

> **Trevin:** I hate these things!
> **Investigator:** Do you mean the model?
> **Trevin:** Yea. I try to practice with them, but I have been taught on paper how to assign the configuration, but they don't teach you how to use the model to determine the configuration.

Indeed, several of these novice participants admitted that they had never used a molecular model to determine R or S configuration, but instead were only familiar with solving these types of problems in two dimensions such as with Fischer projections:

> **Marvin:** I'm not used to doing these problems in actual 3-D. Usually it's just Fischer diagrams.
> **Investigator:** So, you are not really familiar with using models?
> Marvin: Nope.

One would be tempted to think that a physical model would be helpful for determining the R or S configuration of any chiral centers, since it clearly shows all of the groups that must be assigned priority and it allows the problem solver to orient the molecule in the appropriate way for determining the configuration. However, for these participants, this did not appear to hold true. For example, Cherie stated that solving absolute configuration problems on paper was easier because she could more easily see the direction that groups are going. Stull and colleagues (2012) described a similar scenario in a study involving translation between molecular representation types – "participants may not use models if they have learned analytic translation strategies that do not rely on considering the 3-D structure of the molecule. Under these circumstances, using a model may be perceived to be more effortful than alternative strategies" (p. 409). Apparently, the same holds true for solving stereochemistry problems – participants may not use models if they have learned analytic strategies for solving these problem types.

The researcher also got the chance to interview the pilot study instructor (Professor Black), a professor of organic chemistry for about 23 years, about the emphasis placed on molecular models during the course. Professor Black admitted that while model kits were not required, they were recommended. He admitted that this is primarily due to keeping the cost of the course as low as possible. However, Professor Black seemed to have mixed views about the use of models. While Professor Black admitted that molecular models were helpful for students with poor visualization skills and reported bringing molecular models to class when teaching chapters on stereochemistry, he stated that most times students were “encouraged to use models on their own time.” Furthermore, although Professor Black acknowledged the potential benefits of using models, he also held the following view:

> **Professor Black (Pilot Study Instructor):** The models are a crutch. They should be able to visualize simple things, without the use of the model. Usually a week or two after using the model, I expect that they can solve the simple problems focused on in the course on paper.

Rather than placing a great deal of emphasis on the use of molecular models, it seemed that Professor Black placed more stock in showing students step-by-step procedures for solving problems in two-dimensions:

> The model kits, in my opinion, are there to allow them to learn to visualize in 3D. But I teach them how to do it on paper. The model kit only allows them to see why we draw the 2-D representation the way that we do.

Professor Black described showing students algorithms on what to do to answer any question, whether they could rotate it in their head or not, without the use of a model. While the instructor stated that students seemed to enjoy these step-by-step procedures, he admitted that they may not understand why they are carrying out the steps. This may help to explain why participants seemed to be ‘thrown for a loop’ when asked to determine the configuration of chiral centers using a molecular model. That is, students may follow the steps, but not truly understand how these steps relate to the three-dimensional arrangement of the molecule.

Students who follow the algorithms may be successful in solving certain problems, despite possessing the necessary visualization skills. However, Professor Black admitted something interesting:

> I have noticed that students who purchase models and work on homework problems with the models tend to do better on this kind of thing – the visualization stuff. In fact, they tend to better in the class overall, because they have good study habits…not so much that they are working exclusively with models.

Although this may be true, one may argue the opposite – students who purchase molecular models and work with them frequently may develop a better understanding of the three-dimensional arrangement of atoms. This in turn may help these students to develop more accurate mental models, leading to better performance. Williamson and Abraham (1995) argue that the lack of understanding of chemistry concepts may be linked to the students' inability to build complete mental models, and that visual aids might help in concept understanding.

## Concluding Paragraph

In Chapter 3, the researcher described the methodological approach to be used in this dissertation study for each of the four research questions, Q1 to Q4. Chapter 4 presents the data from the experiments conducted during the dissertation study. In Chapter 5, these results are discussed in relation to these research questions.

# CHAPTER 4

# RESULTS

The purpose of this study was to gain a better understanding of how organic chemistry students solve stereochemistry problems. This chapter presents the data collected during the study. These results include data collected using spatial ability measures (MRT), eye-tracking data collected while participants solved stereochemistry problems involving two-dimensional representations, as well as qualitative data collected while participants solved stereochemistry problems involving both two- and three-dimensional representations. Further, organic chemistry performance measures were used to investigate the relationship between spatial strategies and organic chemistry achievement.

## Q1: Spatial Ability Instrument and Strategy Classification

During the first week of the Fall semester, the MRT-A instrument was completed by 137 students enrolled in two sections of a first semester organic chemistry course. The researcher administered the instrument and followed the testing instructions and its prescribed protocols (Peters et al., 1995).

After the overall scores were calculated for each participant, an independent samples t-test was conducted to compare scores on the MRT for males and females.

Means and standard deviations for males and female MRT scores are presented in Table 4-1. There was a significant difference where males outperformed females, t (135) = 2.832, p = 0.005. The magnitude of the differences in the means (mean difference = 2.43, 95% CI: 0.73 to 4.12) resulted in a moderate effect size (d = 0.50). This information is also shown graphically in the form of a box plot shown in Figure 4-1.

Table 4-1

*Observed Gender Differences on Mental Rotations Test-A Score, t(135) = 2.832*

| Gender | N | *M* | *SD* | p value | D |
|---|---|---|---|---|---|
| Male | 48 | 11.6 | 5.20 | 0.005* | 0.50 |
| Female | 89 | 9.16 | 4.55 | | |

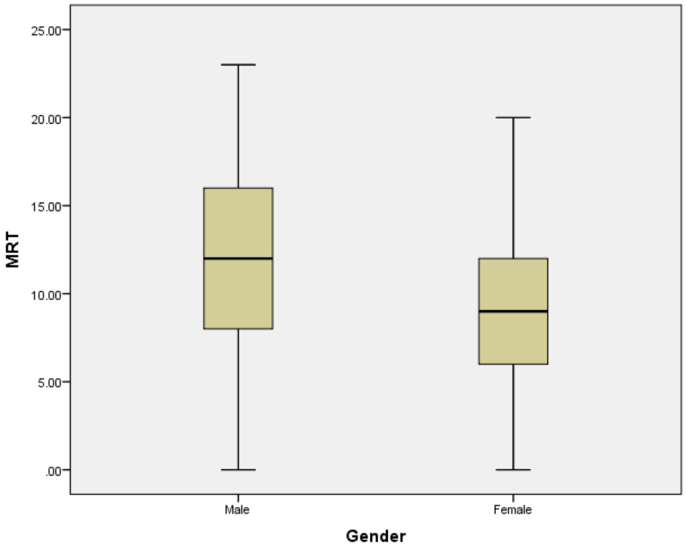


Figure 4-1: Box Plot Showing Gender Differences on Mental Rotations Test-A Instrument

Next, using each participant's response on the MRT-A items, they were classified into one of five groups (denoted as fast rotators, moderate rotators, slow rotators, weak rotators, or analytic strategy users), which was based on the five class model described by Geiser and colleagues (2006). Specifically, Latent Class Analysis (LCA) was used to calculate the optimal probability for each participant belonging to a particular group. For each of the five groups, the *observed distributions* of their response profiles are shown across the first twelve individual MRT-A items (Figure 4-2).

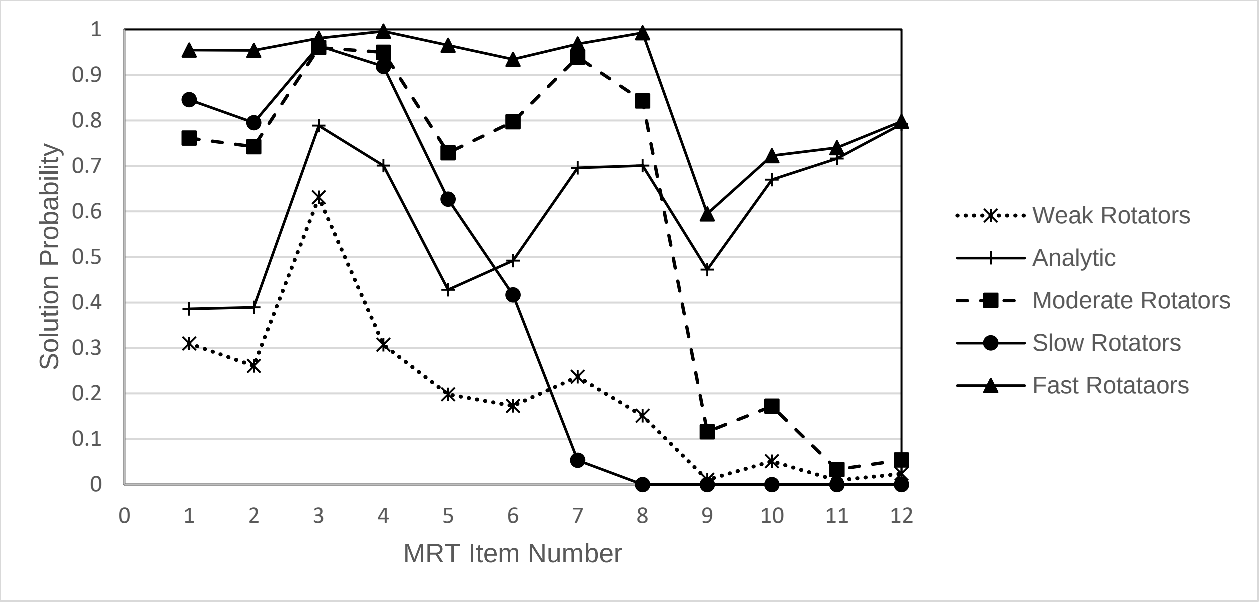


Figure 4-2: Observed Latent Class Profiles (N = 137)

After participants were assigned to their group, the observed distributions of participants were compared to the expected distributions (Table 4-2), which were based on the proportions (i.e., percentage of each group) found in the previous study (Geiser et al., 2006). These proportions were used to predict the expected distributions of the participants in this study (N =137). As can be seen in Table 4-2, a chi-square goodness-of-fit test, $\chi^2 = 17.46$, $p = 0.016$, indicated that there was a highly significant difference between the actual proportions of the participants' strategies as compared with the expected distribution of strategies (Geiser et al., 2006).

Table 4-2

*Comparison of Observed and Expected Distributions of Mental Rotations Test Solution Strategies (Geiser et al., 2006)*

| Group | Observed | Expected |
|---|---|---|
| 1: Poor rotators | 44 | 34 |
| 2: Analytic Strategy | 12 | 20 |
| 3: Moderate rotators | 57 | 35 |
| 4: Slow rotators | 16 | 26 |
| 5: Fast rotators | 8 | 22 |
| Total | 137 | 137 |

Note: $\chi^2$ = 17.46, df = 4, p = 0.0016 (significant differences)

A chi-square test of proportions was used to investigate whether there were different distributions of male and female participants across these five groups. The results indicated that there were no significant differences ($\chi^2$ = 1.78, p = 0.775) in the observed distribution of strategies across male and female novice organic chemistry students (Table 4-3) on the Mental Rotations Test (MRT-A).

Table 4-3

*Observed Gender Distributions for Mental Rotations Test-A Solution Strategies*

| | Number of Participants | | Percentage (%) | |
|---|---|---|---|---|
| Group | Males | Females | Males | Females |
| 1: Poor rotators | 13 | 31 | 27 | 35 |
| 2: Analytic strategy | 5 | 7 | 10 | 8 |
| 3: Moderate rotators | 21 | 36 | 44 | 40 |
| 4: Slow rotators | 5 | 11 | 10 | 12 |
| 5: Fast rotators | 4 | 4 | 8 | 4 |
| Total | 48 | 89 | 100 | 100 |

Note: $\chi^2$= 1.78, df = 4, p = 0.775 (no significant differences)

## Q2: Cognitive Processes While Solving Stereochemistry Problems

Of the 137 participants who completed the MRT-A, 15 volunteers were selected for individual interview sessions (both eye tracking and molecular modeling). The researcher did not know the classification of the participants while conducting the interviews, in order to avoid any influence on the interpretation of strategies. A summary of the number of volunteers interviewed from each of the five groups is shown in Table 4-4. In addition to these 15 novices, data was analyzed from 10 expert participants, who volunteered to be interviewed.

Table 4-4

*Summary of Classifications for Novice Volunteers Used in Eye-Tracking Study*

| Classification | N | Volunteer’s Pseudonyms |
|---|---|---|
| G1: Poor rotators | 7 | Ruthie, Ernestine, Howard, Vanessa, Davina, Kimberly, Crystal |
| G2: Analytic Strategy | 1 | Pamela |
| G3: Moderate rotators | 6 | Brian, Eve, Alicia, David, Donald, Michael |
| G4: Slow rotators | 0 | |
| G5: Fast rotators | 1 | Cherie |
| Total | 15 | |

### Q2A: Eye-Tracking How Problem Solvers Determine the Relationship Between Molecules

For the first set of problems, novices and experts were required to determine the relationship between two molecules (see Appendix C). For these six relationship items (labeled as R1 through R6), the number of transitions (fixation switches) between the two molecules was calculated for novices and experts on each item (Table 4-5). Independent samples t-test were conducted to compare the number of transitions for novices and successful experts on each item. A pattern of more frequent transitions for novices was found, which produced a significant difference for three of the six relationship items (R2, R3, R6). These differences are also presented graphically in Figure 4-3.

Table 4-5

*Differences in Number of Transitions Between Stimuli for Novices and Experts on Solving Each Question*

| Item | Group | N | *M* | *SD* | p value |
|---|---|---|---|---|---|
| R1 | Novice | 15 | 9.87 | 5.78 | 0.463 |
| | Expert | 10 | 7.10 | 5.74 | |
| R2 | Novice | 15 | 32.33 | 11.66 | <0.001* |
| | Expert | 10 | 14.70 | 8.30 | |
| R3 | Novice | 15 | 12.00 | 4.29 | 0.005* |
| | Expert | 10 | 7.10 | 3.03 | |
| R4 | Novice | 15 | 14.80 | 18.04 | 0.829 |
| | Expert | 10 | 13.50 | 6.06 | |
| R5 | Novice | 15 | 12.33 | 5.11 | 0.862 |
| | Expert | 10 | 11.80 | 10.04 | |
| R6 | Novice | 15 | 12.80 | 7.28 | 0.038* |
| | Expert | 10 | 7.50 | 2.55 | |

*Statistically significant at p = 0.05 level

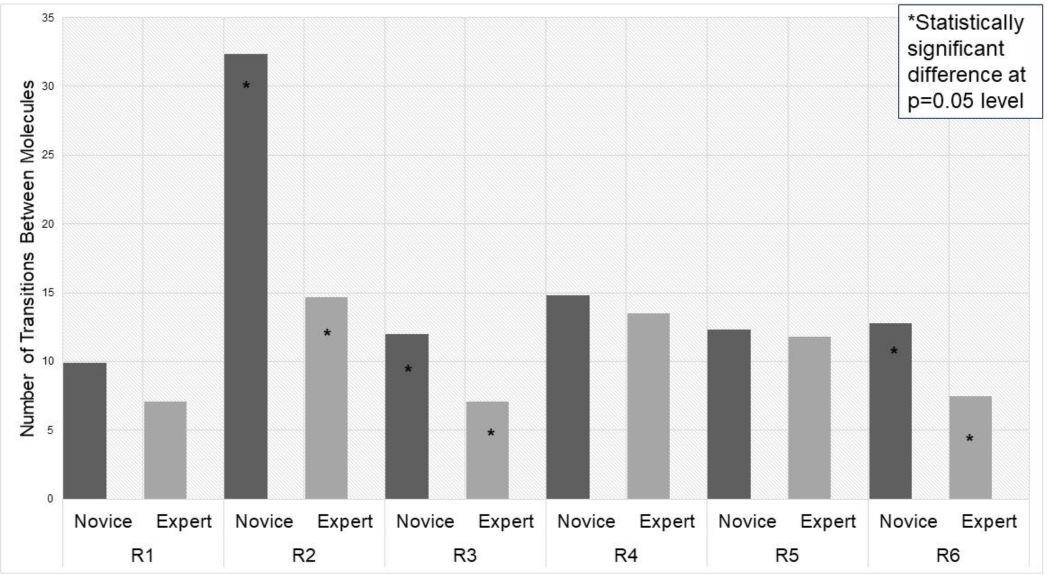


Figure 4-3: Differences in Transitions for Experts and Novices

Furthermore, differences between successful and unsuccessful novices were investigated on these relationship items (R1 to R6). Independent samples t-test were conducted to compare the number of transitions for successful novices and unsuccessful novices on each relationship item (R1 to R6). Table 4-6 shows the means and standard deviations for each item. A statistically significant difference was found for only one of the items, Item R2, between successful and unsuccessful novices (t = 2.192, p = 0.047). This information is also presented graphically in Figure 4-4.

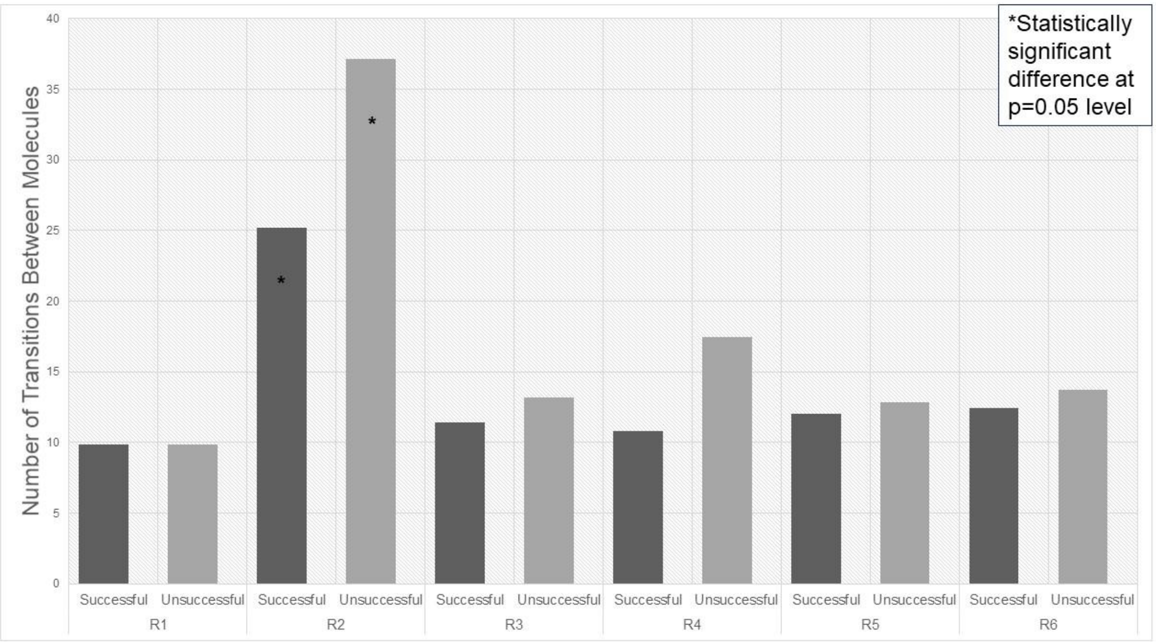
Table 4-6

*Differences in Number of Transitions Between Stimuli for Successful Novices and Unsuccessful Novices on Solving Each Item*

| Question | Outcome Group | N | *M* | *SD* | p value |
|---|---|---|---|---|---|
| R1 | Successful | 8 | 9.875 | 5.14 | 0.995 |
| | Unsuccessful | 7 | 9.857 | 6.87 | |
| R2 | Successful | 6 | 25.17 | 4.79 | 0.047* |
| | Unsuccessful | 9 | 37.11 | 12.62 | |
| R3 | Successful | 10 | 11.40 | 4.74 | 0.465 |
| | Unsuccessful | 5 | 13.20 | 3.34 | |
| R4 | Successful | 6 | 10.83 | 5.78 | 0.507 |
| | Unsuccessful | 9 | 17.44 | 23.00 | |
| R5 | Successful | 9 | 12.00 | 5.22 | 0.769 |
| | Unsuccessful | 6 | 12.83 | 5.38 | |
| R6 | Successful | 11 | 12.45 | 8.02 | 0.773 |
| | Unsuccessful | 4 | 13.75 | 5.62 | |

*Statistically significant at p = 0.05 level

Figure 4-4: Differences in Transitions for Successful Novices Versus Unsuccessful

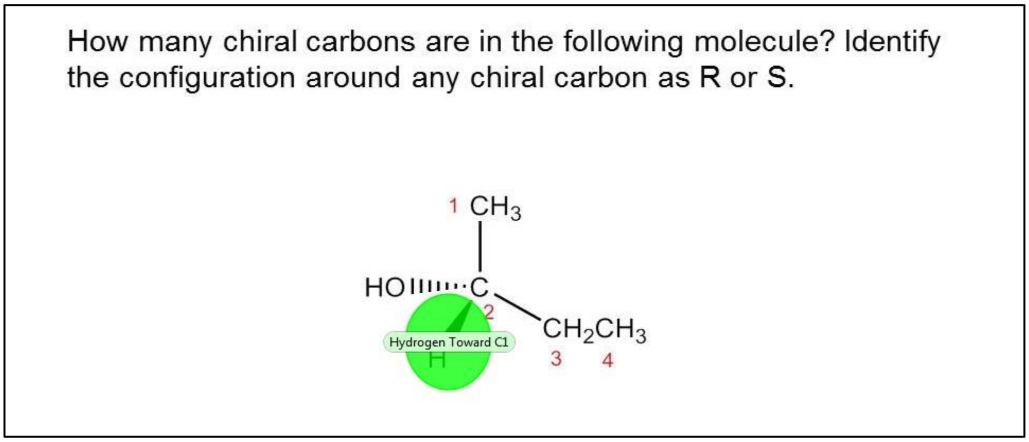


Novices on Solving Relational Problems (R1 to R6)

### Q2B: Eye-Tracking – How Do Problem Solvers Determine Absolute Configuration of Chiral Centers?

For the second set of problems (Items C1 to C5), novice and expert problem solvers were required to determine the configuration of any carbons that were identified as chiral (carbon with four different groups attached). Eye movements were again recorded for each participant and statistical procedures were used to investigate differences in eye movement patterns for successful novice and unsuccessful novice participants.

