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College Students' Understanding of Stereochemistry: Difficulties in Learning and Critical Junctures.

Gary Lester Lyon

Louisiana State University and Agricultural & Mechanical College

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UMI®
COLLEGE STUDENTS' UNDERSTANDING OF STEREOCHEMISTRY:
DIFFICULTIES IN LEARNING AND CRITICAL JUNCTURES

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Curriculum and Instruction

by

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ABSTRACT

Because stereochemistry is an important part of both high school and college chemistry curricula, a study of difficulties experienced by students in the learning of stereochemistry was undertaken in a one-semester college organic chemistry course. This study, conducted over the course of two semesters with more than two hundred students, utilized clinical interviews, concept maps, and student journals to identify these difficulties, which were then tabulated and categorized. Although student journals were not a productive source of information, the types of difficulties that emerged from the concept maps were compared and contrasted with those that emerged from the clinical interviews.

Data from the concept maps were analyzed using Kendall's W, a nonparametric statistic that was deemed appropriate for determining concordance between individual concept maps. The correlation between values of Kendall's W for sets of concept maps and multiple choice questions designed to evaluate the content of these same maps was determined, with values of Pearson's r of .8093 (p = .051) and .7191 (p = .044) for the Fall, 1997 and Spring, 1998 semesters, respectively. These data were used to estimate the occurrence of critical junctures in the learning of stereochemistry, or points at which students must possess a certain framework of understanding of previous concepts in order to master new material (Trowbridge & Wandersee, 1994). One critical juncture was identified that occurred when the topics of enantiomers, absolute configuration, and inversion of configuration were introduced.

Among the more important conclusions of this study to the learning of stereochemistry are the following. Both concept maps and interviews provided useful information regarding difficulties in the learning of stereochemistry; this information was complementary in some aspects and similar in others. Concept maps were useful in diagnosing difficulties in application of terms and definitions, whereas interviews were useful when seeking information about difficulties in the manipulation of chemical
structures. Both concept maps and interviews were superior to student journals as tools to probe student difficulties in the learning of stereochemistry.
INTRODUCTION

The set of concepts known as stereochemistry, or the study of three-dimensional relationships in chemical structures, is an important part of both the high school and college level chemistry curricula. Lecture and laboratory methods and suggestions designed to improve the teaching of stereochemistry abound in the literature (Ayorinde, 1985; Barta, 1994; Beauchamp, 1984; Shubbar, 1990). This may indicate both that instructors view this material as important and that they have an intuitive feeling that their students experience difficulty with its mastery. However, little work has been reported regarding students' alternative conceptions and difficulties in learning stereochemical concepts. This study is an investigation of the use of concept mapping and interviews to explore some of the difficulties encountered by students as they learn the concepts of stereochemistry.

Background. Stereochemistry demands of its learners the ability to mentally translate and rotate structures in three dimensions. The author of this study is fond of telling his chemistry students, "The hardest part of chemistry is representing a three-dimensional molecule on a two-dimensional piece of paper." Intuitively, it seems that success in chemistry should correlate with measures of spatial ability. A modest correlation of success in many areas of chemistry and measures of spatial ability has been found (Bodner et al., 1983; Bodner and McMillen, 1985; Carter et al., 1987; Keig and Rubba, 1993; Pribyl and Bodner, 1987). However, lacking a tool which measures changes in knowledge structure, investigations of this type have been unable to explore either students' initial alternative conceptions or the changes which occurred as students studied and mastered chemical topics. A tool developed for such investigations is concept mapping, which has been described as "a highly selective tool for measuring changes in knowledge structure (Novak, 1990)."

Three potential uses of concept mapping in science learning and teaching have been described (Wallace & Mintzes, 1990). Concept maps have been used as heuristics, or
teaching tools, to promote meaningful learning. Perhaps this is because concept mapping is "an activity which fosters active engagement in every student (Trowbridge & Wandersee, 1994)." In addition, concept maps have been used to foster metalearning, or the ability of a learner to reflect upon and develop his or her own learning strategies. Finally, concept maps have been used as a research tool to investigate acquisition of knowledge, and it has been suggested that they will be useful in the identification of critical junctures, or points at which students must possess a certain framework of understanding of previous concepts in order to master new material (Trowbridge & Wandersee, 1994).

Thus, although the alternative conceptions of students regarding stereochemistry and the changes in knowledge structure which occur during its study have not been thoroughly investigated, a tool for this type of investigation has been developed. This tool, concept mapping, is apparently consistent with both learning theory (Ausubel, Novak, & Hanesian, 1978) and the constructivist view that each learner constructs his or her own unique understanding of concepts (Gowin, 1981).