For Item C1 (Figure 4-5), the hydrogen attached to the carbon labeled as carbon 2 for *R*-2-butanol was defined as an AOI, since participants must have taken into account the position the hydrogen atom (lowest priority group), in order to solve the item correctly.

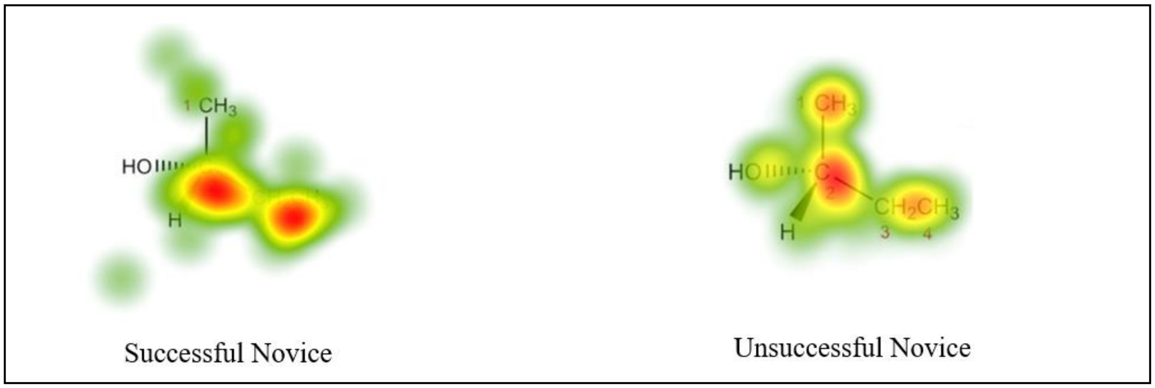


How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

Figure 4-5: Item C1 Area of Interest (*R*-2-butanol)

In Figure 4-6, sample heat maps for Item C1 are shown to compare a successful novice's eye movement patterns with those of an unsuccessful novice. For all novices, an independent samples t-test was used to investigate differences in total fixation duration between successful (N =10) and unsuccessful novices (N = 5) on solving Item

C1. Table 4-7 shows the means and standard deviations for total fixation duration on the hydrogen atom. A statistically significant difference (t = 2.776, p = 0.016) was found for total fixation duration on the C1 AOI between successful and unsuccessful novices.



Successful Novice

Unsuccessful Novice

Figure 4-6: Sample Heat Maps for Item C1 (*R*-2-butanol)

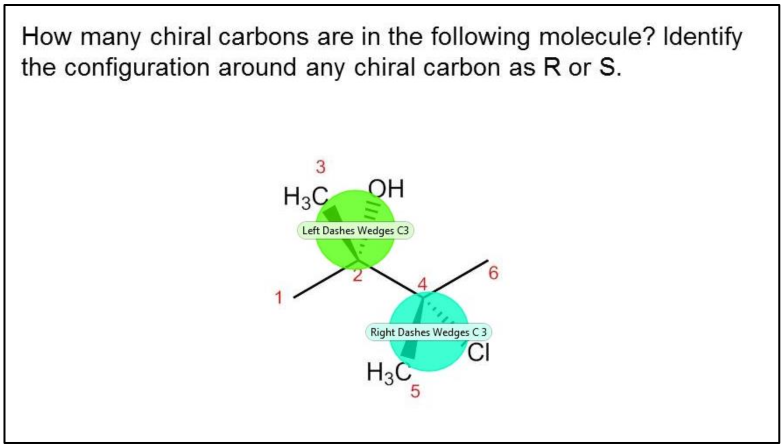
Table 4-7

*Eye-Tracking Metrics for Item C1 (t = 2.776, p = 0.016)*

| Eye-Tracking Metric | Outcome Group | N | *M* | *SD* | p value |
|---|---|---|---|---|---|
| Total Fixation Duration | Successful Novice | 10 | 8.13 | 4.31 | 0.016* |
| | Unsuccessful Novice | 5 | 2.28 | 2.55 | |

*Statistically significant at p = 0.05 level

For Item C3, the carbons that contained dashes and wedges were defined as the AOIs (Figure 4-7). Although the presence of dashes and wedges may draw participants to these carbons, these carbons are not chiral. Table 4-8 shows the mean fixation duration and number of fixations on the AOIs for successful (N = 7) and unsuccessful novices (N = 8). Independent samples t-tests were used to investigate the differences between successful and unsuccessful novices on Item C3 when using these eye-tracking metrics. Statistically significant differences were found for both eye-tracking metrics on this item, with unsuccessful novices fixating on these AOIs for a longer duration and number of times.



How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

Figure 4-7: Item C3 Area of Interest

Table 4-8

*Eye-Tracking Metrics for Item C3 (where t = 2.411 and p = 0.039; and t = 3.691 and p = 0.004)*

| Eye-Tracking Metric | Outcome Group | N | M | SD | p value |
|---|---|---|---|---|---|
| Total Fixation Duration (seconds) | Successful Novice | 7 | 6.11 | 2.76 | 0.039* |
| | Unsuccessful Novice | 8 | 12.78 | 7.25 | |
| Number of Fixations | Successful Novice | 7 | 27.00 | 9.88 | 0.004* |
| | Unsuccessful Novice | 8 | 59.13 | 22.24 | |

*Statistically significant at p = 0.05 level

Next, for Item C5, the carbon labeled as carbon 3 was defined as the AOI (Figure 4-8). Carbon 3 is the only chiral center in the molecule. Although only three groups are explicitly shown attached to this carbon atom, there is actually a fourth group –a hydrogen atom – that is bonded to the carbon atom. To correctly identify carbon 3 as a chiral carbon, problem solvers must consider the implicit hydrogen atom even though it is not shown. Table 4-9 shows the mean fixation duration on the AOI for successful and unsuccessful novices. An independent samples t-tests was used to investigate differences between successful (N = 9) and unsuccessful novices on these eye-tracking metrics. A statistically significant difference was found for total fixation duration (t = 2.317, p = 0.039).

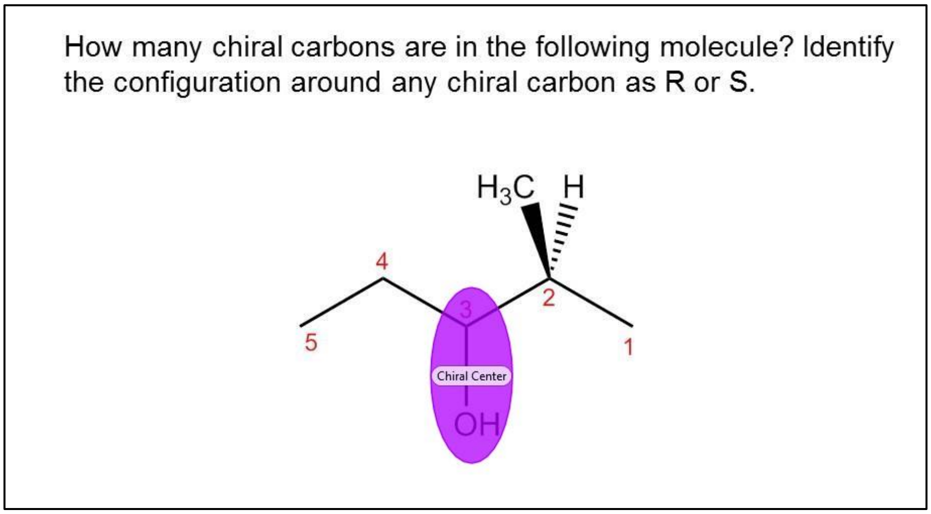
Table 4-9

*Eye-Tracking Metrics for Item C5 (t = 2.317, p = 0.039)*

| Eye-Tracking Metric | Outcome Group | N** | M | SD | p value |
|---|---|---|---|---|---|
| Total Fixation Duration (seconds) | Successful Novice | 9 | 5.35 | 3.41 | 0.039* |
| | Unsuccessful Novice | 5 | 1.33 | 2.41 | |

[*] Statistically significant at p = 0.05 level

[**] Eye-tracker malfunctioned for one participant and their data were omitted.



How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

Figure 4-8: Item C5 Area of Interest (2-methylpentan-3-ol)

## Q3: Strategy Differences When Solving Stereochemistry Problems

In this study, a phenomenographic approach was used to discover the different ways in which novice organic chemistry students approach the phenomena of solving stereochemistry problems. This qualitative process was based on the researcher's immersion in the data and repeated sorting, coding, and comparisons to generate emergent themes. Patterns that emerged during the analysis are summarized below. Direct quotes from the problem-solving interviews are given to support the claims of the researcher. All participants are identified by pseudonyms. Comments made by the interviewer are indicated by his initials "TK."

### Theme #1: Novice Stereochemistry Problem Solvers Prefer Holistic Mental Rotation Strategies

Retrospective think-aloud protocols were used to gather information about the problem-solving strategies of novices (N = 15). The researcher categorized these strategies as either holistic mental rotation or analytic. Holistic strategies were defined as those where participants attempted to mentally rotate the molecules (i.e., around central axes). Strategies were categorized as analytic in instances where participants attempted to apply a heuristic that did not involve rotation of the molecule. Figure 4-9 shows the frequency of each category of strategies used by novices when attempting to determine the relationship between two molecules (Items R1 through R6).

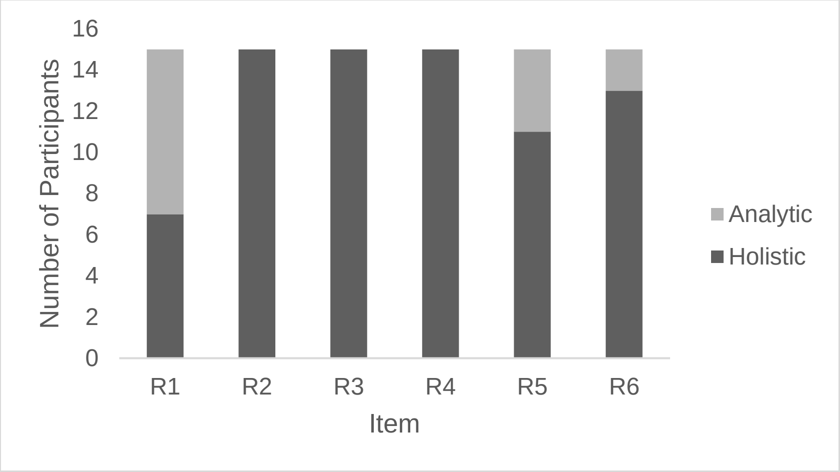
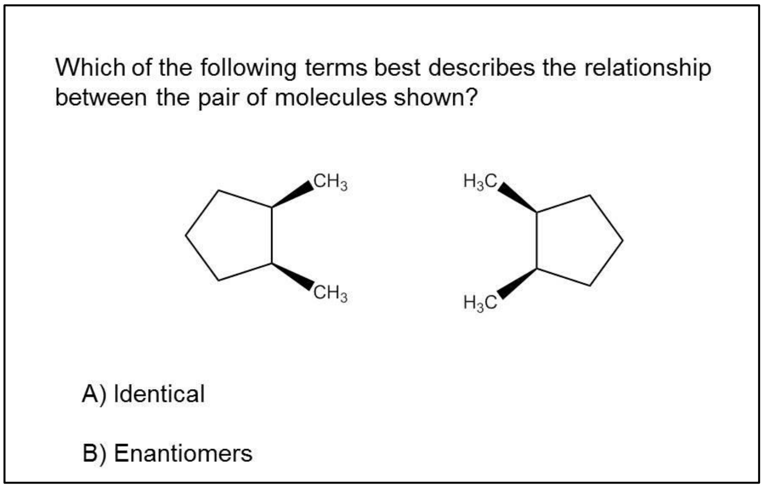


Figure 4-9: Frequency of Strategy Use by Novices (N = 15) When They Determined the Relationship of Molecules

As shown in Figure 4-9, Item R1, had the most diverse mixture of these two strategies (Figure 4-9). The researcher focused on this item (Figure 4-10) and then broke these strategies for each MRT strategy group. The results of this categorization are shown in Table 4-10. Furthermore, sample representative quotes for this item are shown in Table 4-11 in order to illustrate the strategies used by novices in the different strategy groups.



Which of the following terms best describes the relationship between the pair of molecules shown?

A) Identical

B) Enantiomers

Figure 4-10: Item R1

Table 4-10

*Summary of Strategies on Item R1 According to Mental Rotations Test Strategy Group*

| MRT Strategy Group | Analytic Strategy Used (Percent, %) | Holistic Strategy Used (Percent, %) |
|---|---|---|
| G1: Poor Rotator | 6 Novices (86) | 1 Novice (14) |
| G2: Analytic Strategy | 1 Novice (100) | None observed (N/A) |
| G3: Slow Rotator | None observed (N/A) | None observed (N/A) |
| G4: Moderate Rotator | 1 Novice (17) | 5 Novices (83) |
| G5: Fast Rotator | None observed (N/A) | 1 Novice (100) |

Table 4-11

*Strategies for Solving Item R1 According to Mental Rotations Test Strategy Group*

**What is the relationship between these two molecules and describe the strategy that you used to determine your answer**.

| Group | Verbal Utterance | Code |
|---|---|---|
| Poor Rotator (G1) | **Howard:** These are enantiomers.<br>**TK:** That was quick. How did you determine that they were enantiomers?<br>**Howard:** They are already set up to look like mirror images.<br>**TK:** So you didn't attempt to rotate this one?<br>**Howard:** No, I didn't try to rotate this one. But if you pick one up and try to turn it, I suppose you could get them to look identical…well no, because if you flipped it backwards, then the wedges would turn into dashes. So, I still believe that they are enantiomers. | Analytic – incorrect |
| Analytic (G2) | **Pamela:** They are identical.<br>**TK:** Why identical?<br>**Pamela:** Well you can rotate the second one around to look like the first. But there is also plane of symmetry.<br>Investigator: Rotate it around how?<br>**Pamela:** You take the second one and just rotate it 180 degrees. You can see the CH3's line up and they are both coming out of the plane.<br>**TK:** You mentioned a plane of symmetry – what do you mean?<br>**Pamela:** Down the pentagon in between the methyls, there is a plane of symmetry.<br>**TK:** What implication does that have?<br>**Pamela:** It means that it doesn't have…it's a mirror image….so its achiral or something like that.<br>**TK:** Did you talk about that in class?<br>**Pamela:** A little bit… | Analytic – correct |

Table 4-11, continued

| **What are the relationship between these two molecules and describe the strategy that you used to determine your answer.** | | |
|---|---|---|
| Group | Verbal Utterance | Code |
| Moderate Rotator (G4) | **Brian:** How about identical?<br>**TK:** Why would you say that they are identical?<br>**Brian:** If you rotate it about 180 degrees in the plane of the paper, you know what I'm saying? Kinda like this [motions with hands] | Holistic – correct |
| Fast Rotator (G5) | **Cherie:** They are identical.<br>**TK:** Okay. So why identical?<br>**Cherie:** Okay so if you spin one the other way, it will look like the other. | Holistic – correct |

### Theme #2: Strategy Preference Differs According to Expertise

The next theme that became apparent was that strategies differed according to degree of expertise. While novices preferred holistic strategies (Figure 4-9), experts tended to use analytic strategies more frequently than novice participants (Figure 4-11) when determining the relationship between two molecules (Items R1 through R6). Most of the experts (8 of 10, 80%) strove to use an analytic strategy at least once, with about half of them (50%) using an analytic strategy on three of the six relationship items.

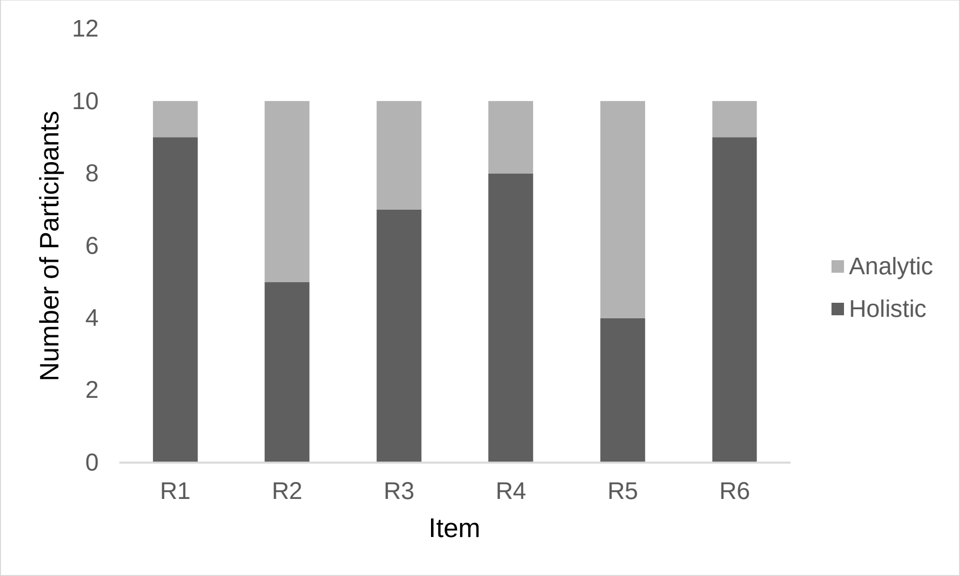


Figure 4-11: Frequency of Strategy Use by Experts (N = 10) When Determining the Relationship of Molecules

In addition to the relationship items (Items R1 through R6), Item C1 (Figure 4-5) was a configuration item where participants could choose to use a holistic rotation strategy to determine the configuration 2-butanol, or they could use an analytic strategy to by-pass any form of mental rotation. Figure 4-12 shows the percentage of successful novice participants that used a holistic mental rotation strategy as compared with the percentage of successful experts that used this strategy on Item C1. As seen in Figure 4-12, all novice participants (100%) chose to use the holistic strategy. On the contrary, 90% of experts chose the analytic strategy. Differences in solution strategies between novices and experts are illustrated through sample representative quotes presented in Table 4-12.

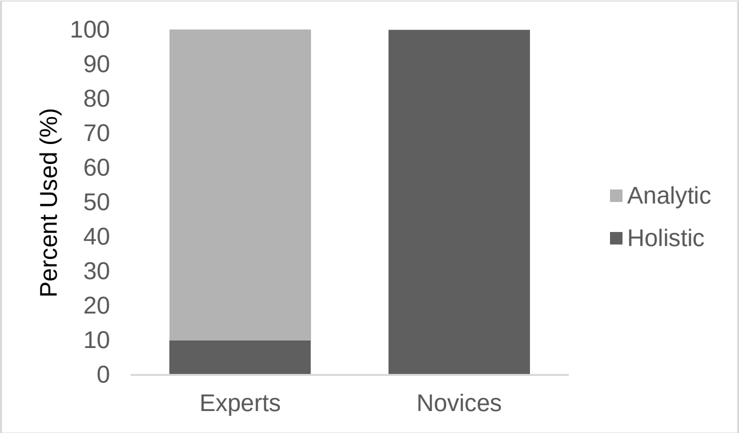


Figure 4-12: Strategy According to Expertise on Item C1

Table 4-12

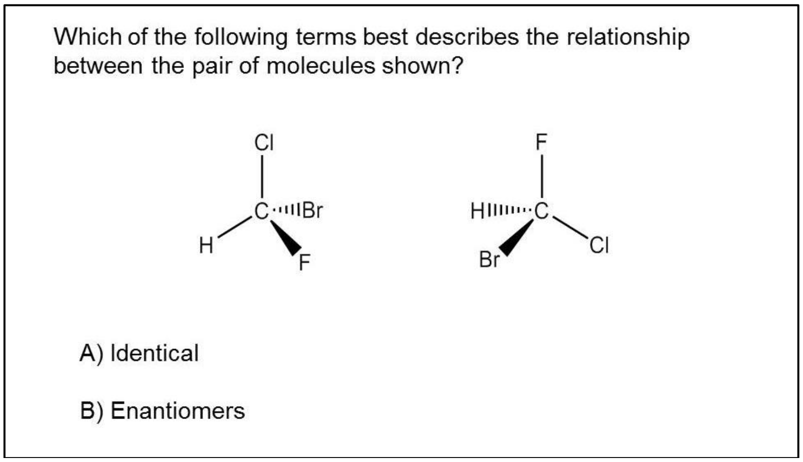
*Strategies for Solving Item C1 Differs by Expertise*

**Describe how you determined the configuration for any chiral centers in the molecule.**

| Participant | Verbal Utterance | Code |
|---|---|---|
| Successful Novice | **Brian:** Carbon 2 is chiral and the configuration would be R. I flipped the entire molecule, and then you would have your H in the back – OH in the front and the ethyl group would switch to this way, if that makes any sense. | Holistic – correct |
| Successful Expert | **Mr. Plum:** The configuration would be R and carbon 2.<br>I am looking at this carbon – the oxygen takes top priority. The methyl that is bonded to a carbon – second priority. The methyl bonded to only hydrogens third. I am going counter-clockwise as far as priority. If I were to step behind the plane, it would be clockwise.<br>**TK:** So did you step behind the plane or did you just switch your answer.<br>**Mr. Plum:** I would say more so switched my answer. | Analytic – correct |

### Theme #3: Experts May Use Multiple Strategies When Solving a Problem

For some items, a few expert participants used both holistic and analytic strategies during the problem-solving process. For instance, some experts used a holistic mental rotation strategy only enough to get the molecules in a position so that an analytic strategy could be applied. According to Table 4-13, when solving item R2 (Figure 4-13), some experts rotated the molecule shown on the left to get the hydrogen (lowest priority group) pointing to the back. After doing so, both molecules were now in the correct position for applying the Cahn-Ingold-Prelog rules (Cahn et al., 1966) to determine their configurations.



Which of the following terms best describes the relationship between the pair of molecules shown?

A) Identical

B) Enantiomers

Figure 4-13: Item R2

Table 4-13

*Experts Use Multiple Strategies to Solve Item R2*

**Describe the strategy that you used to determine your answer.**

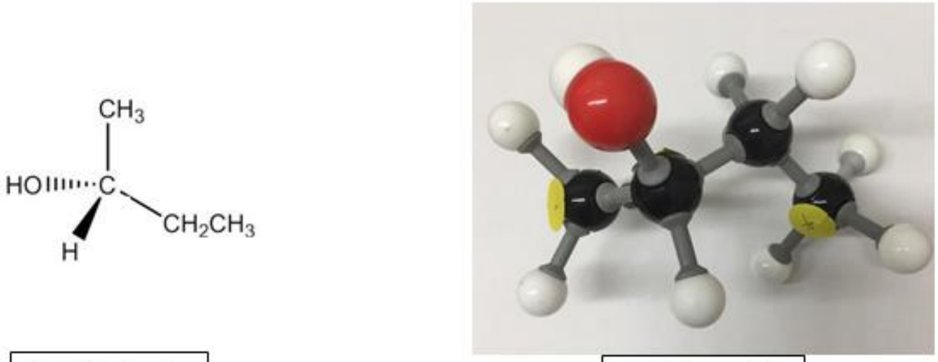
| Participant | Verbal Utterance | Code |
|---|---|---|
| Mr. Blue | In this case, I first rotated the molecule on the left, keeping the chlorine in the same spot. After I rotated it to get the hydrogen in the back, I determined the configuration of both molecules and found that they had the same configuration. | Holistic strategy followed by analytic strategy (determination of configuration) |
| Mr. Green | I rotated the molecule on the left so that the hydrogen is in the back. Then I used the Cahn Ingold Prelog rules to determine the configuration – bromine, chlorine, fluorine in that order. So the left one is counterclockwise S, the right one is also counterclockwise S. | Holistic strategy followed by analytic strategy (determination of configuration) |

In other instances, some experts were able to use multiple strategies to double-check that the solution they received using one strategy was correct: For example, when solving item C1, Mr. Blue described the following:

> To kinda check that that made sense, I did the configuration again, the way it is here, knowing that if the lowest priority group isn't pointing back then it's going to be the opposite configuration. So, I can confirm my answer to myself. So first I rotated and then I checked using the second method."

### Theme #4: Novices Prefer Using Three-Dimensional Models To Determine Configuration

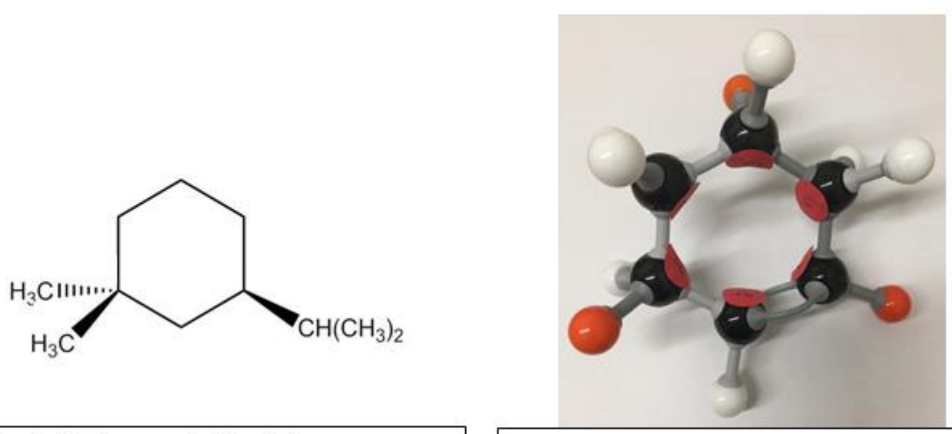
The next theme that was discovered was that novice students preferred to solve stereochemistry problems in three dimensions rather two dimensions. Two pairs of items were compared to determine whether there were any differences in performance on 2-D (items shown on eye-tracker screen) and 3-D (molecular model) representations when determining absolute configuration. For the first pair of items, Item C1 and molecular model #1 (Figure 4-14), the molecules were enantiomers of each other. For the next pair of items, item C4 and molecular model #2 (Figure 4-15), the molecules both contained chiral carbons that were part of a ring structure. Figure 4-16 shows performance on these problem sets. For both problem sets, performance increased when they solved problems using a 3-D model, as opposed to a 2-D representation. Participants were further arranged into several categories based on their performance on these items. Table 4-14 shows the number of participants in each of these categories. Furthermore, Table 4-15, presents representative quotes on students' preferences for representation type when determining absolute configuration.



*(R)*-2-butanol

*(S)*-2-butanol

Figure 4-14: Representation Type Problem Set #1, enantiomers of 2-butanol



1,1-dimethyl-3-(propan-2-yl)cyclohexane

(3*S*,5*S*)-1,3,5-tribromocyclohex-1-ene

Figure 4-15: Representation Type Problem Set #2, molecules with chiral centers as part of a ring structure

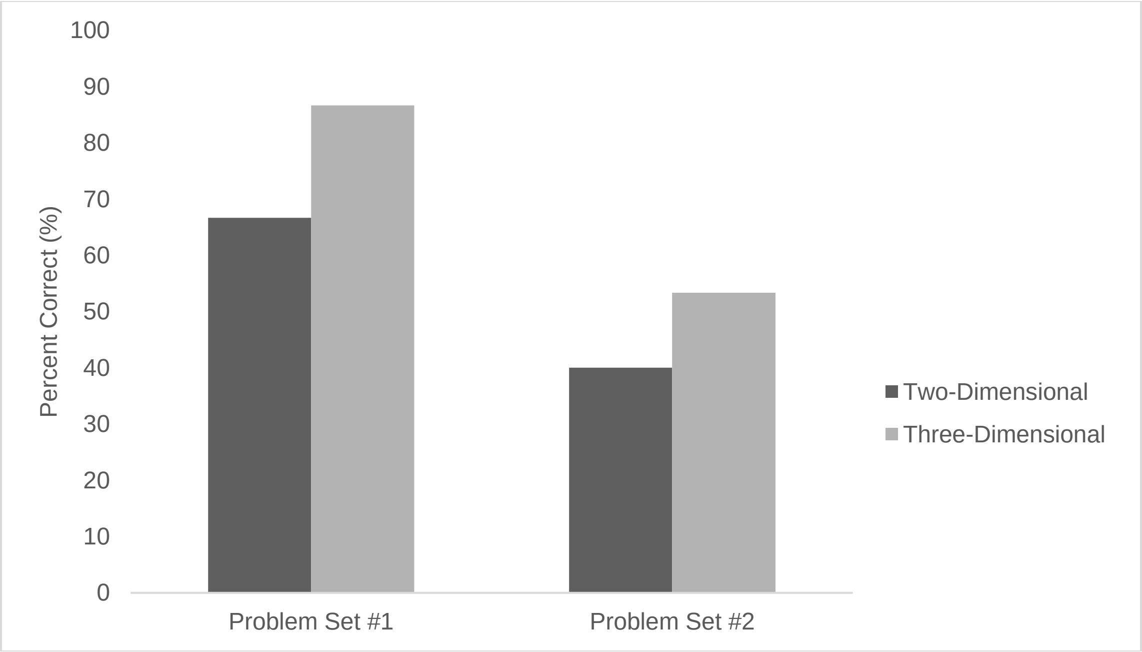


Figure 4-16: Performance of Novice Volunteers by Representation Type

Table 4-14

*Performance on Two-Dimensional and Three-Dimensional Problems*

| Comparison | Category | Number of Novice Participants |
|---|---|---|
| Problem Set #1 (Item C1 and Molecular Model #1) | Could solve both problems correctly | 10 (67%) |
| | Could solve neither problem correctly | 2 (13%) |
| | Could only solve two-dimensional problem correctly | 3 (20%) |
| | Could only solve three-dimensional problem correctly | 0 (0%) |
| Problem Set #2 (Item C4 and Molecular Model #2) | Could solve both problems correctly | 4 (27%) |
| | Could solve neither problem correctly | 5 (33%) |
| | Could only solve two-dimensional problem correctly | 4 (27%) |
| | Could only solve three-dimensional problem correctly | 2 (13%) |

Table 4-15

*Preferences on Representation Type for Solving Stereochemistry Problems*

| **Did you prefer determining absolute configuration for the molecules in two or three dimensions?** |
|---|
| **Brian** (G3, Moderate Rotator)**:** I think with the model kits it's a bit easier. So you can have it physically in your hand and rotate it around. There was one on there I was trying to rotate in my head. And it was tough to look at the one on the screen and try visualize it the different spatial arrangement in my head. So it was easier here – I could just physically rotate it and look at it. |
| **Ruthie** (G1, Poor Rotator)**:** I think working on the screen is easier than the model.<br>**TK:** Why is it easier?<br>**Ruthie:** Because I don't really understand how to move the model. In class, the model kit helps, but like she just didn't explain how to use it really well. |
| **Ernestine** (G1, Poor Rotator)**:** The models were definitely easier, I could manipulate it and move it to where it made sense. I wasn't trying to do it in my head.<br>**TK:** Do you find when it's on paper its usually harder?<br>**Ernestine:** Yes. |
| **Howard** (Poor Rotator)**:** The model kits. Because you could see it and I didn't have to flip it in my mind and I didn't have to visualize it. It allowed me to do it a little faster. |
| **Vanessa** (G1**,** Poor Rotator)**:** The model.<br>**TK:** Why would you say it was easier with the model.<br>**Vanessa:** It's in 3D, so you can see it more easily. Especially when using the wedges and dashes, you can see where exactly they are, and relate them to the molecule. |
| **Davina** (G1, Poor Rotator)**:** I wanna say the one on the computer was easier. Just cause the models seem a little busier and there were all the extra hydrogens and stuff. That made it a little bit harder.<br>**TK:** So the one on the screen was a little cleaner?<br>**Davina:** Yea. And I feel like it showed the priority groups, whereas the model has every single atom on it. |

## Theme #5: Gestures Help Students to Solve Stereochemistry Problems

Another theme that was evident was the role that gestures play while novices and experts solved stereochemistry problems. Several novices and experts made the comment that gestures helped them while solving stereochemistry problems. Sample representative quotes as it relates to gestures are found in Table 4-16.

Table 4-16

*The Role of Gestures When Solving Stereochemistry Problems*

**Brian** (G3, Moderate Rotator)**:** My hands also kinda helped me with this problem. I imagined the molecule as my hand, with my fingers being the atoms.
**TK:** Okay so if the H is pointing toward you, how do you change your fingers?
**Brian:** So then my thumb would be my H and I would rotate the whole thing back. [Makes motion with hands]

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**Davina** (G1, Poor Rotator)**:** Honestly, I kinda just use my hands. If I'm like... if I pull it this way, but other than that I haven't really found any other strategies.
**TK:** So you use your hands a lot?
**Davina:** Even if I don't have a model kit, I try to picture the molecule and try to rotate it as if I did have it in my hands.
**TK:** Is that something that came naturally for you, or did someone show you use to use your hands?
**Davina:** Mmm..I feel like it came natural. Because if I did have a model kit, that's what I would do.
**TK:** So you pretend that you hold it?
**Davina:** Yea.

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**Donald** (G3, Moderate Rotator)**:** My hands help me associate things. If I just do it in my brain, I have to say okay on the right side is the OH group and on the left side is the methyl. And then I have to think about the structure. But I guess if I just have my hand like this, I can just visualize. Okay here is the ring as my fist, and then my thumb is where the OH is and my pinky is where the methyl group is. And so if I were to rotate it, it's still methyl and that would be OH.
**TK:** So you imagine the atoms as your fingers?
**Donald:** Sometimes, especially when they are sticking out or sticking in, this really helps. Because then obviously my thumb is sticking toward me in this orientation, so then this is what it looks like and then if I flip it I can see how it would look. So it's like a physical visualization. Visualization in my mind still works. But when you integrate the two - visualization and the physical aspect – that makes it significantly better for me.

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**Ms. Scarlet** (expert)**:** I am picturing a clock as I make my finger go around. So this is counterclockwise that I am making my finger do right now, so that is S.
**TK:** How does your finger help you?
**Ms. Scarlet:** Because I have to go to each group with my finger and I don't know what my finger is doing until I actually pay attention to it, to know if it is going clockwise or counterclockwise. If you see me taking a test on this, for example, in biochemistry I use my finger all the time and like I literally will be doing this for a long time until I realize whether it's going clockwise or counterclockwise. Or if I don't use my finger, I have to draw arrows on my paper to say which direction.

## The Big Picture – How Novices and Experts Solve Stereochemistry Problems

After analyzing the qualitative data, several major patterns emerged for novice and expert stereochemistry problem solvers. A summary of these patterns for novices and experts are presented in Figure 4-17 and Figure 4-18 respectively.

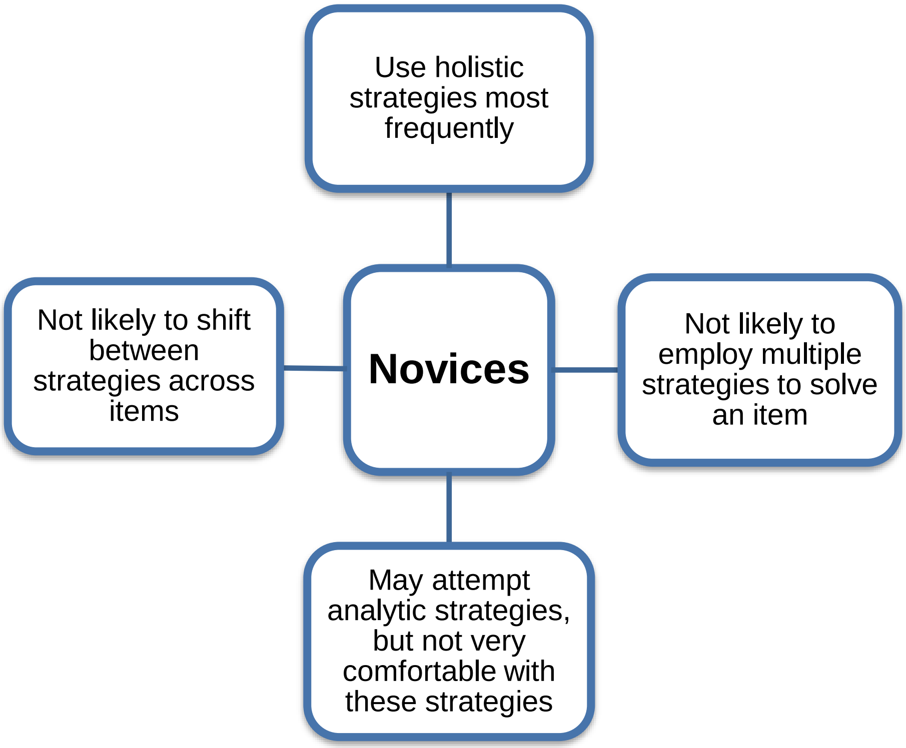

Figure 4-17: Summary of Novice Patterns for Solving Stereochemistry Problems

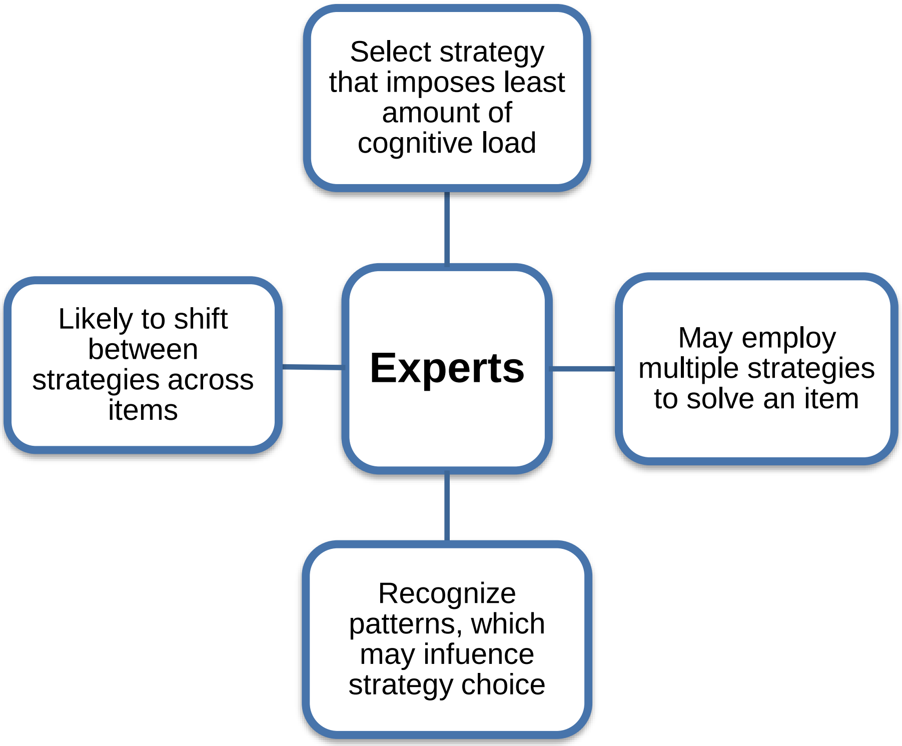

Figure 4-18: Summary of Expert Patterns for Solving Stereochemistry Problems

## Q4: Relationship Between Mental Rotations Test Spatial Strategies and Performance on the American Chemical Society Exam

The relationship between ACS 1st term organic chemistry exam[1] performance measures (total score, stereochemistry sub-score, and non-stereochemistry sub-score) and MRT performance (total score) was investigated using Pearson product-moment correlation coefficient. As shown in Table 4-17, there were significant correlations between total raw score and non-stereochemistry sub-score with MRT total score.

Table 4-17

*Correlations Between 2010 ACS 1st Term Organic Chemistry Examination Performance Measures and Mental Rotations Test-A Score*

| | MRT Total Score | r and p values |
|---|---|---|
| Total Score on the ACS Exam | Pearson Correlation | 0.372 |
| | Significance (2-tailed) | 0.005* |
| Stereochemistry Sub-Score | Pearson Correlation | 0.211 |
| | Significance (2-tailed) | 0.119 |
| Non-Stereochemistry Sub-Score | Pearson Correlation | 0.344 |
| | Significance (2-tailed) | 0.009* |

*Statistically significant at p = 0.05 level

Further, to investigate factors that influence performance on the ACS 1st semester Organic Chemistry Examination (2010 Version), stepwise regression was used to assess

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[1] It should be noted that one of the two sections of participants was inadvertently administered the incorrect examination and consequently results could only be interpreted for the section that received the correct version of the ACS examination. Due to the smaller number of participants populating each group, the slow and moderate rotator group was combined for the purposes of analyzing Research Question 4. There was a significant relationship between these two groups in terms of score on the MRT (r = .327, p = 0.014).

the ability of MRT score and gender to predict ACS exam total score. When evaluating the influence of gender and MRT score on ACS exam total score, gender did not reach the alpha level of 0.05 (p = 0.153) and therefore, was not entered into the equation. MRT score was found to be a significant predictor of ACS total score *b* = 0.503, t(54) =2.949, p = 0.005 (Table 4-18).