Another research tool that has been extensively used to identify and categorize alternative conceptions is the interview. Although alternative conceptions in stereochemistry do not appear to have been extensively investigated, a good deal of work has been done on alternative conceptions in other subdisciplines of chemistry related to stereochemistry (Ben-Zvi, Bat-Sheva, & Silberstein, 1986; Dyche, McClurgm Stepans, & Veath, 1993; Griffiths, 1983; Griffiths & Preston, 1992; Kikuchi & Suzuki, 1985; Peterson & Treagust 1989a; Peterson and Treagust, 1989b; Ross & Munby, 1991; Treagust, 1988; Zoller, 1990). These two tools, the concept map and the interview, will be used in this study of alternative conceptions in the learning of stereochemistry.

**Purpose of the Study.** The effectiveness of concept mapping and student interviews as measures of conceptual change will be measured in college students studying units on stereochemistry as presented in a one-semester organic chemistry course.
Research Questions. The following research questions are addressed in this study.

1) How effective are concept maps as tools for the identification of difficulties and critical junctures in the learning of stereochemistry?

2) What types of difficulties encountered in the learning of stereochemistry can be identified through interviews of students?

3) How do the difficulties in the learning of stereochemistry that are identified by interviews correspond to those identified through concept mapping?

Importance of the Study. Studies which correlate spatial ability and achievement in chemistry do not address students' alternative conceptions and conceptual change. Both concept mapping and student interviews offer tools which may be effective in assessing both students' alternative conceptions and conceptual change as they learn about chemistry in three dimensions.

Definition of Terms. Stereochemistry is all aspects of the study of three-dimensional relationships in chemical structures; however, in this paper, stereochemistry as studied in college level organic chemistry will be limited to the three dimensional chemistry of carbon and its molecules. The stereochemistry of inorganic compounds such as the octahedral complexes of transition metals (Huheey, 1983) is not properly a part of organic chemistry as taught at the sophomore level and is not discussed in this study. Concept mapping is a method derived from Ausubel's assimilation theory (Ausubel et al., 1978) that hierarchically represents the cognitive structure of concept meanings and ideas (Novak, 1990). Critical junctures are points at which students must possess a certain framework of understanding of previous concepts in order to master new material (Trowbridge & Wandersee, 1994). Definitions of chemical terms used in this study are given in Table 1.1. Examples of some types of representations of chemical structures are given in Figure 1.1. Bond-line representations of the conformers of cyclohexane are given in Figure 1.2.
This study uses the term *difficulty* as being more general than the term 'alternative conception.' Alternative conceptions have been defined as concepts that are different from the "acceptable and scientific viewpoint" (Treagust, 1988) and may be stable and difficult to alter (Wandersee, Mintzes, & Novak, 1994). Because this study is not designed to address conceptual change and the stability of the concepts held by students, the term 'difficulty' is used throughout.

**Scope and Limitations.** This study focused on college level students enrolled in a one-semester organic chemistry class at one university carried out over the course of two different semesters. Differences may be observed in freshman level inorganic chemistry students, students enrolled in the traditional two-semester organic chemistry class, and also at the high school level. In addition, although concept maps are assigned and evaluated for all students in both classes (more than two hundred students), only a small number (ten) of students were chosen as interviewees.
<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
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<tbody>
<tr>
<td>antiperiplanar&lt;sup&gt;a&lt;/sup&gt;</td>
<td>An adjective describing substituents on a staggered conformer that are as far apart from each other as possible. Commonly abbreviated 'anti'.</td>
</tr>
<tr>
<td>axial position&lt;sup&gt;b&lt;/sup&gt;</td>
<td>One of six positions occupied by substituents on a cyclohexane ring in which the substituents are parallel to each other and perpendicular to the average plane occupied by the six carbon atoms forming the cyclohexane ring.</td>
</tr>
<tr>
<td>boat conformation&lt;sup&gt;b&lt;/sup&gt;</td>
<td>A conformation of cyclohexane in which the carbon atoms adopt a shape approximating that of a boat.</td>
</tr>
<tr>
<td>bond-line formula&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Also called a line-bond formula, this is a type of structural formula in which carbon atoms are designated as either angles or ends of lines. Hydrogen atoms attached to carbon are not drawn, and all other atoms are drawn in full.</td>
</tr>
<tr>
<td>chair conformation&lt;sup&gt;b&lt;/sup&gt;</td>
<td>A conformation of cyclohexane in which the carbon atoms adopt a shape approximating that of a chair.</td>
</tr>
<tr>
<td>chiral&lt;sup&gt;a&lt;/sup&gt;</td>
<td>An adjective describing any object that is nonsuperimposable on its mirror image, such as the left and right hand. Entire molecules can be described as chiral as can atoms within molecules. The chirality of all molecules in this study is caused by carbon atoms containing four different substituents. Chiral molecules do not possess a plane of symmetry.</td>
</tr>
<tr>
<td>cis-trans isomer</td>
<td>See 'geometric isomer'.</td>
</tr>
<tr>
<td>condensed formula&lt;sup&gt;a&lt;/sup&gt;</td>
<td>A type of structural formula in which bonds are not always shown, and atoms of the same type bonded to one other atom are grouped together.</td>
</tr>
<tr>
<td>configurations&lt;sup&gt;c&lt;/sup&gt;</td>
<td>Two or more representations of different stereoisomers.</td>
</tr>
<tr>
<td>conformer&lt;sup&gt;b&lt;/sup&gt;</td>
<td>Also known as a conformational isomer. Conformers are different orientations of the same molecule caused by the free rotation that occurs around sigma (single) bonds.</td>
</tr>
<tr>
<td>dash formula&lt;sup&gt;b&lt;/sup&gt;</td>
<td>A structural formula in which each atom is denoted by its chemical symbol and bonds between atoms are denoted by lines.</td>
</tr>
<tr>
<td>dash notation&lt;sup&gt;b&lt;/sup&gt;</td>
<td>A notation used to denote bonds that point behind the plane of the paper.</td>
</tr>
<tr>
<td>diastereomer&lt;sup&gt;c&lt;/sup&gt;</td>
<td>Stereoisomers that are not enantiomers.</td>
</tr>
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Table 1.1 (cont.)

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
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<tbody>
<tr>
<td>eclipsed</td>
<td>An adjective describing a conformer in which the substituents on two neighboring atoms being studied are as close together as possible.</td>
</tr>
<tr>
<td>empirical formula</td>
<td>A chemical formula that lists the types of atoms in a molecule and their numerical ratio.</td>
</tr>
<tr>
<td>enantiomer</td>
<td>Stereoisomers that are nonsuperimposable mirror images. In this study, all enantiomers are caused by the presence of chiral carbon atoms within molecules.</td>
</tr>
<tr>
<td>equatorial position</td>
<td>One of six positions occupied by substituents on a cyclohexane ring in which the substituents are roughly in the same plane occupied by the six carbon atoms forming the cyclohexane ring.</td>
</tr>
<tr>
<td>Fischer projection</td>
<td>A shorthand notation used to represent chiral molecules.</td>
</tr>
<tr>
<td>geometric isomer</td>
<td>A type of diasteromer resulting from hindered rotation around a chemical bond. This hindered rotation may be caused by the presence of either a multiple bond or a cyclic structure.</td>
</tr>
<tr>
<td>isomers</td>
<td>Chemical structures having the same numbers and types of atoms but varying in the orientation of their atoms in space.</td>
</tr>
<tr>
<td>Lewis structure</td>
<td>A type of structural formula that represents each bonding electron as a dot. A single bond is shown as a pair of dots, a double bond as two pairs of dots, and a triple bond as three pairs of dots.</td>
</tr>
<tr>
<td>meso</td>
<td>Adjective describing a molecule containing two chiral centers and a plane of symmetry.</td>
</tr>
<tr>
<td>molecular formula</td>
<td>A chemical formula that gives the actual number of atoms in a molecule with no representation of the order in which the are attached to one another.</td>
</tr>
<tr>
<td>Newman projection</td>
<td>A method of depicting conformers that is specifically designed to depict conformers and the free rotation around a sigma bond.</td>
</tr>
<tr>
<td>optical diastereomer</td>
<td>A term used in this study to denote diastereomers that are not geometric isomers.</td>
</tr>
<tr>
<td>sawhorse diagram</td>
<td>A method of depicting the three-dimensional structure of molecules.</td>
</tr>
<tr>
<td>staggered</td>
<td>An adjective describing a conformer in which the substituents on two neighboring atoms being studied are as far apart as possible.</td>
</tr>
<tr>
<td>Term</td>
<td>Definition</td>
</tr>
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<td>--------------------------</td>
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</tr>
<tr>
<td>stereoisomers</td>
<td>Structures containing the same number and types of atoms bonded by the same bonds but having different three-dimensional structures that are not interchangeable.</td>
</tr>
<tr>
<td>structural formula</td>
<td>A chemical formula that shows the order of attachment of the atoms in a molecule.</td>
</tr>
<tr>
<td>structural isomers</td>
<td>Isomers that vary because their atoms are attached in a different order.</td>
</tr>
<tr>
<td>wedge notation</td>
<td>A notation used to represent bonds that point above the plane of the paper.</td>
</tr>
</tbody>
</table>

\(^{a}\)Definition derived from Fessenden & Fessenden (1994).

\(^{b}\)Definition derived from Bailey & Bailey (1995).