Additionally, the influence of MRT score on stereochemistry sub-score and non-stereochemistry sub-score was examined. As can be seen in Table 4-18, MRT score significantly predicted non-stereochemistry sub-score, *b* =0.437, t(54) = 2.693, p =0.009. However, MRT score was not a significant predictor of ACS stereochemistry sub-score *b* = 0.066, t(54) = 1.584, p = 0.119.

Table 4-18

*Regression Analysis Showing Influence of Mental Rotations Test Total Score on ACS exam performance measures*

| | *B* | p value |
|---|---|---|
| Total | 0.503 | 0.005* |
| Stereochemistry | 0.066 | 0.119 |
| Non-stereochemistry | 0.437 | 0.009* |

*Statistically significant at p = 0.05 level

To explore differences between MRT strategy groups (G1 to G5) on the ACS organic chemistry examination (2010 Version), a one-way multivariate analysis of variance (MANOVA) was conducted (Table 4-19). Two dependent variables were used: stereochemistry and non-stereochemistry sub-scores on this examination. Strategy group on the MRT was the independent variable. There was no statistically significant difference due to MRT strategy groups on the overall MANOVA statistic, *F* (3,52) =

1.294, p = 0.267*;* Wilk's Λ = 0.864. Thus, the individual ANOVA p-values (Table 4-19) were not investigated.

Table 4-19

*One-Way MANOVA Looking at Differences in Performance Measures According to Mental Rotations Test Strategy Classification*

| Source | Dependent Variable | SS | Df | MS | F | p value |
|---|---|---|---|---|---|---|
| MRT Strategy | Stereochemistry | 6.315 | 3 | 2.105 | .767 | .518 |
| | Non-stereochemistry | 271.328 | 3 | 90.443 | 2.124 | .108 |

## Summary

Quantitative and qualitative results were presented in this chapter in order to characterize novices' and experts' strategies for solving organic stereochemical problems. In Chapter 5, these data will be interpreted for each of the four research questions.

# CHAPTER 5

# DISCUSSION

The overall purpose of this study was to gain a better understanding of the cognitive processes that occur when students solve stereochemical problems. In this chapter, the data analyzed in Chapter 4 are discussed with respect to previous research studies. Chapter 5 is organized based on the four research questions presented in Chapter 1. Implications for teaching and research based on this study are presented following the discussion.

## Research Question 1

Were there significant differences in the observed distribution of solution strategies between male and female novice organic chemistry students when solving problems on the Mental Rotations Test-A (MRT-A)?

The results (Table 4-1) showed that there was a gender difference on MRT-A overall score. As can be seen from Figure 4-1, males scored significantly higher than females ($p = 0.005$), which produced a moderate effect size ($d = 0.50$) for the difference in the means. This was consistent with other studies who found gender differences on the MRT (Geiser et al., 2006; Linn & Petersen, 1985). For example, in the study conducted by Geiser et al., 2006, there was a large effect size ($d = 0.72$) for the gender difference.

Additionally, these results were not surprising as the ability to mentally rotate an object has been found to produce one of the largest gender differences in cognitive literature (Linn & Petersen, 1985; Parsons et al., 2004; Voyer, Voyer, & Bryden, 1995).

To further investigate differences in gender on the MRT-A, participants were classified into one of five groups according to their strategies for solving items on this instrument (Geiser et al., 2006). Figure 4-2 shows the profiles of each strategy group based on their solution probabilities for solving items on the first 12 items on the MRT-A. Further, a summary of the observed number of participants in each class can be found in Table 4-2. Results indicated that there was a highly significant difference ($p = 0.016$) in the distribution of spatial strategies across the five groups as compared with the distribution of these strategies originally found by Geiser and colleagues (2006). One likely reason for this discrepancy is that the prior study had a very broad pool from which participants were drawn ($N = 1,695$). However, in the current study, participants were selected based on a clearly defined criterion – enrollment in a lecture section of first semester of organic chemistry. It is likely that in the current study, participants' mental rotation strategies were highly specialized due to their previous experiences in STEM courses, which were required as pre-requisites.

In this study, the distributions of these spatial strategies for male and female students on solving items on the MRT was also investigated (Table 4-3). While females appeared to be over-represented in the poor rotator class in comparison to males, a chi-square test of proportions indicated that there was no significant difference in the distribution of spatial strategies for these male and female organic chemistry students when solving problems on the MRT, $\chi^2 = 1.78$, $p = 0.775$.

In the current study, females were found in high numbers in the poor rotator group (G1), which agrees with results from the study conducted by Geiser and colleagues (2006) who found that females were more often assigned to the group with the poorest performance. Additionally, the present study found that females were shown in the highest proportion in the moderate rotator group (G3). On the other hand, Geiser and colleagues (2006) found that females were overrepresented in the slow rotator group (G4) and slightly overrepresented in the analytic group (G2).

The fact that female participants in the present study were not found in higher numbers in the analytic group (G2) was surprising. While Geiser and colleagues (2006) found this group to be only slightly overrepresented by females, other prior studies have found that females have a greater tendency than males to use analytic strategies (Heil & Jansen-Osmann, 2008; Moè, 2009). Therefore, it was expected that more females would have populated this group.

## Research Question 2

When novice organic chemistry students were solving stereochemical problems, could a) eye-tracking methods and b) molecular modeling serve as tools to reveal their cognitive processes?

### Q2A: Eye-Tracking Method

The analysis of eye-tracking data can be used to provide information on a participant’s overt visual attention, which has been shown to be related to their cognitive processes (Topczewski et al., 2016). Eye-tracking methods were used to investigate the cognitive processes that occur while problem solvers attempted to work stereochemistry problems.

For the first set of items (R1 through R6, i.e., the relationship item problem set), problem solvers were required to determine whether two molecules were identical or enantiomers. For these items, the number of transitions made between the two molecules was of particular interest. The number of transitions, also called fixation switches, can give insight into active processing of information within the visual-spatial working memory (Hyun & Luck, 2007). A transition was coded whenever a fixation on any region of one molecule AOI (i.e., Area Of Interest) was immediately preceded by a fixation on any region of the other molecule AOI (Figure 3-3). These transitions can be viewed as a refresh rate within the visuospatial working memory, which is necessary to keep up the fading object representation within the working memory (Hyun & Luck, 2007). Furthermore, transitions between the molecules can be inferred as an attempt to integrate the features of the two molecules (Hinze et al., 2013; Johnson & Mayer, 2012). This is often important when determining the relationship between a pair of molecules.

First, when the number of transitions made between a pair of molecules for experts and novices were compared, the results (Table 4-5) suggest that experts made fewer transitions between two molecules when they attempted to determine the relationship between the molecules. Although statistically significant differences were only found for half (50%) of the items regarding relationship (i.e., R2, R3, and R6) between experts and novices, an overall pattern of fewer transitions was observed for all items (Figure 4-3).

When solving these types of stereochemistry problems, the higher number of transitions for novices suggests that they experienced greater amount of cognitive load as compared to experts. That is, the number of fixations increases when the cognitive load of a task is increased (Tang & Pienta, 2012). This finding is not surprising, as experience with solving these types of problems would likely reduce the amount of mental effort required to solve stereochemistry problems. For novices, these problem types were unfamiliar, which resulted in more cognitive effort being required on their part to solve these problems.

Related to this, a lower number of transitions for experts may suggest that they are better at keeping an internal representation of the molecules fresh within their working memory while attempting to determine the relationship. This factor may have reduced the cognitive load imposed on the experts by these problems. To determine the relationship of the molecules using holistic rotation strategies, the individual must maintain an active representation of all the parts of the molecule, and the interrelations of these parts, while simultaneously rotating the molecule within working memory (Kaufman, 2007). Overall, these results support the idea that experts are able to solve problems more efficiently, and thus reduces the need for back and forth transition between molecules.

An alternative inference is that this pattern may suggest that experts tend to use more analytic strategies rather than holistic strategies when determining the relationship between molecules. The use of more analytic strategies, such as looking for planes of symmetry or using an algorithm (such as Cahn-Ingold-Prelog nomenclature rules – Cahn et al., 1966) reduces the need to keep all of the various parts of the molecules within working memory in order to attempt to bring them into congruence. This in turn diminishes the need for experts to transition back and forth between the molecules. This is consistent with a prior study by Stieff (2007) which found that experts use analytic strategies more frequently and consistently than novices do. This particular study also found that novice students relied more on holistic mental rotation strategies when solving problems. This inference can help explain why the results indicated that novice students needed to make more transitions between the molecules when attempting to determine their relationship. Conversely, when using analytic strategies, fewer transitions between the molecules may be required during the problem-solving process.

Next, the number of transitions between molecules were compared for successful and unsuccessful novices. Again, there was a pattern of fewer transitions for successful novices as compared to those of unsuccessful novices (Figure 4-4). However, a statistically significant difference was found only on Item R2 (Table 4-6). Interestingly, this item was calculated as the most difficult one (item difficulty index of 0.54) in the relationship item problem set (R1 to R6). It is not surprising that this item was the most difficult because it required participants to keep track of the largest number of atoms when rotating the molecules. For instance, in the other items, participants could ignore the ring portion of the molecule and thus reduced the pieces of information that had to be kept in working memory while solving the problem.

As all novice volunteers reported using a holistic strategy for this item (Figure 4-9), the fact that the number of transitions made by novices on this item was substantially more than for any of the other items supports the idea that this item required them to frequently refresh the parts of the molecules and the interrelations of these parts within working memory. Furthermore, as successful and unsuccessful novices differed in the number of transitions on this item, it appears that successful novices were more efficient than unsuccessful novices at keeping the information about molecules within working memory and therefore reducing cognitive load.

Overall, however, there was no clear pattern of differences in the number of transitions between molecules for successful and unsuccessful novices. A similar number of transitions for all novices, regardless of success on the item, may indicate that both successful and unsuccessful novices use similar strategies when determining the relationship between molecules. Therefore, successful and unsuccessful novices require a similar number of transitions between the molecules. However, it seems that successful novices are more effective at using these strategies.

For the set of problems related to determining the absolute configuration of molecules (configuration items C1 through C5), eye tracking contributed information about the cognitive processes that occur when problem solvers identify chiral centers and determine their configuration. For these items, regions of the molecule that were deemed important to the problem-solving process were defined as AOIs. As AOIs were unique to each molecule, AOIs were analyzed individually for each molecule.

When determining the configuration of a chiral center, an important step in the problem-solving process is to consider the direction of the lowest priority group around this center. To investigate any differences in the problem-solving process between successful and unsuccessful novices due to completion of this step, Item C1 was used. For Item C1 (Figure 4-5), the lowest priority group was not oriented in the way that the Cahn-Ingold-Prelog rules (Cahn et al.,1966) dictate. That is, the lowest priority group (the hydrogen atom) is pointed toward the problem solver instead of pointing away. The researcher defined this hydrogen atom as an AOI because an important step in the problem-solving process is to consider the direction in which the hydrogen is pointed.

The total fixation duration for successful novices as compared with unsuccessful novices on this item was computed (Table 4-7). There was a statistically significant difference found ($p = 0.019$), with unsuccessful novices fixating on the hydrogen atom less frequently than successful novices. This may indicate that the unsuccessful novices failed to consider the direction in which the hydrogen was pointed during the problem-solving process. Long fixations in a certain region often indicate that participants find the region to be important or relevant to the problem (Tang et al., 2014). Thus, it was interesting that successful novices fixated more on the hydrogen atom than did their unsuccessful counterparts.

The sample heat maps shown in Figure 4-6 for a successful novice (e.g., Brian) and an unsuccessful novice (e.g., Vanessa) also point to differences in eye movement patterns between successful and unsuccessful novices. From the heat maps, it appears that the unsuccessful novice fixated on other groups more so than the hydrogen atom. However, the successful novice on this item fixates on the hydrogen atom for a considerable duration. Furthermore, this fact was supported by their account of how they solved the problem. Brian described attempting to flip the entire molecule to get the hydrogen atom in the back. In contrast, Vanessa made no mention of the hydrogen atom in her explanation of how she solved the item.

Next, Item C3 (Figure 4-7) was used to investigate whether participants are automatically drawn to carbons that have atoms attached with dashes and wedges. In stereochemistry problems, dashes and wedges are often used to imply a three-dimensional arrangement of atoms. Consequently, these areas may be particularly attractive to problem solvers. However, the use of dashes and wedges does not always indicate a chiral center. Item C3 was interesting because although there are two carbons (carbons labeled as 2 and 4) where groups are shown with wedges and dashes, there are actually no chiral centers in this molecule. On closer inspection, the successful problem solver would observe that despite the presence of wedged and dashed groups, neither carbon 2 nor carbon 4 had four different groups attached. That is, both of these carbons have two methyl groups attached, but represented in different ways. To determine whether carbon 2 and carbon 4 were more attractive to unsuccessful problem solvers, the total fixation time and number of fixations were calculated on carbon 2 and carbon 4. The eye-tracking data (Table 4-8) show that unsuccessful novices spent a statistically significant longer ($p = 0.039$) duration fixating on carbon 2 and carbon 3 than did successful novices. Furthermore, the results showed that unsuccessful novices made a statistically significant higher ($p=0.004$) number of fixations on the wedged and dashed substituents.

The finding that unsuccessful novices had longer fixation durations and made more fixations on these AOIs may have resulted from attempting to determine the absolute configuration for these carbons. That is, the successful novice problem solvers correctly verified that there were not four different substituents attached to each carbon before ‘wasting’ their cognitive resources to determine the absolute configuration. Conversely, after incorrectly identifying carbon 2 and carbon 4 as being chiral, the unsuccessful novice problem solvers proceeded to determine the absolute configuration. It was interesting that six out of the eight (75%) unsuccessful novices discovered their error upon attempting to assign absolute configuration. Attempting to assign absolute configuration for these non-chiral carbons ‘forced’ them to consider the identity of the substituents more carefully than they had done initially.

Further, Item C5 (Figure 4-8) was used to investigate whether participants could correctly identify a chiral carbon without the wedged and dashed notation being shown.

For Item C5, there was only one chiral center – the carbon labeled as carbon 3. Although the wedged and dashed notation was used for carbon 2, it was not a chiral center due to two methyl groups being attached. Carbon 3, the only chiral center in the molecule, may have been overlooked due to the lack of wedged and dashed notation used for this carbon. Furthermore, the fourth substituent of carbon 3 (hydrogen atom), was not shown. By convention, it is common for the hydrogens in skeletal representations to be omitted, however, this may make it easy for problem solvers to neglect such atoms when attempting to determine chirality. For this item, it was interesting to see if successful and unsuccessful novices differed in determination of whether or not this carbon was a chiral center. Thus, carbon 3 was defined as an AOI. Results shown in Table 4-9 revealed that there was a statistically significant longer fixation duration on this AOI (p=0.039) for successful novice problem solvers than for unsuccessful novice participants.

### Q2B: Molecular Models

To investigate the impact that physical molecular models had on novice students' ability to solve stereochemistry problems, novices were asked during the physical model session to solve stereochemistry items that were similar to problems given during the eye-tracking session. Two different problem sets, as described below, were used to investigate differences in how novices solved stereochemistry problems presented in two- and three-dimensions.

For Problem Set #1 (Figure 4-14), the two- and three-dimensional representations were enantiomers (*R*- and *S*-2-butanol). Results (Figure 4-16) showed that overall, novices (N = 15) performed better with the molecular model than they did with the 2-D problem (Figure 4-16). These results were consistent with results found by Stull and colleagues (2012), who proposed that using physical (concrete) models to enact and support cognitively difficult tasks can enhance problem solving.

When novices were asked about how molecular models helped them to solve problems such as determining the configuration of a chiral center, one of the reasons given was that it was easier to manipulate the physical model than it was to manipulate a two-dimensional representation mentally. Looking again at Item C1 (Figure 4-5), some participants were unsuccessful because they failed to (or were unable to) manipulate the molecule in the appropriate way to determine its absolute configuration. For example, Ruthie, Davina and Kimberly, three novices who had all been identified as poor rotators, were unsuccessful at determining the absolute configuration for the 2-D representation, but were successful at determining the configuration for the 3-D model. According to their retrospective think-aloud for solving the item, it was evident that Ruthie and Davina had not taken into account the position of the lowest priority group. However, when given the molecular model problem, these participants positioned the molecule in the correct way for determining the absolute configuration. Kimberly’s performance was a little different from Ruthie and Davina because she noticed that the 2-D representation of the molecule was not positioned so that the lowest priority group was pointed away from her and she described trying to rotate the molecule to the correct position, but was not confident that she had done so accurately:

> Um what I was trying to do is assign priority to all of the groups coming off of the carbon that I think is the chiral center and then I try to flip it so that the lowest priority group is in the back. I hope that I flipped it in the right way because sometimes I can’t.

Although Kimberly was unable to rotate the 2-D representation correctly, she correctly manipulated the 3-D molecular model. She explicitly mentioned positioning the molecule in the appropriate way:

> **Kimberly:** Carbon 2 would be chiral – and so then it would be S. Because the OH is on top.
> **TK:** So you positioned it so that the OH is on top?
> **Kimberly:** Well really, position it so that the hydrogen is in the back.

Thus, while Kimberly knew that she needed to rotate the 2-D representation, she was unable to do so successfully. The physical model, however, may have allowed her to use her cognitive resources to determine the absolute configuration rather than devoting her resources to mental rotation of the molecule. This finding is consistent with the assertion by Stull and colleagues (2016) – a physical model can help to reduce the demand on working memory and lower cognitive load. A physical model accomplishes this as it represents the molecule externally so that students do not need to imagine and maintain a three-dimensional representation in their working memory. This, in turn, allows students to visualize the three-dimensional relations between atoms in a molecule, and thus makes manipulating molecules an easier task.

For Problem Set #2 (Figure 4-15), the novices were required to identify any chiral carbons for molecules that contained a ring structure. Similar to Problem Set #1, results (Figure 4-16) showed that for Problem Set #2 slightly more novices were able to successfully solve the 3-D problem (53%) involving chiral centers within a ring compared to those who were able to successfully solve the 2-D item (40%). This trend indicated that overall performance increased with the use of a physical model. Conversely, the results (Table 4-14) showed that for some participants, performance appeared to be adversely impacted with the use of a physical model. That is, they were able to solve the 2-D problem, but not the corresponding 3-D problem. Although overall more novices solved the 3-D problem more successfully than the 2-D problem, one reason for this may have been that the 3-D problem was more challenging in that it required the problem solver to locate and assign absolute configuration for two chiral centers (as opposed to only one chiral center in the 2-D item). However, another possibility for some novices performing poorer on the 3-D problem was something inherent about the physical model. This was supported by statements made by Davina, a "poor rotator," when asked about her preference for solving problems in two or three dimensions:

> **Davina:** I wanna say the one on the computer was easier. Just cause the [molecular] models seem a little busier and there were all the extra hydrogens and stuff. That made it a little bit harder.
> **TK:** So the one on the screen was a little cleaner?
> **Davina:** Yes. And I feel like it showed the priority groups, whereas the [molecular] model has every single atom on it.

This was consistent with results from Huk (2006) with 106 biology students, who found that not all students benefited from 3-D models. That is, while students with high spatial abilities benefited from the presence of 3-D models by helping them to free up space in the working memory, the presence of 3-D models resulted in cognitive overload for students with low spatial abilities. On the contrary, a study by Stull and colleagues (2012) with organic chemistry students found that while concrete molecular models can be beneficial while problem solving for both students with high and low spatial abilities, some students need direct instruction to be able to take advantage of molecular models. Ruthie, another "poor rotator," expressed this preference (Table 4-15) for solving problems in two dimensions rather than three dimensions – "I don't really understand how to move the model. In class, the model kit helps, but like the instructor just didn't explain how to use it really well."

In the study by Stull and colleagues (2012), some students were unable to use molecular models because they did not remember the correct conventions of the models (such as what the colors of the balls mean) or they could not chunk the units in the model that are identified as chunks in the 2-D representation. For example, a methyl group ($CH_3$) may be viewed as a single unit in a 2-D representation, but in a 3-D representation, a methyl group is presented as a much larger entity. As Davina alluded to, showing every atom as its own separate unit may serve as a source of extraneous cognitive load, making the problem more difficult for some students to solve. According to Johnstone (1983), when all bonds between atoms are explicitly drawn or shown (such as in a molecular model), students may not perceive groups such as $CH_3$ as a single entity.

It was also interesting that overall performance decreased overall for Problem Set #2, as compared with Problem Set #1. When attempting to determine the absolute configuration for molecules in which a chiral center is part of the ring, if two substituents have the same immediate substituent atom, the problem solver must evaluate atoms progressively further away from the chiral center until a point of difference is located. This additional evaluation criterion may have decreased performance on Problem Set #2, because it may have added to the cognitive load imposed on the problem solver. Several novices seemed to struggle with this item, expressing that it was difficult to keep track of so many atoms, which, in turn, made the item more challenging.