\(^{c}\)Definition derived from March (1977).
a) Dash, condensed, and bond-line formulas of ethanol.

\[
\text{Dash formula} \quad \text{CH}_3\text{CH}_2\text{OH} \quad \text{Condensed formula} \quad \text{OH} \\
\text{Bond-line formula}
\]

b) Newman projections of the staggered and eclipsed conformers of ethanol

c) dash formula of 2-chlorobutane

d) (R)- and (S)- enantiomers of 2-chlorobutane using dash and wedge

e) sawhorse diagrams of the (R)- and (S)- enantiomers of 2-chlorobutane

f) Fischer projections of the (R)- and (S)-enantiomers of 2-chlorobutane

**Figure 1.1.** Some types of molecular representations used in this study.
a) Bond-line representations of the chair and boat conformations of cyclohexane.

b) Bond-line representations of the chair conformation of cyclohexane, showing the positions of equatorial and axial substituents. Equatorial substituents are marked with an 'e', and axial substituents with an 'a'.

Figure 1.2. Conventions used in the representation of cyclohexane.
REVIEW OF LITERATURE

Introduction to the Literature. The most important secondary source used in preparation of this review was the Current Index to Journals in Education of the Educational Resources Information Center (ERIC) which was used as a guide to locate most of the primary journal articles consulted. Bibliographies in these articles were then consulted for further sources of information. Papers were obtained from the Document Reproduction Service of ERIC. Bibliographies on concept mapping by Al-Kunifed and Wandersee (1990) and alternative frameworks and science education by Pfundt and Duit (1988) were consulted when writing the appropriate sections. More recent works on these topics were obtained through ERIC.

Because the learning of stereochemistry would appear to require extensive visualization of three dimensional structures, the nature of spatial ability and its correlation to performance in stereochemistry will be addressed. Several investigators have demonstrated a modest correlation between various measures of spatial ability and success in stereochemistry, whereas others have found little correlation (Bodner & McMillen, 1985; Bodner & McMillen, 1986; Carter, 1985; Carter, LaRussa, & Bodner, 1987; Pribyl & Bodner, 1985; Pribyl & Bodner, 1987; Treagust, 1980). The limitations of the value of this type of information will be mentioned before discussing research on alternative conceptions.

Although alternative conceptions in stereochemistry do not appear to have been extensively investigated, a good deal of work has been done on alternative conceptions in other subdisciplines of chemistry related to stereochemistry (Ben-Zvi et al., 1986; Dyche et al., 1993; Griffiths, 1983; Kikuchi & Suzuki, 1985; Peterson & Treagust, 1989a; Peterson & Treagust, 1989b; Ross & Munby, 1991; Treagust, 1988; Zoller, 1990). One powerful technique for investigating alternative conceptions that has had extensive use in the sciences is concept mapping (Cliburn, 1990; Fraser & Edwards, 1985; Novak, Gowin, & Johansen, 1983; Novak & Gowin, 1984; Novak, 1990; Pendley, Bretz, &
Novak, 1994; Ross & Munby, 1991; Roth & Roychoudhury, 1993; Vargas & Alvarez, 1992; Wallace & Mintzes, 1990). The potential of concept mapping as a tool to assess alternative conceptions in stereochemistry will be further discussed.

The Nature of Spatial Ability. The limited ability of intelligence tests to predict specific aptitudes has led psychologists to investigate cognitive models that describe these aptitudes. One psychological construct that has been extensively investigated is spatial ability (Pellegrino & Hunt, 1991). Early factor-analytic studies of spatial ability were derived from studies of mechanical aptitude, and many of these studies identified a spatial factor that was separate and distinct from verbal ability (McGee, 1979).

Spatial ability is not readily defined as a single skill; multivariate studies have identified and defined several major factors. In his review of studies on spatial abilities, McGee (1979) identified two factors that emerged in factor analytical studies. Pellegrino and Hunt (1991) expanded the list of factors to three, which are here described. The best defined factor is spatial relations ability, or the ability to mentally translate or rotate objects (Pellegrino & Hunt, 1991), which is called visualization by McGee (1979). A second factor, named spatial visualization by Pellegrino and Hunt, is the ability to deal with problems which require imagining the motions of internal parts of an image. Third is spatial orientation, or the ability to perceive how an image would appear from a different orientation. This last factor is difficult to separate from spatial relations (McGee, 1979; Pellegrino & Hunt, 1991).

The correlation between spatial ability and success in science, mathematics, and technology has been investigated for many years. In 1957, the United States Employment Service included performance on spatial ability tests as a predictor of success in engineering, mathematics, chemistry, botany, physics, and several other scientific and technical disciplines (Dyche et al., 1993). Meta-analysis of literature dealing with spatial visualization, verbal ability, measures of general intelligence, and performance in science has revealed that both spatial visualization and verbal ability
predict additional variance in achievement in science beyond that shared with general intelligence (Piburn, 1993). However, the performance of spatial ability tests as academic predictors has been described as "generally disappointing (McGee, 1979; Pellegrino & Hunt, 1991)."

**Relation of Spatial Ability to Performance in Chemistry.** Intuitively, it seems that spatial ability should be an important predictor in a discipline such as chemistry that relies heavily on three-dimensional representations. However, this does not always appear to be true. Several studies have demonstrated a statistically significant correlation between spatial ability and performance in various aspects of chemistry, but the correlations were not generally large (Bodner & McMillen, 1985; Bodner & McMillen, 1986; Carter, 1985; Carter et al., 1987; Pribyl & Bodner, 1985; Pribyl & Bodner, 1987; Treagust, 1980).

Bodner and McMillen (1986) investigated the relationships between spatial ability and chemistry in one thousand eight hundred students in the first semester of a two-semester freshman chemistry course at Purdue University. A battery of four tests was used to measure spatial ability. Statistically significant coefficients of correlation (Pearson's r) between 0.29 and 0.35 were observed when the composite spatial ability was correlated with stoichiometry exam scores, crystal structure exam scores, a free-response quiz on crystal structure, and the comprehensive final exam. These results indicate that between 8.4% and 12.3% of the variance in these scores is accounted for by spatial ability. Somewhat surprisingly, no apparent correlation between performance in measures of the stereochemistry of covalent molecules and measures of spatial ability was demonstrated in this study. One explanation for this apparent correlation between spatial ability and performance in measures of stereochemistry may be that students can correctly answer many stereochemical problems by the application of the rote rules that are given in many organic chemistry texts. An example is "If any two groups around a chiral atom are interchanged, the mirror image of that carbon is formed" (Bailey and Bailey, 1995, p. 204).
Carter et al. (1987) used analysis of variance to study the relationship of two measures of spatial ability with performance on various items from a freshman chemistry course of two thousand five hundred students at Purdue University. Statistically significant correlations between spatial ability and all four unit exams were observed. The largest correlations were in the range of 0.30 (roughly 9% of the variance in some chemistry subscores correlated with spatial ability), and many of the correlations were much lower. Similar results have been reported on correlation of success in organic chemistry with spatial ability scores (Pribyl & Bodner, 1987).

Although the studies listed above demonstrate some relationship between spatial ability and achievement in chemistry, and in some cases, a relationship between spatial ability and achievement in stereochemistry, they do not address the difficulties such as the representation and naming of three-dimensional molecular structures on a two-dimensional surface that give students problems in the learning of stereochemistry. This observation parallels the statements of Gauvain in studies on spatial development in everyday thinking, who advocated that researchers concentrate less on the nature of representations and investigate instead how activities are conducted in large scale space (Gauvain, 1991). It appears that researchers interested in the development of alternative conceptions in fields requiring three-dimensional reasoning (such as stereochemistry) need a more powerful tool than simple measures of spatial ability.

One other factor may help explain why spatial ability appears to be a poor predictor for success in the study of stereochemistry. If students learn to manipulate two-dimensional representations of three-dimensional chemical structures through rote algorithms, the student may have little need for spatial ability or reasoning. A study of requisite knowledge for problem solving in chemistry concluded, "Rules for producing correct solutions to problems work simply because they are rules; the rules of an algorithm. If such rules are given to students to follow, no confrontation with the chemistry of why they work is needed (Lythcott, 1990)."
The Nature of Stereochemistry. Fessenden and Fessenden (1994) defined stereochemistry as follows. "Stereochemistry is the study of molecules in space, that is, how atoms in a molecule are arranged in space relative to one another." Some idea of the importance that teachers of chemistry attach to this subject is illustrated by the number of articles dealing with stereochemical topics which have appeared in the *Journal of Chemical Education*. Examples include articles on relationships between isomers (Black, 1990), history of stereochemistry (Grossman, 1989; Shallenberger & Wienen, 1989) various chemical demonstrations and syntheses (Ballester & Perpinan, 1988; Jackman & Rillema, 1989; Rowland, 1983; Wasacz & Badding, 1982), applications of graph theory to stereochemistry (Hansen & Jurs, 1988), methods of model construction (Yamana, 1987; Yamana, 1989a; Yamana, 1989b) and methods for assigning stereochemical configurations (Eliel, 1985). The three-dimensional nature of stereochemistry becomes clear to beginning organic chemistry students upon encountering tetrahedral carbon atoms, Fischer and Newman projections, planes and axes of symmetry, structural, geometric, and optical isomers, and enantiomers and diasteromers.

Chemists have many notations and methods to denote different aspects of the same three-dimensional structure. Keig and Rubba (1993) note that for a structure as simple as that of water, a chemist may use the chemical formula, H₂O, to identify the constituent atoms composing the molecule and express their ratio, the chemist may choose to draw the Lewis structure to convey information regarding covalent bonding and bond order, or the chemist may use a ball-and-stick model (or a drawing) to represent the shape of the molecule and convey information regarding bond angles. These multiple representations may add to the difficulties students experience in dealing with the structures, shapes, and three-dimensional properties of chemical structures.