As stated previously, 93% of novices in this study stated that they preferred using the model kit to determine configuration. Conversely, in the researcher's pilot study the majority of participants (78%) expressed challenges with using molecular models to determine absolute configuration. It is interesting to note that there was a 180 degree turn around from the pilot study. One crucial factor may help to explain these findings: there were two different instructors, one for the pilot study and another one for this study. The pilot-study instructor, Professor Black, did not seem to place as much emphasis on the use of model kits as did the instructor for this study. While the pilot-study instructor recommended that students practice with model kits on their own time, he admitted that he did not provide many opportunities for model kit use during class time. Furthermore, Professor Black did not allow students to use molecular models while taking exams:

> **TK:** Do you allow students to bring them to the exam?
> **Professor Black:** No, I don’t.
> **TK:** Why not?
> **Professor Black:** Because they should be able to do it on paper. The model kits, in my opinion, are there to allow them to learn to visualize in 3-D. But I teach them how to do it on paper. The model kit only allows them to see why we draw the 2-D representation the way that we do.

In stark contrast, several of the participants in this dissertation study mentioned using model kits during class time and were even allowed to take them to their examinations. To investigate this phenomenon further, the researcher interviewed the instructor of the dissertation study, Professor Pink, about the emphasis she placed on molecular models during the course:

> **Professor Pink (Dissertation Study Instructor):** I frequently took a model kit with me to class, during topics such as Newman projections, cyclohexane conformations, elimination reactions and almost every class period during stereochemistry topics such as chirality. I had them ‘model as I modeled’- that is, I would show the students my model and would have them also build their own. I also allow them to use them on the exam.

Professor Pink strongly recommended that her students purchase molecular model kits, but she did not require them. She stated that roughly half of the class would bring model kits to class. However, Wu and Shah (2004) stated that students benefit equally from viewing models either as a demonstration by the instructor or directly manipulating the models themselves. Therefore, even students who did not own a model kit may have benefited from the instructor's demonstration of the model. It is also likely that this increased exposure to model kits (either through demonstration or direct manipulation) made students more comfortable with using them to solve stereochemistry problems such as absolute configuration. Consequently, they could tap into the benefits of model kits in a way that the participants could not in the pilot study.

This difference in focus on molecular models may also be related to the strategy type that these instructors emphasized during instruction for solving stereochemistry problems. For example, Professor Black (pilot study instructor) seemed to emphasize step-by-step analytic procedures for solving problems on paper. When following these step-by-step procedures, visualizing the molecule may not be a vital part of solving the problem. However, Professor Pink (dissertation study instructor) seemed to emphasize more holistic rotation strategies, such as always rotating the molecule in the proper orientation before determining the configuration. For this strategy, visualizing the molecule is likely to be an important part of the problem-solving process and hence, a molecular model may be especially helpful.

Given the above rationale, what happens when students do not have model kits available to them? While solving the two-dimensional problems in this study, participants were not allowed to use a model kit. However, some participants were observed using their hands to mimic models while solving these problems, which seemed to be beneficial to some novices (Table 4-16).

. When questioned about this strategy, a few of the participants mentioned that their Supplemental Instruction (SI) instructor had shown them how to use their hands to solve problems during a review session. For example, Brian (a moderate rotator, G3), stated the following:

> **Brian:** I went to an SI session and the SI instructor said something about the fingers and like how you can visualize it and rotate it. So I was doing that for a little while and so that kinda helped.
> **TK:** So the finger thing helped?
> **Brian:** Yes, once I kind of got that down, I was like okay I can kind of see it.

Ruthie (a poor rotator, G1) also echoed these sentiments:

> **Ruthie:** Our SI taught us this thing to do with our hands which is easier.
> **TK:** So does your instructor not use this hand method?
> **Ruthie:** No.
> **TK:** But you find that way easier? What other strategies do you use – or is it just the hand thing that helps?
> **Ruthie:** The hand thing is really helping me.

The researcher interviewed the SI instructor further about these hand strategies. The SI instructor described using her hands and fingers to represent molecules. When asked about the origins of this strategy, she said that while taking organic chemistry, she wanted to be able to come up with a way of physically visualizing molecules other than having to use a molecular model.

> **SI instructor:** I didn't want to rely on a model kit because I could practice with it, but I couldn't bring it to the test. And so I figured out a way to use my hands instead.
> **TK:** But did you also use molecular models?
> **SI instructor:** No, I never got a model. I wanted to be able to do it in my head because I felt that I would get to rely on it too much and I didn't want to rely on it as a crutch.

Using one's hands to represent molecules and fingers to represent atoms seems like a useful approach, especially when a molecular model is not available. This is in keeping with the assertion by Siloac (1999), that using the hands to observe chiral molecules provides a molecular model that the student can apply anywhere. A student's hands may be a great alternative to a model kit:

- if they cannot afford one
- if they are not allowed to bring a model kit to the examination, or
- if it would take too long to build a model of the molecule using the kit.

Furthermore, using the hands to represent molecules is consistent with assertions made by Hegarty and colleagues (2005) in that the hands can be used to represent an object that must be mentally transformed. In this way, hand motions can be used to reveal something about the motion of an object itself or the effects of moving the object. For example, by perceiving their hands as the molecule and the individual atoms as their fingers, some participants were able to move their hands to mimic the rotation of the molecule. This was especially useful when it was necessary to re-position the molecule (such as when determining the absolute configuration of the molecule to ensure the lowest priority group was pointed toward the back). By using their hands to accomplish this, they could more easily visualize the effects of re-positioning the molecule. For example, they could predict the new position of individual atoms based on where their fingers were pointed.

Additionally, hand gestures may have also offered cognitive advantages while solving stereochemistry problems. Hegarty and colleagues (2005) argue that gestures may be beneficial while solving spatial problems in that they allow information to be offloaded onto the motor system and consequently help to free working memory resources for other aspects of the problem-solving process. An example of this was when

Ms. Scarlet (an expert) described using circular hand motions to help her keep the priority groups in the correct sequence:

> **Ms. Scarlet:** I am picturing a clock as I make my finger go around. So this is counterclockwise that I am making my finger do right now, so that is the S configuration.
> **TK:** Can you describe how your finger helps you?
> **Ms. Scarlet:** Because I have to go to each group with my finger in the order of their priority, and I don't know what my finger is doing until I actually pay attention to it, to know if it is going clockwise or counterclockwise. If you see me taking a test on this, for example, in biochemistry I use my finger all the time and like I literally will be doing this for a long time until I realize whether it's going clockwise or counterclockwise. Or if I don't use my finger, I have to draw arrows on my paper to say which direction.

This is analogous to an example provided by Hegarty and colleagues (2005), in which they describe a problem solver making clockwise motions when solving a problem related to a gear system in order to keep track within working memory of the way that certain gears move. In this way, when solving visuospatial tasks that require the internal maintenance of information, an individual may use gestures to maintain some of this information, thus freeing space in working memory for other aspects of the problem-solving process (Hegarty et al., 2005).

## Research Question 3

Do the strategies used to solve organic stereochemical problems differ for successful novice students versus unsuccessful novice students? Do the strategies used to solve organic stereochemical problems differ for experts versus novice students?

### Q3A: Successful versus Unsuccessful Novice Students

Eye-tracking data revealed some key differences in eye movement patterns for successful and unsuccessful novice participants. To further characterize differences between successful and unsuccessful novices, descriptions of their strategies for solving stereochemistry problems were collected using retrospective think-aloud protocols.

Of interest was whether a problem solver’s spatial strategies for determining relationships between non-chemical objects (blocks on the MRT-A) were similar to strategies used to determine relationships between chemical objects (molecules). Using similar methods to Geiser and colleagues (2006), novice participants were classified (Table 4-2) according to their strategies for solving items on the MRT-A.

The first set of problems, Items R1 through R6 (Appendix C), required novices to determine the relationship – identical or enantiomers – for a pair of molecules. These stereochemistry tasks were analogous to solving items on the MRT-A, in that novice volunteers were required to make decisions about their relationships. Furthermore, just as participants could use multiple strategies to solve items on the MRT-A, they could employ multiple strategies to arrive at their answers for these stereochemistry items. These strategies included holistic strategies such as imagining the molecules in the mind and manipulating them as needed to determine whether they could be brought into congruence, or more analytic strategies such as searching for planes of symmetry or chiral centers.

As observed in Figure 4-9, novices overwhelmingly used holistic strategies over analytic strategies to determine the relationship between molecules, regardless of their strategy classification based on the MRT-A. For Item R1 (Figure 4-10), however, there was the greatest division in strategy type used by novice participants. For this item, problem solvers could mentally rotate one of the molecules about 180 degrees to determine that it was identical to the other. Alternatively, the problem solver could have used an analytic strategy to solve the problem. One such strategy would be to search for a plane of symmetry within the molecule and figure out that 1,2-dimethylcyclopentane is a meso compound, meaning that although it contains chiral centers it is an achiral molecule.

Because of these distinct strategies that could be used for Item R1, transcripts of novices' explanations for how they solved the item were coded as either holistic or analytic (Table 4-10). As seen in their descriptions of solution strategies in Table 4-11, novices used different approaches to solve this item. In all, about half of novices attempted to use holistic mental rotation strategies, while the other half attempted to use strategies which did not involve mental rotation. Unfortunately, the majority of these novices were unable to use these alternative strategies to arrive at the correct answer. For example, although an incorrect strategy, Ernestine (classified as a poor rotator) attempted to lay the molecules over each other without rotating them, as she believed this to be a method taught by the course instructor. Howard, another poor rotator, also came to an incorrect conclusion – the molecules were enantiomers simply from the fact that the molecules already looked like mirror images. This novice's mistake was that he did not take into consideration the full criteria for a pair of enantiomers – they must be non-superimposable mirror images. However, after being questioned further about his strategy, he attempted to rotate it but could not figure out a way to do so in which the molecules appeared identical.

For another novice, Pamela (classified as an analytic strategist) used an analytic strategy to arrive at the correct answer:

> **Pamela:** Well you can rotate the second one around to look like the first. But there is also a plane of symmetry.
> **TK:** You mentioned a plane of symmetry – what do you mean?
> **Pamela:** Down the pentagon in between the methyls, there is a plane of symmetry.
> **TK:** What implication does that have?

> **Pamela:** It means that it doesn't have…it's a mirror image….so its achiral or something like that.
> **TK:** Did you talk about that in class?
> **Pamela:** A little bit…

Interestingly enough, this analytic strategy matched her classification in the analytic strategy group, which was based on her strategies for solving items on the MRT-A. Consequently, it appeared that Pamela was the only novice to use an analytic strategy to successfully solve this item. She was also the only novice who was able to use an analytic strategy to arrive at the correct answer for Item R5 (see Appendix C). On this item, she almost immediately reported that the molecules were enantiomers by observing that the molecules as presented looked like non-superimposable mirror images of each other and hence enantiomers. Although she did not use analytic strategies consistently for all items, she applied these strategies successfully whenever she did.

It appears that holistic rotation comes most naturally to novice problem solvers. Stieff (2007) argues that the routine use of holistic strategies such as mental rotation, in daily tasks, may make students more likely to use them in the chemistry classroom (such as when solving stereochemistry problems). Consequently, for novel stereochemistry tasks, holistic strategies are preferred until students discover or become more comfortable with using alternative analytic strategies (Schwartz & Black, 1996; Stieff, 2007). As novices used holistic mental rotation strategies most frequently to determine the relationship between molecules, this suggests that major differences between successful and unsuccessful novices were related to differences in their abilities to mentally rotate the molecules rather than differences in their strategy choice. In most cases, this "leveled the playing field" for novices in terms of their strategy – all participants had to rely on their abilities to mentally rotate the molecules.

Of the relationship items, Item R2 (Figure 4-13) was calculated to have the highest item difficult index (0.54), indicating that it was the most difficult item for participants. This item was interesting, as all novice participants attempted to use a holistic mental rotation strategy. As previously stated, novices seemed to only differ in their abilities to mentally rotate the molecules accurately. Unlike the other items where participants could 'ignore' parts of the molecule while problem solving, this item required participants to keep track of all parts of the molecule within working memory. Ruthie, a poor rotator, expressed these sentiments:

> The tetrahedral ones like these give me problems more than the others, as there is more rotation involved. I can't leave part of the molecule in one spot. At least with a ring, the majority of the atoms in the ring aren't changing and so I don't have to rotate their positions.

As successful and unsuccessful novices differed in their frequency of transitions on this item, R2, this may be due to differences in their respective working memories. For items where parts of the molecule could be ignored, there was less of a difference observed between successful and unsuccessful novices in terms of their working memory. However, since Item R2 (Figure 4-13) forced participants to keep an accurate account of all parts of the molecule in working memory, mental rotation imposed more cognitive load on unsuccessful problem solvers. One possibility is that unsuccessful novices were unable to chunk pieces of the molecule in the same way that successful novices could. For example, Cranford and colleagues (2014), assert that novice organic chemistry students may look at the structure of a molecule and see distinct atoms, distinct bonds, and electron pairs. Unfortunately, when a representation is viewed from this perspective, the total cognitive load associated with this representation may be quite high, and leaves little free working memory capacity for the actual manipulation (such as through mental rotation) and use of the representation to solve problems. However, as expertise begins to develop, the molecule may now be viewed as clustered groups of atoms, bonds, and electrons. When the representation is viewed in this way, the overall cognitive load associated with using it is substantially decreased, which allows more cognitive resources to be allocated to other aspects of the problem-solving process (Cranford et al., 2014).

Furthermore, mental rotation speed may have accounted for some differences between successful and unsuccessful novices. Both Howard and Vanessa, who had been identified as poor rotators, were unable to solve Item R2 (Figure 4-13) in the given time. Consequently, the screen automatically advanced on them. Interestingly, these were the only instances for all items where a novice was unable to complete their solution process in the given time. Vanessa asserted that although she was unable to arrive at an answer, she felt that she could if given more time. Howard felt that having to manipulate the molecule, while keeping track of all the atoms was a difficult task to do within the given time.

As participants used holistic mental rotation strategies most frequently, it is likely that differences in their abilities to use such strategies accounted for the largest differences between successful and unsuccessful novices. However, as mentioned previously, in a few instances some novice participants attempted to use strategies other than mental rotation. Though, they were largely unsuccessful in their efforts to apply an analytic strategy correctly.

On this note, novices may have been reluctant to use analytic strategies because they had not practiced them enough to be confident with using them. Other reasons for students' limited attempts at using analytic strategies could be that these strategies were not readily obvious to novices or were more difficult for them to apply. For example, for some items, participants could determine the absolute configuration, R or S, of both molecules to determine whether they were identical or enantiomers. However, determining the absolute configurations for both molecules within the given time may have been more challenging for these novices than attempting to rotate them mentally. This inference is supported by statements made by David, a moderate rotator:

> I think the flipping molecules visually is easy, but assigning S or R is kind of tough because you have to remember which way it is facing to do it in the correct order and all that stuff. Relationship is about imagining in your head. And as long as you understand how the groups are supposed to move in relation to each other, you have it right. With the S and R you have to remember some extraneous factors like clockwise and counterclockwise. If you are having a bad day and get them swapped you kind of screw yourself over.

Consequently, unsuccessful novices may not only struggle with mental rotation, but may also struggle when attempting to apply alternative analytic strategies. To help students be more successful with using analytic strategies, Stieff (2007) recommends training students to use these strategies and calls for greater attention to be placed on the use of analytic strategies during instruction to benefit students who apply visuospatial strategies inappropriately.

For some absolute configuration problems, C1 through C5 (see Appendix D), the ability the ability to mentally rotate the molecule also played a key factor in success. As discussed in the previous section, one of the key steps in solving these types of problems involves the correct placement of the lowest priority groups. For example, Ruthie, a poor rotator, did not take into account the position of the hydrogen atom on item C1 (Figure 4-5):

> **Ruthie:** Carbon 2 was the only one that had four different groups attached, and the configuration would be S – the OH and the $CH_2CH_3$ next and then the $CH_3$ and then the H.

Although she had determined her priority groups in the correct order, Ruthie made no mention that she had considered the position of the hydrogen atom. On the other hand, Kimberly, also a poor rotator, realized that the molecule was not positioned so that the lowest priority group was pointed away from her. However, she was unable to mentally rotate the molecule in the correct way. Ultimately, mental rotation played a key difference between successful and unsuccessful novices on this item – that is, unsuccessful novices did not or could not mentally rotate the molecule as part of their solution process.

In most of the other cases for the configuration items, novices were unsuccessful largely because they did not consider key features of the molecules. This pattern was supported by eye-tracking data discussed in the previous section. In some instances, unsuccessful novices failed to carefully inspect groups attached to the carbons that they considered to be chiral. For example, in Item C3, 53% of novices erroneously determined carbon 2 and carbon 4 (or at least one of these) to be chiral. It was only after inspecting the groups more carefully, when determining the configuration, that most of the unsuccessful novices (75%) realized that these carbons did not contain the necessary requirements (4 different groups) to be chiral. Vanessa's description was a good example of this:

> **Vanessa:** So there are 2 chiral centers – 2 and 4.
> **TK:** What's the configuration?
> **Vanessa:** Okay, just carbon 4.
> **TK:** What's the configuration?
> **Vanessa:** Wait…are there no chiral centers? Is that an option?
> **TK:** Yes. Okay why no chiral centers?

> **Vanessa:** I was thinking 2 and 4…but these two are both $CH_3$ groups.
> **TK:** So you only discovered that when you tried to determine the configuration?
> **Vanessa:** Yeah when I tried to do R and S. There are two $CH_3$ groups – I wouldn't know which one had priority over the other.

While this type of stereochemistry problem may not be impacted by a student's mental rotation abilities, one other type of spatial ability factor – closure flexibility – may help to account for differences between successful and unsuccessful novices. Closure flexibility is concerned with the speed of apprehending and identifying a visual pattern, often in the presence of distracting stimuli (Wu & Shah, 2004). In some stereochemistry problems, such as Item C3, participants must observe that there is a pattern of repeating groups within the molecule. Making these types of observations may be difficult for some students. However, it is also plausible that some students have trouble with all the different ways that a methyl group can be represented, such as a line and as $CH_3$ in this case. Taber (2009) argues that organic chemistry uses a range of symbols in representations that learners must be able to interpret. Consequently, remembering all of these symbolisms can present challenges to novice organic chemistry students.

For Item C5 (Figure 4-8), six of the fifteen novices (40%) were initially drawn to carbon 2 as a chiral center. This was most likely since the wedged and dashed notation was used for groups attached to this carbon – which is often used to indicate directionality around chiral centers. However, again most unsuccessful participants (67%) realized their mistake when attempting to determine the configuration. Crystal, a poor rotator, admitted that she did not carefully inspect the identity of the groups before making the determination that it was a chiral center:

> **Crystal:** Carbon 2 would be a chiral center.
> **TK:** What is its configuration?
> **Crystal:** Actually, 2 is not a chiral center.

> **TK:** Okay. So why were you initially thinking it was a chiral center?
> **Crystal:** Just because I didn't notice that there were two methyl groups attached. I guess I just kind of went by it too fast.

Successful novices, on the other hand, were able to rule out carbon 2 as it did not meet the criteria of a chiral center. Furthermore, successful novices seemed to have a good grasp of the information conveyed by the representation. That is, before identifying carbon 3 as a chiral center, they needed to correctly infer that carbon 3 had a hydrogen atom attached, even though it was not explicitly shown. For a few of these novices, it appeared that they had trouble with this interpretation. This was reflected in Alicia's (a moderate rotator) comments:

> **TK:** Why isn't carbon 3 a chiral center?
> **Alicia:** Because I'm thinking that there is no hydrogen attached to carbon 3.
> **TK:** So what are the groups attached to that carbon?
> **Alicia:** OH and then carbon 2 and then carbon 4…

On this point, Taber (2009) reminds us that aspects of symbolic representation that are familiar and taken for granted by experts are not always well understood by students. Therefore, it is not surprising that some novices had trouble remembering that an additional hydrogen is attached to carbon 3. This may further suggest that some students have trouble constructing well-structured 3-D mental images from 2-D drawings.

### Q3B: Experts versus Novices

We now turn our attention to expert stereochemistry problem solvers. While novice organic chemistry students preferred holistic strategies, expert chemists shifted between strategies more frequently. It appeared that experts were able to readily recognize patterns when solving stereochemistry problems, often prompting them as to which strategy type may be more appropriate. Recognizing such patterns seems to develop from experience with solving these types of problems. For example, when solving Item R5 (see Appendix C), Mr. Green (an expert) simply looked at the pattern of dashes and wedges, noting that if the chiral centers are shown in the same position for both molecules but are pointed in the exact opposite direction for one of the molecules, then the two molecules are enantiomers:

> **Mr. Green:** Enantiomers. For this one, I'm looking at the wedges and dashes being opposite for both and it isn't otherwise…like you can't rotate it to where they line up.
> **TK:** Did you try to rotate this one?
> **Mr. Green:** No. I was just looking the dashes wedges being opposite for both. If all of the chiral carbons…. if one group is shown pointing opposite and the other group is also shown as the opposite wedge or dash and it's not a meso compound, then they have to be enantiomers. So no, I did not try to rotate it.