One indication of some of the difficulties involved in the teaching and learning of stereochemistry may be the number of different types of models devised by chemists to represent the three-dimensional nature of molecules. A model can be thought of as a
representation in three dimensions of some projected or existing structure, showing the proportions or arrangements of its component parts. In this case, the structure is a molecule.

Models are not perfect replicas that differ only in scale. The atomic theory from which our ideas of molecules is derived is itself a model of the nature of matter. Of necessity, molecular models must represent a "classical" rather than quantum mechanical view of molecular structure and can, therefore, at best only convey to the user some idea of the molecular nature of the substance. The limitations of molecular models must be emphasized in their use and it has been said that a molecular model can either display one aspect of structure extremely well or be a moderately successful compromise showing a number of structural features (Walton, 1978).

Traditionally, the aspects of molecular structure displayed in models are constitution, configuration, conformation, and chirality. Constitution refers to what atoms are present in a structure, configuration refers to the spatial arrangement of atoms and bonds, conformation refers to differing spatial arrangements resulting from rotation around sigma bonds, and chirality refers to the property of a structure that is not superimposable upon its mirror image (Walton, 1978).

Molecular models are generally classified as static or dynamic, with static models being by far the most common. Static models are in turn classified as being either space-filling, ball-and-spoke, or skeletal, although this can be thought of as a continuum, with space-filling models at one end and skeletal models at the other.

Space-filling models attempt to accurately portray the geometry of the model (including appropriate bond angles) as well as the relative sizes of the individual atoms within the molecule. Sizes of atoms in these models are usually related to their covalent radii. Models of this type are frequently called Stuart type models (after one of their early developers) or CPK (Corey-Pauling-Kuhn) models. Like most models, they do not portray atoms or molecules in motion. They perhaps have the most effective "look" of a
molecule, and are the most effective models for demonstrating steric hindrance, which occurs when the "spatial arrangement of the atoms of groups at or near the reacting site of a molecule hinders or retards a reaction" (Solomons, 1996, p. 249). Some of these models have pieces that allow the illustration of hydrogen bonding. The disadvantage of these models is that they are not very "transparent," that is, most of the volume of the model is taken up by spheres representing atoms, and it is not easy to see the inner atoms. For example, the model of the simple molecule methane, CH\(_4\), appears to be mostly hydrogen (H) atoms, and the important central carbon atom (C) is almost totally obscured. This problem becomes much worse for larger molecules. In addition, unshared electron pairs are not readily represented using space-filling models (Walton, 1978).

Ball-and-spoke models (sometimes called ball-and-stick models) are surely the most commonly-used models in teaching. A very common ball-and-spoke model set is the Prentice-Hall Molecular Model Set for Organic Chemistry\(^\text{TM}\) that was used in this study. These models represent the relative positions of atoms using spheres (usually made of wood), but the spheres are all the same size, and are relatively much smaller than those used in space-filling models. These models portray bond angles very accurately and do a fair job of showing bond lengths, but give up altogether the idea of depicting covalent radii of atoms. The spheres representing atoms only locate their relative positions in space. These models do an excellent job of illustrating molecular geometry because most of their volume is empty space; that is, it is not difficult to see all of the atoms in a structure (Walton, 1978).

Skeletal models (for example, the popular Dreiding models) do not actually represent the individual atoms at all; rather, only bonds are represented. The position of atoms is determined by the points at which bonds intersect. These models are very convenient to build, especially for organic chemists dealing with complicated structures, and are very lightweight. They are not as inclined to come apart as are many types of ball-and-spoke
models. In addition, some models, in particular Framework Molecular Models\textsuperscript{TM} (FMM), can be used to show unshared electron pairs. They do an excellent job of illustrating both bond angles and bond lengths (Framework Molecular Models contain plastic tubing that can be cut using a knife to the exact bond length required), but to beginners they can be confusing because they do not actually depict any atoms (March, 1977).

A few attempts have been made to construct models illustrating the dynamic aspects of molecules. Some use magnets and some use various types of moving joints to illustrate molecular motion. Most of these models are specific to some phenomenon. For example, the Berry pseudorotation of five-coordinate compounds (a phenomenon of the interconversion of trigonal bipyramidal and square pyramidal geometries) has been modeled (Walton, 1978); however, this is something that the beginning student is very unlikely to encounter. Five-coordinate compounds are unusual (Huheey, 1983).

Alternative Conceptions and the Learning of Science. One important factor affecting student learning is the set of concepts that the student brings into the classroom. This conclusion has been reached by researchers from a cognitive perspective, a developmental perspective, a behavioral perspective, and a constructivist perspective (Griffiths & Preston, 1992). Concepts that are different from the "acceptable and scientific viewpoint" have been variously labeled as "misconceptions," "alternative conceptions," "preconceptions," "alternative frameworks," and "children's science (Treagust, 1988)." Other terms that are sometimes used interchangeably are "naive beliefs," "naive theories," "naive conceptions," "intuitive beliefs," "intuitive science," and "learners' science (Boo, 1998)." These terms have similar but slightly different meanings. The two most commonly-used terms are probably "alternative conceptions" and "misconceptions." The term misconception generally refers to "a vague, imperfect, or mistaken understanding of something (Wandersee, Mintzes, & Novak, 1994)." These "misconceptions" are held to be difficult to teach away and the implication is that they have little value and should be
eradicated. The term "alternative conception," now preferred by many researchers, refers to constructions built by the learner which may be very fruitful and make natural events and objects intelligible to the learner, and also confers "intellectual respect" to the person holding these conceptions (Wandersee et al.).

Much work in alternative conceptions has a theoretical basis in the work of David Ausubel, who developed a theory of verbal learning and "advance organizers" that ultimately lead to his assimilative theory of cognitive learning (Ausubel, 1960; Ausubel, 1962; Ausubel et al., 1978). Although he was not opposed to discovery learning, Ausubel contended that direct didactic instruction was the most common method of teaching, and would likely remain so. Thus, investigation of how learning occurs when students are taught by this method was likely to be fruitful. Ausubel developed a theory of reception learning based on this need. (DeBoer, 1991; Novak, Ring, & Tamir, 1971; Novak, 1979). Reception learning occurs when "the content of the learning task (what is to be learned) is presented to rather than independently discovered by the learner (Ausubel, 1963).

Ausubel claimed that concepts are continuously brought into the mind's conceptual framework and integrated with older conceptual structures, and he made a distinction between rote reception learning and meaningful reception learning (DeBoer, 1991). In the former, new knowledge is not associated with previously learned concepts. This isolated, rotely learned knowledge is thus easily lost. Meaningful reception learning occurs when new knowledge and new concepts are associated with ideas or concepts already in the learner's cognitive structure.

Instead of completely separating rote-reception learning from meaningful-reception learning, Ausubel's theory places them in a continuum, in which rote-meaningful learning may be described as learning subject matter verbatim, requiring only that the learner provide stimulus-response associations, whereas meaningful-reception learning is more meaningful, idiosyncratic, and requires the learner to associate new material with that
which is already known (Cliburn, 1990). When new knowledge is accepted, it is associated with a general subsuming concept already present. Although the individual's cognitive structure is enriched, the acquired information may no longer be dissociable from the cognitive structure. After a time, the discrete pieces of information learned may no longer be available to the learner. This obliteration of recall of specific knowledge is called "obliterative subsumption," and is distinctly different from the loss of information that occurs when material is learned by rote and cannot enrich the cognitive structure. Association of concepts in the cognitive structure is claimed to be hierarchical, with the most general concepts higher in this hierarchy and the subsuming concept at the top (Novak et al., 1971).

Ausubel's theory of meaningful reception learning evolved as a result of his work on "advance organizers," that he claimed could help to provide a cognitive structure for the learner when none existed (Ausubel, 1960). Advance organizers are "brief introductory instructional episodes," and are designed by the teacher with the intention of facilitating meaningful learning by organizing relevant concepts so that they may be more readily assimilated into the student's existing cognitive structure (DeBoer, 1991). Providing this type of structure is seen as a powerful aid to meaningful reception learning and a means to provide "anchorage" for information previously learned by rote (Novak et al., 1971).

The theory of meaningful reception learning predicts that structured teaching will promote meaningful learning and this learning will be greatest when it is tailored to the individual student's current cognitive structure. Because of this, individualized instruction will be more beneficial than group instruction. Another consequence of meaningful learning theory is that the degree of existing knowledge of a subject influences performance at subsequent educational levels. This is a much greater determinant than are general ability, personality, or interest levels, which may help explain why tests of spatial ability have in general been poor predictors of success in the learning of stereochemistry. In general, pretests that fail to account for the learner's
cognitive structure have little predictive validity, and any predictive validity of educational achievement decreases as the time between two related measures of academic ability increases. Finally, prior learning that helps the learner build and draw upon subsuming concepts is beneficial (Novak et al., 1971).

**Types of Studies in Alternative Conceptions Research.** Three broad areas of alternative conceptions research have been identified: descriptive studies, explanatory studies, and studies attempting to foster conceptual change (Hashweh, 1988). The majority of these studies are descriptive. In this type of study, the researcher describes directly observable phenomena and may construct a model or theory regarding students' knowledge. This researcher is involved in hypothesis formulation and testing. Descriptive studies often do not offer suggestions for instructional strategies, and purely descriptive studies that are not based on a model of conceptual change cannot be expected to offer strategies for inducing such change. Instead, descriptive studies "should aim to identify and describe student preconceptions (Hashweh)." In contrast, explanatory studies should attempt to explain conceptual stability and change, and studies that attempt to implement conceptual change should test the explanations fostered by these explanatory studies (Hashweh).