This is similar to when expert chess players carry out an initial 'perceptual phase,' where they become familiar with the structural patterns of the pieces before starting to look for a good move in the 'search phase' of the problem-solving process (Simon & Chase, 1973). Expert stereochemistry problem solvers seem to also inspect the 'board' for patterns in an attempt to determine the most appropriate move (strategy). The strategy chosen by an expert seemed to be the one that imposed the least amount of cognitive load on their part, which was often an analytic strategy. For example, one graduate student seemed to use mental rotation strategies as a last resort during the interview session:

> **TK:** It appeared that you used strategies other than mental rotation whenever possible. Would it be accurate to say that you use mental rotation as a last resort?
> **Ms. Scarlet:** Yes. Trying to rotate a molecule in my head doesn't work out so well for me. I can't rotate it unless it's an easy flip. And rotating circularly in any way is beyond me.

Indeed, novices overwhelmingly used mental rotation strategies on configuration items, while experts tended to use simpler analytic strategies to arrive at the same answer. Based on descriptions of their solution strategies (Table 4-12), Item C1 was a good example of this distinction. For this item, holistic strategies included mentally repositioning the molecule from a stationary point of view (allocentric spatial processing), or mentally repositioning themselves to view the molecule from a different perspective (egocentric spatial processing). On the other hand, an analytic strategy could also be used to avoid any form of mental repositioning – the problem solver could determine the configuration using the arrangement of the groups as presented, but the actual configuration would be opposite of the one obtained through this method. As can be seen from Figure 4-12, for this item, all successful novices reported that they had used a holistic strategy to get the molecule into the proper orientation for determining absolute configuration. Unsuccessful novices on the other hand, made no mention of the direction in which the lowest priority group was pointed. Conversely, when looking at the strategies for solving this item used by experts, 9 out of 10 experts (90%) used an analytic strategy. This analytic strategy was as follows: first, determine the configuration for the molecule as presented, and then give the ‘opposite’ answer. That is, if they determined the absolute configuration as *S*, then the actual answer was *R*. Ms. Scarlet’s explanation clearly shows this strategy:

> **Ms. Scarlet:** 2 is chiral. The OH group gets priority, then the carbon labeled as 3, and then the carbon labeled as 1 and then the hydrogen. But its opposite, so what I did was I determined the configuration normally and then whatever letter I said, I flipped it. So, looking at my finger, I am going counterclockwise. So, because the H is coming at me, the opposite would be clockwise, so R.

The only expert who used a holistic strategy to determine the configuration actually followed up with an analytic strategy to verify that his solution to the problem was correct:

> **Mr. Blue:** To kinda check that that made sense, I determined the configuration again, the way it is here, knowing that if the lowest priority group isn’t pointing

> back then it’s going to be the opposite configuration. So I can confirm my answer to myself. So in the first method I rotated the molecule and then I checked my answer using the second method.

This is in keeping with Gluck and Fitting (2003) who proposed that individuals often use more than one strategy to solve a task, for example, to double-check a solution. Indeed, as seen in their descriptions of solution strategies (Table 4-13), some expert stereochemistry problem solvers employed multiple strategies during the problem-solving process. For example, on Item R2 (Figure 4-13), Mr. Blue and Mr. Green reported that instead of rotating the molecules to determine if they were identical, they only rotated the molecule on the left enough to get it into the appropriate position for determining the absolute configuration. Once the molecule on the left was rotated in the appropriate orientation, they used the Cahn-Ingold-Prelog rules (Cahn et al., 1966) to determine the configuration of both molecules. When asked about why this was, Mr. Green (expert) admitted that he did not want to rely on his visualization ability solely, when an analytic strategy was simpler to use:

> **Mr. Green:** I try to rotate it enough so that I can be confident in determining configuration. I don’t want to trust my visualization ability, when I know I can just determine R/S.

It appeared then that some experts used one strategy only enough to then continue the problem-solving process with another strategy. Star and Rittle-Johnson (2008) argue that an important learning outcome in problem-solving domains is the development of flexible knowledge, where learners know multiple strategies and are able to apply them adaptively to a range of situations. Consequently, this flexibility in strategy choice is often a hallmark of expertise (Hegarty, 2010; Star & Seifert, 2006).

While some experts attempted to use analytic strategies whenever possible, for some items it appeared that holistic strategies were preferred. It is possible that for some items, an analytic strategy was not practical to use. For example, on Item R4 (see Appendix C), to determine the relationship between the molecules, using the analytic strategy of determining the absolute configuration, they had to determine the configuration of the two chiral centers in each molecule. This ‘double duty’ may have imposed more cognitive load than attempting to use the holistic strategy. Furthermore, this is consistent with assertions by Hirnstein and colleagues (2009) that solving mental rotation tasks using analytic strategies often takes more time and can therefore lead to poorer performance on tasks which include time restrictions. However, according to Star and Rittle-Johnson (2008), expert problem solvers know which strategies are more efficient than others under particular circumstances.

Therefore, experts seemed to make judgments about which strategy would be more effective, before applying a strategy (or multiple strategies) in a way that novice participants did not. While novices appeared confined to one strategy, most experts could transition seamlessly between the two strategies:

> **TK:** Why did you switch your approach this time?
> **Mr. Blue:** On that last question, I second guessed myself, even though I ultimately came to what I believe the correct conclusion. I thought, let’s see if trying it a different way would get me to a more solid conclusion in my mind. And ultimately, I still did the rotations around one axis. In this case, I first rotated it keeping the chlorine in the same spot and then rotated it keeping the hydrogen in the back. So, I guess in the end, I wound up doing the same thing, but just the fact that I was second guessing myself at all made me want to try something new.

This strategy agrees with Hegarty (2010) who points out that flexibility in strategy choice between visualization and a more analytic thinking process is one important component of spatial ability. That is, individuals with high spatial levels can readily switch between a more visual strategy and an analytic strategy.

In this current study, novices did not seem to exhibit as much flexibility in their strategy choice. For only one item, Item R1 (Figure 4-10), did a substantial amount of novice problem solvers attempt to use an analytic strategy. However, for many of these novice students, these analytic strategies failed. Over time, these novice stereochemistry problem solvers might become more comfortable with using analytic strategies, providing an alternative to the more cognitively challenging holistic strategies. When questioned about why they failed to utilize more well-known analytic strategies, it appeared that they had not encountered these strategies during lecture. It seemed that the course instructor had emphasized mental rotation strategies over analytic strategies. There may have been a good reason for this, as one expert participant recounted his past experiences where using an analytic strategy to determine absolute configuration had resulted in problems:

> **Mr. Green:** Switching my answer rather than attempting to rotate the molecule has gotten me in trouble in the past. For example, when I forget to do the switch to my answer or I am trying to assign eight chiral centers all at once and I forget to do the opposite for some.

It is not clear why there was little focus on analytic strategies during the lecture, however, if analytic strategies are not taught during the lecture, novices, such as Donald (moderate rotator) may be afraid to venture out and try these strategies on their own:

> **TK:** Why do you rotate the molecule instead of switching your answer in situations like this?
> **Donald:** I remember the instructor saying you have to grab the hydrogen and bring it to the back before you can determine the configuration.
> **TK:** But if you know it’s gonna be the opposite, why not just change your answer?

> **Donald:** I guess it's just reassurance. I'm still not comfortable with figuring it out and so I guess it's just my way to check for sure. The way we learn it in class, and especially for students like me who this is their first time taking an organic chemistry class, the way we are taught...I don't wanna say that it's set in stone...but venturing out to use another method is kinda dangerous, especially since right now I'm not as well versed in solving these types of problems.

Since many of the experts interviewed in this study relied on analytic problem-solving strategies, it is unclear whether these novices who had not been shown analytic problem-solving strategies were placed at a disadvantage. Although continued practice with the mental rotation of molecules may help these novice students, it is also plausible that poor rotators may never be able to solve some items correctly using holistic mental rotation strategies.

The fact that many experts favored analytic strategies over holistic mental rotation was surprising for several reasons. First, it was believed that accurate mental rotation abilities would be one trait possessed by experts as it relates to solving stereochemistry problems. However, in many cases, experts attempted to avoid mental rotation at all costs. Additionally, the researcher expected that mental rotation abilities of problem solvers would be one of the major distinguishing factors between expert and novice problems solvers. However, as many experts appear to frequently shift between these two strategies, strategy choice on stereochemistry problems may be an even more important contributor to success.

## Research Question 4

Are novice students' spatial strategies for solving mental rotation tasks related to their achievement on the ACS organic chemistry examination?

The final research question involved examining whether a student's spatial strategies for solving mental rotation tasks were related to their performance in an organic chemistry course. To do so, the relationship between MRT-A performance (both classification and total score) and ACS organic chemistry exam scores (total raw score, stereochemistry sub-score, and non-stereochemistry sub-score) were investigated. According to Table 4-17, several interesting relationships were found.

First, there was a moderate, positive correlation between MRT-A Total Score and ACS total raw score ($r = .314$, $n = 56$, $p = 0.019$). This suggests that students with higher spatial abilities performed better on the 2010 version of the ACS Organic Chemistry examination than those with lower spatial abilities. This result is consistent with a correlational study in which a slight ($r = 0.209$, $p < 0.05$) but significant relationship between mental rotation as measured by the Purdue Visualization of Rotation Test (PVROT) and achievement on the 2004 version of the ACS organic chemistry exam (Harle & Towns, 2010).

Next, for the stereochemistry sub-score, its relationship with the MRT-A total score was not significant ($r = 0.211$, $n = 56$, $p = 0.119$). This result was surprising because both variables directly involved spatial abilities. However, Hegarty (2010) made the assertion that although students with high spatial abilities may perform well on psychometric measures of spatial visualization tasks, this ability does not automatically translate into their ability to imagine structures and processes on much more complex tasks (such as problems related to stereochemistry).

Alternatively, this could support the assertion by Uttal and Cohen (2012) that as domain specific knowledge increases, the need for the abilities measured by typical spatial ability tests tend to diminish. In this study, one possibility is that during the remainder of the semester the students learned to apply more analytic strategies for solving stereochemistry problems. In a study conducted by Stieff et al. (2012), in the beginning of the course, students tended to use more holistic strategies. However, by the end of the course there was an increased use of analytic strategies. Furthermore, it was found that students with high spatial abilities continued to use more holistic strategies, while students with low spatial abilities shifted to using more analytic strategies. Therefore, some students may have used strategies other than mental rotation to successfully solve stereochemistry items on the ACS organic chemistry exam and so there was no direct relationship found between mental rotation ability as measured by the MRT and the ability to solve stereochemistry problems. According to Stieff (2007), "mental rotation skill is not a prerequisite for organic chemistry…students who use mental rotation can learn to apply analytic strategies to solve the same tasks with equal accuracy and efficiency as mental rotation" (p. 233). This may be especially true for stereochemistry tasks, where analytic strategies are often emphasized during instruction.

On the other hand, it was interesting that there was a moderate, positive relationship between MRT-A total score and the non-stereochemistry sub-score (Table 4-17). This suggests that overall, students with higher spatial abilities perform better on concepts within an organic chemistry course than students identified as having low spatial abilities. It is not readily apparent how spatial abilities impact students' performance in areas of organic chemistry that are non-spatial in nature; however, these findings are consistent with findings of other studies. For example, in a general study of spatial abilities and problem-solving skills, Bodner and McMillen (1986) investigated general chemistry students' performance both on spatial and non-spatial items. Their study found that high levels of spatial abilities were significantly correlated with performance on all item types – both spatial and non-spatial. That is, spatial abilities partially explained students' performances on non-spatial chemistry problems as well as the spatial chemistry problems. Furthermore, Carter et al. (1987) found that students with high spatial ability appeared to have higher scores on novel problems that required problem solving skills rather than rote memory. It follows that on a standardized examination, such as the ACS organic chemistry examination, students are presented with a wide range of novel problems since these problems are not written by their course instructor. Thus, those students with high spatial abilities may have used them to solve the many novel problems on the ACS final examination.

Wu and Shah (2004) provided several possible explanations as to why some studies have found correlations between spatial ability and non-spatial problems, which may provide some insight into the current findings. One explanation that provides support for these findings is that problem solvers restructure problems mentally in their spatial domain when solving chemistry problems (Wu & Shah, 2004). Furthermore, although some problems may be perceived as being non-spatial in nature, these problems may actually involve spatial thinking. Additionally, the comprehensive use of visual representations for both spatial and non-spatial questions may require students to utilize their spatial thinking skills in order to answer the questions (Wu & Shah, 2004). Finally, it has been shown that high spatial ability students tend to draw figures while problem solving, which seemed to help them solve problems, even though the drawings were not required by questions. On the other hand, low spatial ability students drew fewer figures and were more likely to have incorrect drawings with non-symmetric and inappropriate structures (Pribyl & Bodner, 1987; Wu & Shah, 2004).

In this study, stepwise regression was used to evaluate the influence of gender and MRT-A score on total ACS exam score (Table 4-18). It was found that gender did not make a significant contribution to total ACS exam score ($b$ = -.193, t(54) = -1.451, p = 0.153). However, MRT score was a significant predictor of total ACS exam score ($b$ = 0.503, t(54) =2.949, p = 0.005). This was interesting because a student's performance on the MRT at the start of the semester could be used to predict their performance on the ACS examination overall. However, upon further analysis, MRT score was only found to be a significant predictor of non-stereochemistry sub-score ($b$ =0.437, t(54) = 2.693, p = 0.009), but not a significant predictor of their performance on the ACS stereochemistry sub-score ($b$ = 0.066, t(54) = 1.584, p = 0.119). Although an unexpected finding, this may support the idea that as expertise develops, there is a shift to more analytic strategies to solve spatial tasks (Stieff et al., 2012). That is, by the end of the semester, as students have become more familiar with applying analytic strategies, they are able to depend less on their spatial abilities to solve stereochemistry problems.

When looking at how students' strategies for solving items on the MRT impacted performance on the ACS examination, there was a non-significant difference for the strategy groups on the ACS performance measures of stereochemistry and non-stereochemistry sub-scores (Table 4-19). Therefore, it appears that performance on the MRT was a more important marker of success on the ACS exam than was strategy group. However, one of the limitations for answering this research question was the small sample size (n =56). Unfortunately, the course instructor inadvertently administered the incorrect examination in one of the sections and so results could only be used for the section that received the correct version of the exam. Consequently, this may have resulted in insufficient power to detect significant differences. With a larger sample, significant differences may have been found between the groups for scores on the ACS examination.

## Overall Conclusions

This study investigated differences in the cognitive strategies of expert and novice students while solving organic stereochemical problems. Eye-tracking data pointed quantitatively to differences in eye-movement patterns for expert and novice participants. Further, eye-movement patterns differed for successful and unsuccessful novices. As eye movements can be considered direct and non-biased indicators of attentional allocation, and attentional allocation is one indicator of cognitive activity (Tai et al., 2006), these results shed some light into key differences in cognitive processing of information during stereochemistry problem solving.

For the set of relationship items (R1 through R6), there was a pattern of fewer transitions for experts as compared with novices. While eye tracking does not inform the researcher as to why a participant looks in a certain region, it may have pointed to differences in the working memory of experts and novices. As experts are able to chunk information, this allows them to hold more pieces of information within working memory and reduces the amount of times that they transition between molecules in order to refresh information. However, from qualitative data, it appeared that experts frequently used analytic strategies when determining the relationship between two molecules. Novices on the other hand, used mental rotation strategies more consistently. Consequently, it is also plausible that experts made fewer transitions because they used analytic strategies. Such analytic strategies minimize the need to keep parts of both molecules fresh within working memory, which is supported by fewer number of transitions made during problem solving.

While it was expected that differences in an individual's ability to determine the relationship between two molecules would be explained by their ability to mentally rotate the molecules, as expertise develops, it becomes possible to rely less on these abilities. That is, some experts seemed to use analytic strategies whenever possible, instead of mental rotation strategies. Therefore, for students who may struggle with mental rotation, all hope may not be lost. To a certain extent, analytic strategies can be learned, which can help to compensate for a student's inability to mentally rotate a molecule. Even if mental rotation is not something that students struggle with, analytic strategies may be advantageous as they may reduce the cognitive load of a problem, which allows the problem solver to use fewer cognitive resources or devote them to other aspects of the problem-solving process.

Overall, the importance of mental rotation cannot be minimized for solving stereochemistry problems. In this study, experts still often needed to use their mental rotation strategies during the problem-solving process. Experts appeared to use this strategy in cases where an analytic strategy was not practical, or as a 'stop-gap measure' until they could continue the problem-solving process using an analytic strategy. For novices who frequently employ mental rotation as their strategy of choice, mental rotation abilities appear to be of even greater importance. Until novices become familiar with alternative strategies, they rely on these mental rotation abilities. Consequently, it is at this point that mental rotation abilities may account for the largest differences between successful and unsuccessful novice stereochemistry problem solvers.

For the configuration items (C1 through C5), eye-tracking data also showed different eye movement patterns for successful and unsuccessful novices. For example, unsuccessful novices fixated less on key features of the molecule, such as lowest priority groups, when they were attempting to determine the configuration. Failure to take into account such features adversely impacted performance on these items.

In addition to eye-tracking methodology, this study utilized a phenomenographic approach to characterize the qualitatively different ways that novices solve stereochemistry problems. For the purpose of comparison, expert chemists were also interviewed about their strategies for solving stereochemistry problems. Summaries of novice and expert patterns for solving stereochemistry problems are provided in Figure 4-17 and Figure 4-18 respectively. While most novices appear confined to using holistic strategies, experts are much more flexible in their strategy choice and often select the strategy that imposes the least amount of cognitive load on their part. As expertise in solving stereochemistry problems develops, the problem solver begins to recognize patterns that may influence their strategy choice. Furthermore, experts are able to use multiple strategies to solve a stereochemistry problem and become more comfortable with shifting between strategies across items.

This study also investigated how representation type impacted performance on stereochemistry problems. In this dissertation study, novices overwhelmingly preferred using molecular models over two-dimensional representations to solve stereochemistry problems such as determining the configuration of chiral centers. Furthermore, performance was improved when novices were allowed to use a model kit. That is, more novices could solve the three-dimensional problem than the corresponding two-dimensional problem. However, it should be noted that not all students improved their performances with the model kit and some students actually preferred solving the stereochemistry problems using 2-D representations.

Finally, this study looked at the relationship between students' performance on the MRT-A instrument (at the start of the semester) and the 2010 version of the first semester ACS organic chemistry examination. There was a significant relationship found between these two performance measures. However, upon further analysis, MRT score correlated with non-stereochemistry sub score, but did not correlate with stereochemistry sub-score on the ACS organic chemistry examination. Two possibilities may exist to explain this phenomenon. First, through practice, students may become more adept at solving spatial problems. That is, students – especially those who may be identified as slow or moderate rotators – may become more comfortable with using holistic mental strategies during the semester. Consequently, by the time they took the ACS examination at the end of the semester, there were no appreciable differences between strategy groups for solving stereochemistry problems. Alternatively, there may have been a shift to specialized analytic strategies for solving stereochemistry problems during the semester. Such a shift to analytic strategies would result in students identified as being adept at mental rotation (such as fast and moderate rotators) now having several methods in their arsenal for solving stereochemistry problems on the ACS final examination. Other students (such as poor rotators) may now be more comfortable with using an analytic method for solving stereochemistry problems. As the experts in this study tended to favor analytic strategies, the latter explanation may be more likely.

## Limitations of This Study

The results of this study must be interpreted with respect to its limitations. One important limitation was the relatively small sample size for the eye-tracking study. Although the sample size was small, it is not uncommon for eye-tracking studies (Havanki & VandenPlas, 2014). Eye-tracking methodology is labor intensive, and it produces copious amounts of data even with small numbers of participants (Havanki & VandenPlas, 2014). Nonetheless, the small sample size may have limited several aspects of the study. Specifically, the statistics comparing eye-movement data between groups of interest were difficult to interpret because of the small size of each group. For example, although eye-tracking metrics showed a pattern of differences for some groups, these differences did not reach statistical significance. It is possible that a larger sample size may give more power to detect such differences.

Next, this study utilized retrospective think-aloud methods, where participants were asked to recall their thought processes immediately after they had solved each problem. While the participant described their strategies immediately after solving the problem, they may have left out key steps in their solution process when describing their strategies. Consequently, this factor may have impacted the conclusions drawn from these descriptions.

## Implications for Chemistry Instruction

The current findings have several implications for how we teach chemistry. Eye-tracking and qualitative data suggest that expert and novice problem solvers differ in their strategies for solving stereochemistry problems. Experts tend to be more flexible and to select the strategy that imposes the least amount of cognitive load on their part, which is frequently an analytic strategy. Consequently, novice organic chemistry students may benefit from an increased emphasis on analytic strategies during instruction. As instruction may influence the strategies that students use, presenting a focused number of analytic strategies for solving stereochemistry problems and providing opportunities to practice these strategies may be most beneficial to students, especially those who may be classified as analytic or as poor rotators. Analytic strategies may also be beneficial for students that are adept at mental rotation who over time may learn to shift between analytic and holistic strategies as needed. Therefore, such alternative strategies may be advantageous for all students.

However, there may be a downside to these analytic strategies. While analytic strategies may help students to solve a problem correctly, they may do little to help students to visualize the three-dimensional arrangement of atoms or the spatial relationships between molecules. Furthermore, using these procedures may not provide opportunities for visualization or spatial ability skills to be improved through practice. Therefore, instructors must decide whether visualization is most important for their students when determining the relationship between molecules or whether it is more important for them to simply arrive at the correct answer.

One other implication for chemistry instruction is to provide opportunities for students to become familiar with physical models such as molecular model kits, either through demonstration by the instructor or through direct manipulation by the students themselves. In this study, most students benefitted from the use of a model while solving stereochemistry problems. However, it appears that students must have experiences with models or they are not able to tap into the advantages of molecular model kits. Furthermore, if molecular models are not practical for students due to cost, having to carry it around all the time, or the time it takes to build them – their hands may serve as an ideal substitute. A student's hands cost nothing to use, are always with them and can be 'assembled' into a model more rapidly than a molecular model can. Instructors may also want to consider allowing students to use model kits during quizzes and examinations. If students practice with model kits, they may benefit from being able to use them while problem solving. Knowing that some students struggle with mental rotation, allowing students to use model kits may help reduce the cognitive load of various problems, especially those related to stereochemistry.

In addition to the use of physical models, students may benefit from instructors emphasizing features of molecules that are key for solving stereochemistry problems. For example, ensuring that the lowest priority group is pointed in the appropriate direction and ensuring that 'implicit hydrogens' are taken into account when determining absolute configuration. Instructors should assess their students' abilities to identify such features of simple molecules, before moving on to more complex molecular structures.

## Implications for Future Research

In terms of future research, there are several aspects that may be worth considering further. The first of these is to investigate the extent to which instruction influences strategy choice and performance when solving stereochemistry problems. As instructors can choose to emphasize using either holistic or analytic strategies, how are organic chemistry students impacted when instruction emphasizes one strategy over the other for solving stereochemistry problems? Do students benefit more from increased focus on analytic strategies over holistic strategies?

Furthermore, only one component of spatial ability – mental rotation – was investigated in relation to performance on stereochemistry problems. However, as mental rotation is only one component of spatial ability, it may be interesting to look at how other components of spatial ability impact performance on stereochemistry problems. Furthermore, as a significant relationship was not found between performance on the MRT and stereochemistry sub-score on the ACS organic chemistry examination, using multiple spatial ability measures may help to paint a clearer picture of the relationship between spatial ability and performance on stereochemistry items.

Next, one other theme that may be worth exploring is the extent to which learning disabilities have an impact on chemistry students' spatial abilities and by extension their ability to solve visuospatial problems. Some participants mentioned struggling with stereochemistry problems due to learning disabilities such as dyslexia. This may help to provide an even better understanding of the ways that learning disabilities impact students enrolled in organic chemistry courses.

Additionally, it may be of interest to follow students identified as poor rotators throughout their chemistry journey. That is, how do their spatial abilities impact them in future chemistry courses. What are the ways by which they find to cope with their inabilities to perform visuospatial tasks in advanced chemistry courses? Do their struggles with spatial abilities continue to adversely impact them or are their spatial abilities improved over time with experiences in chemistry courses?

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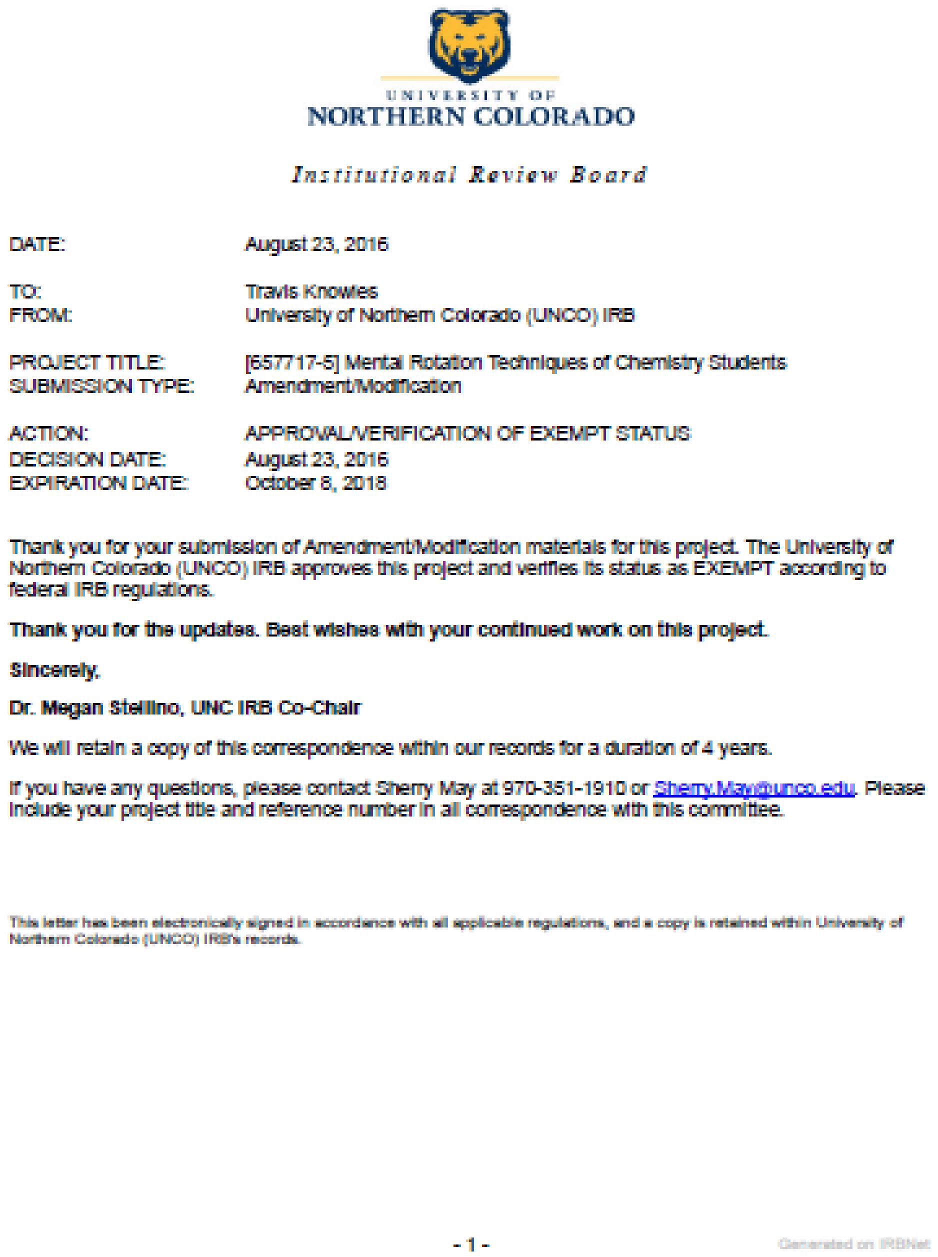
# APPENDIX A

# INSTITUTIONAL REVIEW BOARD APPROVAL LETTER



UNIVERSITY OF
NORTHERN COLORADO

*Institutional Review Board*

DATE: August 23, 2016

TO: Travis Knowles
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [657717-5] Mental Rotation Techniques of Chemistry Students
SUBMISSION TYPE: Amendment/Modification

ACTION: APPROVAL/VERIFICATION OF EXEMPT STATUS
DECISION DATE: August 23, 2016
EXPIRATION DATE: October 8, 2018

Thank you for your submission of Amendment/Modification materials for this project. The University of Northern Colorado (UNCO) IRB approves this project and verifies its status as EXEMPT according to federal IRB regulations.

**Thank you for the updates. Best wishes with your continued work on this project.**

**Sincerely,**

**Dr. Megan Stellino, UNC IRB Co-Chair**

We will retain a copy of this correspondence within our records for a duration of 4 years.

If you have any questions, please contact Sherry May at 970-351-1910 or Sherry.May@unco.edu. Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.

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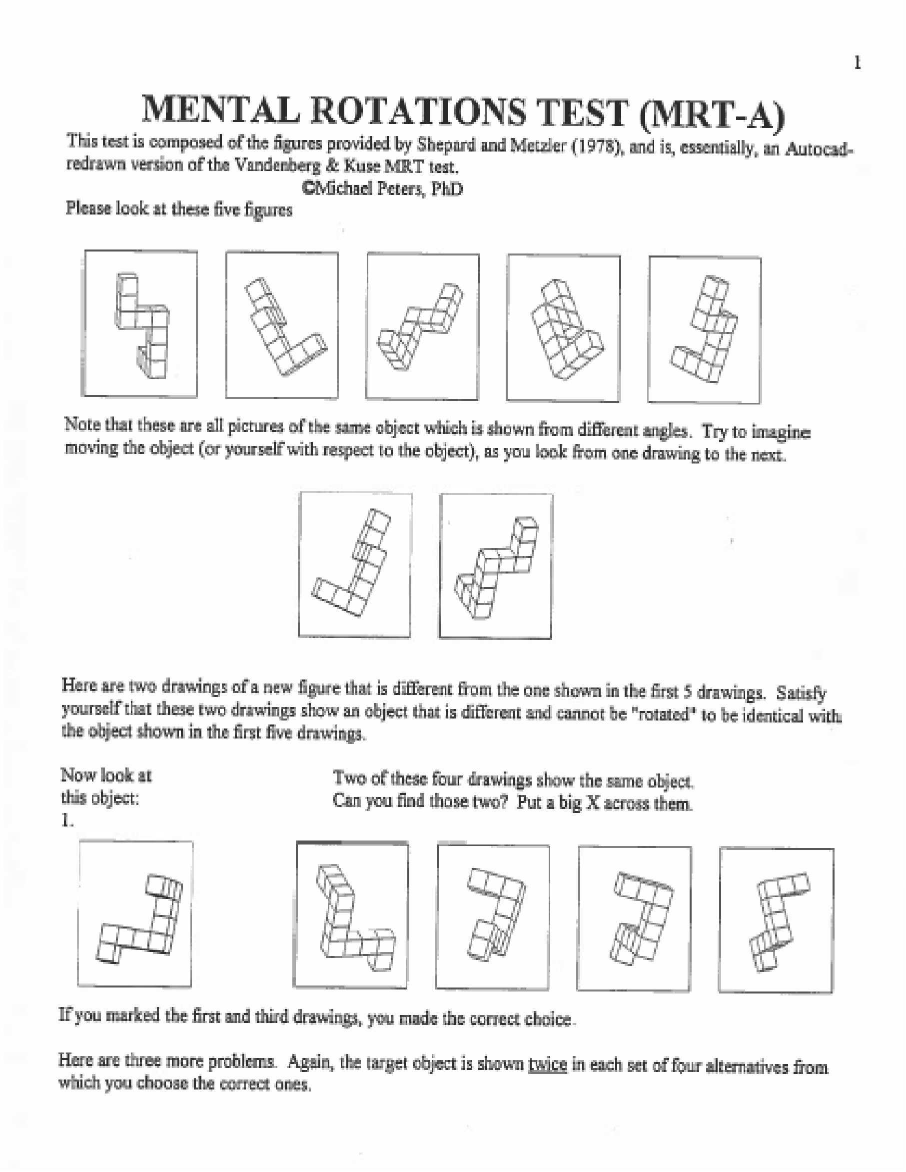
# APPENDIX B

# SAMPLE ITEMS FROM THE MENTAL ROTATIONS TEST



# MENTAL ROTATIONS TEST (MRT-A)

This test is composed of the figures provided by Shepard and Metzler (1978), and is, essentially, an Autocad-redrawn version of the Vandenberg & Kuse MRT test.

Please look at these five figures

Note that these are all pictures of the same object which is shown from different angles. Try to imagine moving the object (or yourself with respect to the object), as you look from one drawing to the next.

Here are two drawings of a new figure that is different from the one shown in the first 5 drawings. Satisfy yourself that these two drawings show an object that is different and cannot be "rotated" to be identical with the object shown in the first five drawings.

Now look at this object:

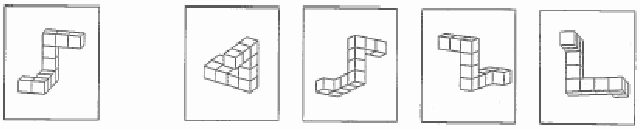
1.

Two of these four drawings show the same object. Can you find those two? Put a big X across them.

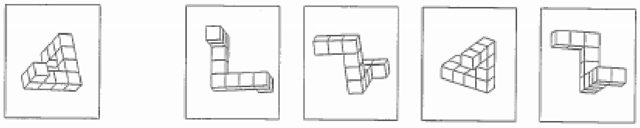
If you marked the first and third drawings, you made the correct choice.

Here are three more problems. Again, the target object is shown twice in each set of four alternatives from which you choose the correct ones.

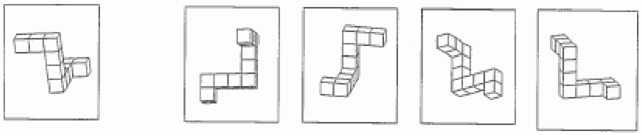
1.a



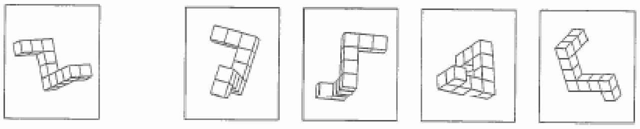
2.a



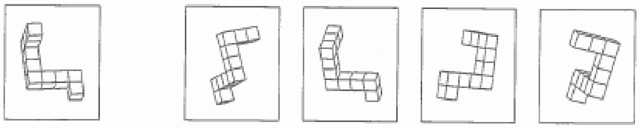
3.a



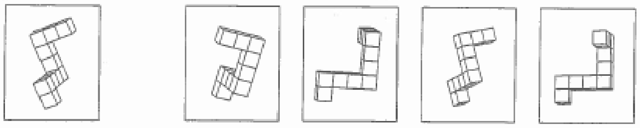
4.a



5.a



6.a

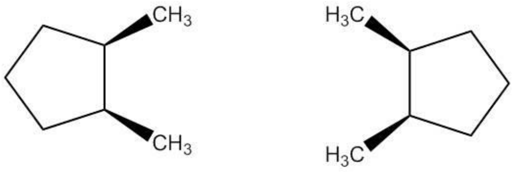


# APPENDIX C

# RELATIONSHIP ITEMS: ORGANIC MOLECULES USED IN THIS STUDY

R1:

Which of the following terms best describes the relationship between the pair of molecules shown?



A) Identical

B) Enantiomers

R2:

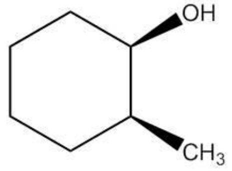
Which of the following terms best describes the relationship between the pair of molecules shown?

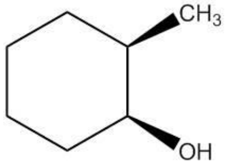
A) Identical

B) Enantiomers

R3:

Which of the following terms best describes the relationship between the pair of molecules shown?



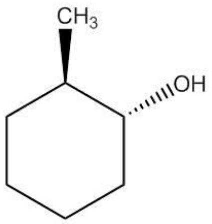


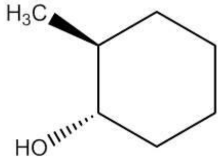
A) Identical

B) Enantiomers

R4:

Which of the following terms best describes the relationship between the pair of molecules shown?



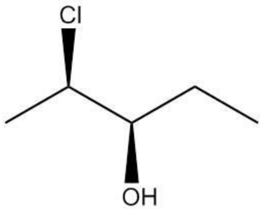


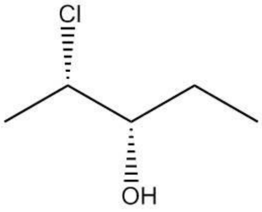
A) Identical

B) Enantiomers

R5:

Which of the following terms best describes the relationship between the pair of molecules shown?



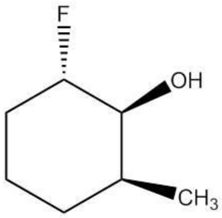


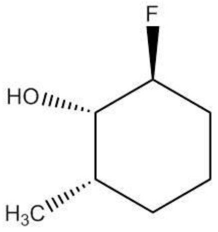
A) Identical

B) Enantiomers

R6:

Which of the following terms best describes the relationship between the pair of molecules shown?





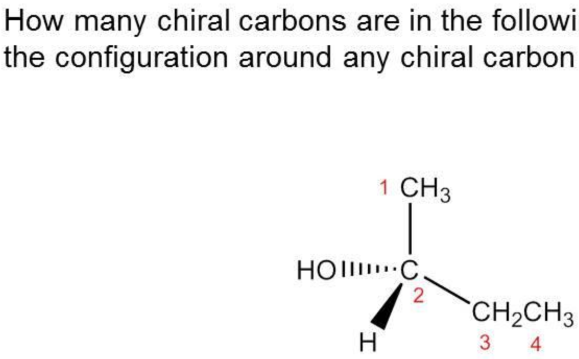
A) Identical

B) Enantiomers

# APPENDIX D

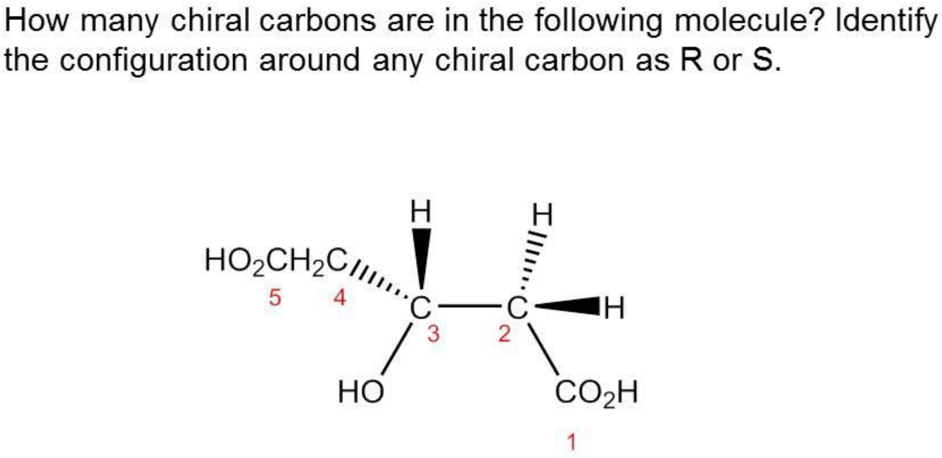
## ABSOLUTE CONFIGURATION ITEMS: ORGANIC MOLECULES USED IN THIS STUDY

C1:



How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

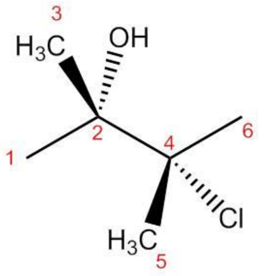
C2:



How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

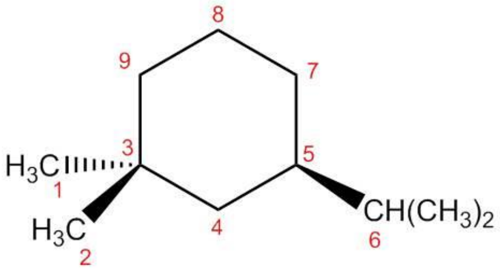
C3:

How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.



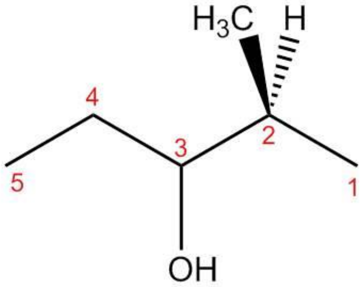
C4:

How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.



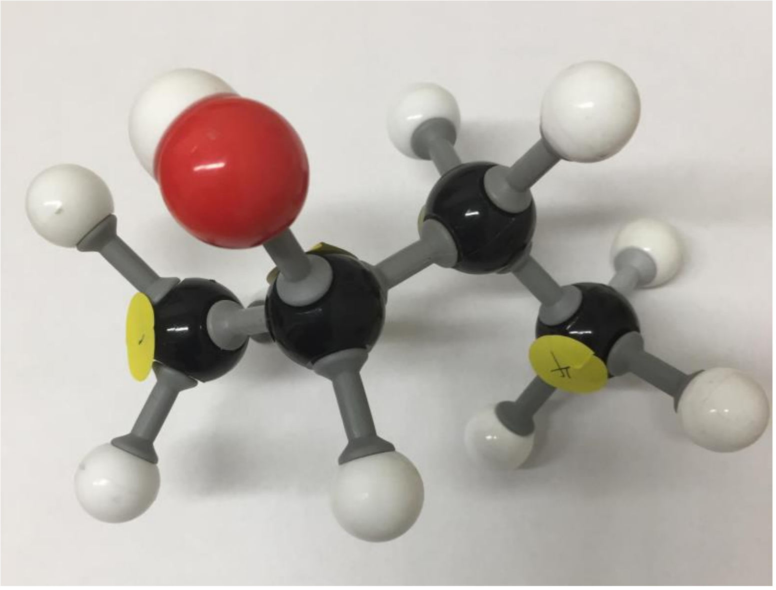
C5:

How many chiral carbons are in the following molecule? Identify the configuration around any chiral carbon as R or S.

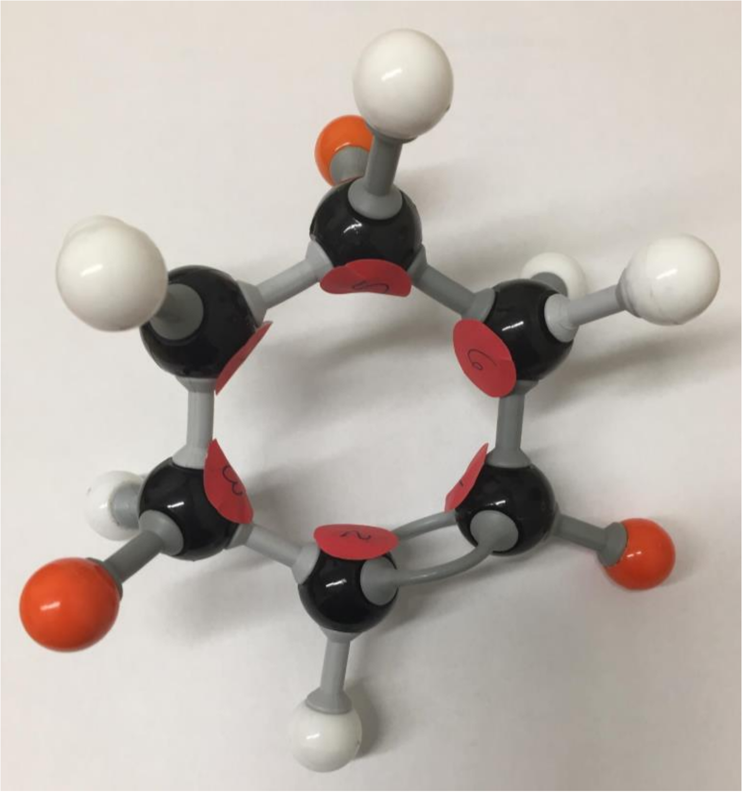


# APPENDIX E

# MOLECULAR MODELS: ORGANIC MOLECULES USED IN THIS STUDY



Molecule #1: (*S*)-Lactic Acid



Molecule #2: (3*S*,5*S*)-1,3,5-tribromocyclohex-1-ene

# APPENDIX F

# SAMPLE TRANSCRIPTS

Participant S-014

<u>Practice R:</u>
P: I believe they are enantiomers.
I: Why enantiomers?
P: Because even if you rotated it any certain way they couldn't be superimposed just because the CH is coming at us – well I guess if you rotated it. Well yeah if you rotated it they would be the same. I thought they were enantiomers because how they are now they are not superimposable.
I: As they are now but-
P: If you rotated them they would be superimposable so they are identical.
I: Remember you have to try to rotate them to see if you can get them to be identical. And if not they are enantiomers. Can you see – yeah now you can see they are identical.
P: Yeah.
I: So how would you have to rotate it be identical?
P: You would have to – so you would have to grab the central carbon and do it this way so the CH is coming at you, the H is going back and then your OH and CH2 are in opposite positions. Is that a good enough answer?
I: Yes. Let's go on.

<u>R1:</u>
P: These are identical because-
I: So why identical?
P: Because if you rotated it you could superimpose them.
I: Good. So those would be – how would you have to rotate it?
P: You would have to just like-
I: Turn in like in the plane of the paper?
P: Yeah.
I: Good. Let's go on.

<u>R2:</u>
P: These are enantiomers.
I: So why enantiomers?
P: Because even if you rotate it like – I guess if you rotate them just switched the molecule they would be identical. So can I change my-
I: Why?
P: If you like – this is hard because they are a mirror image but they are not mirror image because the bond or like the chemistry is different. So I am not one hundred percent.
I: Can those be mirror images of each other?
P: Yes.
I: Okay so they are – can you rotate them to be the same?
P: Yes.
I: How? How can you rotate them to be the same?
P: I think you just have to like go like this.
I: So if you flipped it over then?

P: It would be – I am sorry. I suck at this. Um if you flipped it over it would be non-superimposable because-
I: So they are non-superimposable.
P: Then they are enantiomers.
I: Then they are enantiomers.
P: Okay. Sorry.
I: You are fine. Let's go on.

<u>R3:</u>
P: So it is not a mirror image. They rotated it so it would be identical.
I: Why identical?
P: Because even – well it is not a mirror image. And even if you – I think it just because they are rotated like – it is not a change of stereochemistry.
I: So it is just rotated but not a change of stereochemistry. So you can rotate it to become-
P: Yeah. Like it is a change in stereochemistry but like you know what I mean? They are just rotated.
I: The configuration you mean?
P: Yeah.
I: So did you determine R and S?
P: You could because it is a chiral center.
I: But is that something you did?
P: No.
I: So you just tried to rotate it and saw you could rotate those to be identical? Is that what you said?
P: I guess they are not identical because here the Br and F are next to each other but here they are apart.
I: So could you rotate those – or how were you thinking of rotating them at first to be the same?
P: I was going to say bring the Br from behind forward.
I: Uh huh. So you were just looking at the Br but nothing else?
P: And the hydrogen because here the hydrogen is just in the plane and then went back. But the fluorine – I don't know. I am sorry. I really suck at these.
I: No you are fine. But what you did is you tried to rotate it to bring the bromine forward.
P: Yeah.
I: But you didn't pay enough attention to the other atoms.
P: Yeah.
I: So now looking at it you would think they are?
P: Enantiomers
I: Enantiomers. Okay. Can you get those two images to look like mirror images of each other? Is there any way?
P: No.
I: Well how do you know they are enantiomers?
P: Well the reason I said no is because like they are – I mean not different molecules but just the molecules are arranged differently around the center carbon. Like the Br and F are together here but they are not on the other one. So a mirror image is just flipping it.

I: Well to flip it to look like the mirror image.
P: Yes.
I: But can you flip one to look like the mirror image of the other? If you said they are enantiomers? No?
P: No.
I: Okay.
P: I am sorry.
I: So that one was just process of elimination.
P: So is it an enantiomer?
I: Yeah. So these should be enantiomers. But let's go on.

R4:
P: So these are identical.
I: Okay. Why identical?
P: If you rotate it – like if you turn it toward the CH3 above the OH – no that won't work. The reason I am struggling is if I do a mirror image of this one it is like I know you could not superimpose the mirror image onto that. So I think enantiomer but I am basically confused because it is not a mirror image. That is how I know how to do it.
I: Can you rotate those to become identical?
P: No. Because the OH and CH3 are flipped.
I: Can you rotate them in any way to become-?
P: Yes.
I: How?
P: This way.
I: So you flip it over?
P: Yes.
I: But if you flip it over is the OH pointing towards you?
P: No. It would be back.
I: And the CH would be?
P: So they are enantiomers. The CH3 would be forward. No the CH3 would be back too. So identical then? Right?
I: No.
P: They would be enantiomers?
I: Uh huh.
P: I thought if like you flipped it then the stereochemistry just changes but they are still identical.
I: If the stereochemistry changes then they are not identical.
P: So then they are enantiomers.
I: Yeah. So mirror images of each other.
P: How are they mirror images?
I: You would have to flip them to see that they are mirror images.
P: So mirror images you can flip more than just this way?
I: Uh huh.
P: You can flip them this way too?
I: Uh huh.

P: Okay. We were just taught to do it this way.
I: That is the only way? So just one flip?
P: Well yeah but some teachers have shown us to put a line there an flipped it then they would be enantiomers because if you flipped it this way the OH would be going back and the CH3 would be going back and you could not superimpose that onto the original.
I: Uh huh.
P: But then comparing it to this that is not the mirror image. That is what is screwing me up.
I: You mean as drawn now?
P: If I had to draw a mirror image I can figure it out but since I am given something that is not really the mirror image. Does that make sense?
I: Okay. So you are saying because you are not given something that is in the right orientation to look like the mirror image?
P: No. Like just like when I am saying it is a mirror image I know it is not superimposable. But if this was the mirror image flipped to this, they would be superimposable because my OH-
I: Are you trying to decide whether the one on the right is the mirror image like already or like – what id giving you problems? Let's try to understand that.
P: Like if I were to make a mirror image of this one based on what we talked about going this way, I would know the mirror image would be like – the CH3 and OH would be going back. And that's not superimposable into this. I would know it is an enantiomer. But like with this one-
I: The one on the right?
P: Yes. Since it is given to me where they are coming forward, I know that is not the correct mirror image. Do you know what I mean? Like I mean it is a mirror-
I: Can it be a mirror image? I might now be now but if you rotated any way can it be?
P: Yes.
I: That's your answer?
P: Yes.
I: Okay. Let's go on.

<u>R5:</u>
P: These are identical because if I rotated this this way and made a mirror image they would be superimposable.
I: Identical. And you said because why?
P: If I were to rotate this-
I: The one on the left.
P: This way and then do a mirror image of it they would be superimposable because they have the same stereochemistry.
I: When you say stereochemistry?
P: Like the CH3 is facing toward and this is back.
I: So they would be identical?
P: Yes.
I: So you could rotate those to become identical with the exact same directions of atoms sticking off?

P: Well if I rotated it this way and then did the mirror image then they would be identical. As they are now if I were to do the mirror image. I am just going to stick with identical because if I rotated it this way this would be the mirror image. Well no they wouldn't be superimposable. I lied. Yes they would. Sorry.
I: Final answer?
P: Yeah.
I: So if you rotated it this way then what?
P: This would be my mirror image.
I: Uh huh. That would be your mirror image. Then those would be enantiomers but you said they were identical?
P: No. Sorry. So if I rotated it this way then this would be my mirror image. By superimposable when I am flipping-
I: So if they are mirror images of each other then?
P: They are enantiomers.
I: Well no. So there you have the mirror images and non-superimposable. Yes those would be the mirror images but if you flipped it could you superimpose it on the other?
P: No.
I: So they would be?
P: Enantiomers.
I: enantiomers.
P: So if I flip it do you mean like get it back to the original?
I: No. Rotate it and then flip it like a pancake. Like turn it over. So if you turned it over would they be superimposable because you have to align the atoms.
P: Rotated it this way and then flipped it onto it.
I: Would those be?
P: No.
I: Okay. So why did you say identical first because you rotated it and then what?
P: Was thinking if I put it over it, it would be superimposable. But it is an enantiomer.
I: Okay. Let's go on.

<u>R6:</u>
P: These are enantiomers because they are not superimposable.
I: Okay. So enantiomers because they are non-superimposable?
P: Right. So if I were to flip this like a pancake, on this one, the OH would be facing towards me. CH3 would be facing towards me but on this one the OH is away and the CH is away.
I: If you flipped that like a pancake OH would still be towards you?
P: No. It is just hard because the way she like taught us, is the only thing that changes it whether it is like a wedge or a dash is rotating it. Not mirror imaging it.
I: No you can still flip it.
P: Like this?
I: Uh huh.
P: Like the way I was taught, that wouldn't change. Like the structures she has drawn she – I mean unless I am wrong. She has still shown that if I were to flip this it would still be a wedge and it would still be a CH3 on these two it would still be.

I: Okay. If we flipped it like a pancake what happens to the OH? Is it still pointing at you?
P: No. It would be back into the plane.
I: What about the CH3?
P: It would be back into the plane.
I: What about the F?
P: It would be back – no it would be forward.
I: Is that identical or an enantiomer?
P: They are identical.
I: They are identical. And you said they were first enantiomers because what?
P: They were not superimposable but now they are identical just because if I were to flip them like a pancake they would change.
I: So you are saying you were never taught to flip it like a pancake?
P: No we were taught to flip it like a pancake but like on my drawings that I have from examples from class, if I were to flip this like a pancake the OH was still facing toward me. The CH3 was still facing toward me. The F was facing back. That didn't change about it. The only way we could change, whether it was a wedge or a dash, was by rotating it. Unless I am wrong. But all of my examples are like that.
I: So you were doing it like how you learned in class. Not trying to imagine what it would look like.
P: Yeah.

<u>Practice C:</u>
P: There is one chiral center.
I: Is it R or S?
P: It would be S.
I: What is the number of the chiral center?
P: Two.
I: Two and S. So why two and why S?
P: This one can't be – or one can't be a chiral center just because it is not SP3 hybridized.
I: Uh huh.
P: Two can be a chiral center because it is SP3 hybridized and has four different molecules off of it. CH3 cannot be a chiral center because it has three hydrogens off of it.
I: Good. How did you know it was S?
P: Because when you assign priority OH is first and then it would be the carbon with the OH off of it and then the CH3. And it is going counterclockwise.
I: Good.

<u>C1:</u>
P: So there would be one chiral center.
I: Which number?
P: Two.
I: And what is the configuration?
P: S.
I: Why S?

P: Because when you assign priority the OH is first, the then CH2, CH3 and then the CH3.
I: Good. Let's go on.

C2:
P: I think there is one chiral center.
I: Which one?
P: It would be three.
I: What is the configuration?
P: R. Yeah R.
I: Why R?
P: Because if you assign priority OH comes first, then the CH2, CO2H and then this molecule over here, the CH2CO2H.
I: So which one wins out of those two?
P: Oh it would be two. So it would actually be S because this is directly connected to another C. This is connected – well this C is connected to an O2. This C is connected to a C with hydrogens so I think this would have priority.
I: Wait. You said – so I am looking at the configuration wrong. Three you said? On its left side it is connected to what?
P: A C that is connected to a C with two Hs on it.
I: Uh huh. And then on the right side?
P: It is connected to a C with two Hs but connected to a C connected to an oxygen.
I: And then on the left hand side?
P: It is connected to a C with two Hs. Oh wait on the right hand side?
I: On the left.
P: Yeah. The left is connected to an OH which would have first priority.
I: An OH? Oh I see. That OH then?
P: Is connected to a carbon, connected to another carbon with two Hs, connected to an oxygen.
I: Okay. Let's go on.
P: Is that wrong?
I: I will tell you after.
P: Okay.

C3:
P: So one chiral center.
I: What is the configuration?
P: It is R.
I: So why R?
P: When you assign priority it is Cl first and then – actually it would be S because Cl would be first then this carbon chain and then the CH3. So it would be S.
I: What would be the fourth group?
P: The methyl. Well four is not a chiral center.
I: Let's go on.
P: Sorry.

I: Why is it not a chiral center now?
P: Because it has two methyl groups.
I: So let's go on. Which would be a chiral center in this one?
P: I don't think there would be a chiral center.
I: Okay. Good.

<u>C4:</u>
P: I don't think there would be any chiral centers in this one.
I: No. Okay. Why not?
P: I know it is not going to be any of the CH2s. It can't be one because it is a CH3. It can't be three because there are two methyl groups off of it. Five you are connected to CH2s like on both sides so it couldn't be that. Six you have a C with an H and two methyl groups.
I: Uh huh.
P: That's why.
I: Okay. Let's go on.

<u>C5:</u>
P: You have two.
I: What is the configuration around them?
P: Around three it would be I think S. And then around two it would be – actually two is not a chiral center.
I: Okay. So why were you initially thinking it was a chiral center?
P: Just because I didn't like I know one is a methyl group but I was just kind of like I went by it too fast.
I: So I think three would be the only chiral center.
I: Why did you say S?
P: Because when you set priority OH is first, and then the carbon connected to CH – a CH3. I counted it as S because you have OH first and then number two has a carbon connected to the CH3 and H and then on the left hand side it is a CH2 and a CH3.
I: Okay. Good. How did you know the hydrogen was pointing back?
P: Because of the wedges.
I: No I mean on number three. What is the fourth group on carbon three?
P: It is an H.
I: How did you know it was pointed back? Did you just make that assumption?
P: Yeah. Because it is not denoted otherwise.
I: Okay. Good. Let's go.

I: Can you tell me if this molecule has any chiral centers and what is the configuration around any if it does?
P: It would have two. Would be a chiral center. And then the configuration – this would be one, this would be two and this would be three so it would be S.
I: I noticed in the other ones you didn't make sure your hydrogen was going back. So how come you suddenly remembered this rule?
P: Because it is here in front of my face.

I: Just because it is here in front of your face.
P: And I accounted for it. Those I didn't.
I: Okay. Why didn't you account for it?
P: Probably just on some of them it probably just wasn't shown so I just didn't account for it. And then on the other ones I just probably forgot to.
I: Forgot to. Okay. But this one, seeing it up close was a good reminder?
P: Yeah. And being able to actually rotate it.
I: Rotate it. Okay. And then can you tell me any chiral centers on these molecules and the configuration of them?
P: I know it is not one and two because they are not SP3 hybridized. Six has two hydrogen so it is not that. I don't think it would be five because it is connected to two CH2s. So I would say-
I: That is a bromine.
P: So three would be a chiral center because it is attached to a CH2, a CH and it has a bromine and a hydrogen.
I: What is the configuration around it?
P: Put the hydrogen back, bromine, I think the CH would have higher priority than the CH2 so then one, two, three so it would be S again.
I: Why would you say this one has priority?
P: Higher priority?
I: Yeah.
P: Just because it has – I mean I would guess because it has a double bond making it like not – I would just say I don't know how to explain it. It just seems more like influential in the molecule than just a CH2. Is that wrong?
I: Okay. So that was kind of a guess. So there is a tie right. We have two carbons but this carbon is connected to carbon, carbon, hydrogen. So the double ones count for two bonds. A carbon to carbon, carbon to hydrogen. This one is carbon, hydrogen, hydrogen. So this one wins.
P: Okay. Because it is connected to a carbon, carbon one.
I: Also when there is a tie in the rank, you have to go to the next one.
P: Uh huh.
I: You can't just say these two are the same. They are not actually. You have to go along the rank to see if they are the same.
P: Okay.
I: And then the one you were asking me about (talks to self why figuring out problem). Actually there is no chiral centers in this one because this is a CH2, this is a CH2 and this is Co2H. This is CO2h. So everything attaching is the same just drawn out differently.
P: Okay.
I: So comparing the two exercises so the ones on the screen or these physical models, which do you think was easier if you had to say? The physical models?
P: Yes.
I: Why?
P: Just because it is here in front to me and I can play with it. I don't have to guess how things are going to be rotated or like I can see what changes can be made. I don't just assume that they are going to be made.

I: Does seeing the rotations and changes come easy for you or not at all?
P: No.
I: Do you use model kits when you study and did you use it for the last exam?
P: Yeah.
I: So the model kits help you?
P: Uh huh.
I: Good. So are there any other strategies that you use to help you?
P: Study for like chiral centers?
I: Yeah. Or to solved these types of problems?
P: Knowing like – I need to focus more on like priority to nonpriority. But other than the model kits I don't really use anything else.
I: How has stereochemistry been going for you?
P: The enantiomers suck. I suck at that. You saw that.
I: So the relationship between the two?
P: Yeah. And go ahead.
I: Priority. Is that easier for you?
P: The obvious ones are. I am not sure between halide and like an alcohol which would have priority. I am pretty sure it is an alcohol. Is it?
I: Between oxygen and chlorine you would have to look at the molar mass.
P: Okay.
I: And then other than the relationship, other aspects give you a problem?
P: Like with the chirality or enantiomers?
I: Which one seems to give you more problems?
P: Like the enantiomers.
I: The relationship problems?
P: Yeah. Like mirror images I can do okay with. It is just like if I draw it out it helps me more. What I was confused with on that when we did the mirror image class, the wedges and dashes didn't change in the mirror image. I don't know if that was just like mine or she planned it like that. That is what was confusing me. But it would make sense that they would switch. And then rotating. I have never been good at rotating bonds unless it was in front of me.
I: The model. Okay. So how has organic been going for you. You said in 111 and 112 you had some problems. But is 331 any better?
P: Yeah. It is – like what was hard for me in organic or not organic but CHEM 111 and CHEM 112 was like the equations and math part of it. But like with organic it is like mostly mechanism and that kind of stuff which I like because it more like memorizing. Not memorizing steps but if you understand the steps it is better.
I: So memorization you like the memorization stuff more?
P: Yeah.
I: What about like NMR and stuff like that? Does that come easy for you?
P: I like IR better than NMR because it is more obvious. Like the OH is bigger and the NH2. Like NMR and - or CNMR and HNMR like I can figure it out if I am given the chemical formula. But when I am not given the chemical formula it is kind of hard.
I: Well this has been extremely helpful.
P: I am sorry I suck.

I: You are fine. Thank you so much.
(End of interview)