Alternative conceptions studies have also been categorized as either nomothetic or ideographic. A nomothetic study attempts to compare student knowledge to a standard that is deemed acceptable to the scientific community (Driver & Easley, 1978; Wandersee et al., 1994). These studies are often experimental in nature and may rely on pencil-and-paper tests analyzed quantitatively using inferential statistics. In contrast, idiographic studies probe one or more student's understanding of natural phenomenon, using qualitative methods of analysis such as the unitizing and categorizing of data (Lincoln & Guba, 1985). Idiographic studies typically study small numbers of students in great detail. These methods need not be mutually exclusive and may be combined in a single study (Wandersee et al., 1994).
Some Conclusions Derived from Alternative Conceptions Research. Alternative conceptions can be remarkably stable, in part because they can be fruitful and useful to the holder, and changing alternative conceptions is frequently a difficult task (Treagust, 1988). "These preconceptions are amazingly tenacious and resistant to extinction (Ausubel et al., 1978)." However, not all alternative conceptions appear to be equally stable, and attempts to modify students' ideas using well-planned conventional instruction are frequently successful. Wandersee et al. (1994) concluded, "Accordingly, we think a working knowledge of discipline-specific alternative conceptions research might well be considered basic to the professional preparation of master science teachers.

Research indicates that alternative conceptions are acquired in at least three different ways. They are acquired from nature, from language and from instruction (Gabel, 1989). Children sitting on metal chairs will frequently say that these chairs are colder than are upholstered chairs in the same room. This is an example of an alternative conception acquired from nature. Alternative conceptions acquired from language frequently arise because some words in everyday use have different meanings when used in a scientific context. An example is the "melting" of sugar. The acquisition of alternative conceptions through formal instruction may occur when concepts are presented without proper context. When this occurs, students may simply memorize trivia. Alternative conceptions may also be acquired through formal instruction when what is presented is beyond the developmental level of the student (Gabel, 1989).

If the material presented is beyond the developmental level of the student, then it may be that the student does not possess what has been termed "requisite knowledge" of the subject. A study of requisite knowledge in the solving of chemistry problems concluded that "It is possible, though not our intention, for students to produce right answers to chemistry problems without really understanding much of the chemistry involved. This is a most unsettling piece of information (Lythcott, 1990)." Rote memorization of rules that lead to correct answers may be the type of trivia that is memorized when concepts are
presented without proper context. Lythcott concludes, "If such rules are given to students to follow, no confrontation with the chemistry of why they work is needed. The 'problem' with this sort of problem solving is neither the solvers nor the algorithms, but in the prescription to follow the rules (Lythcott)."

Some alternative conceptions correspond to ideas once held by scientists that have been abandoned for better explanations. Examples from the discipline of chemistry include the belief that matter is continuous, the belief that the shapes of molecules are reflected in macroscopic shapes of matter, and the belief that atoms are animistic, alive, and sensitive (Griffiths & Preston, 1992). Novices at times hold beliefs about burning and combustion that parallel the discarded phlogiston theory, and have been shown to occasionally have conceptions of gases that parallel those of Aristotle (Gabel, 1989). Of particular interest to this study is the alternative conception that shows particles in intact groups rather than in smaller groups after a molecule has decomposed (Gabel & Samuel, 1987).

Researchers have also concluded that alternative conceptions are not specific to any age, ability, gender, or race. The frequencies of some alternative conceptions appear to change very little with time, although some alternative conceptions in certain domains appear to be more resistant to change than are others. Perhaps the previously-mentioned diversity of alternative conceptions is in part caused by the diverse set of personal experiences, culture, language, and teaching experiences in any group of learners. In addition, many teachers hold the same alternative conceptions as their students. Some of these conclusions seem to offer little hope to the practicing teacher; however, one final conclusion of many researchers is that in some cases conceptual change is possible if classroom teaching involves strategies that can facilitate conceptual change (Wandersee et al., 1994).

Alternative Conceptions Research Related to Chemistry and Stereochemistry. Recent studies on alternative conceptions in chemistry have focused on many topics, including
oxidation, chemical reactions, equilibrium, the mole, solubility, transformation of matter, conservation of mass, thermodynamics, chemical and physical changes, and stoichiometry (Peterson & Treagust 1989a). At a more advanced level, studies have been done on alternative conceptions of orbital shapes (Kikuchi and Suzuki, 1985), Markownikov's rule (Newton, 1987), and unexpected molecular symmetries (Heilbronner, 1989), although some of these latter studies might equally be considered to be corrections of textbook errors or errors perpetuated by instruction rather than alternative conceptions of students. Little work has been done on alternative conceptions in stereochemistry, but the related fields of atomic and molecular structure have been investigated (Ben-Zvi et al., 1986; Gabel & Samuel, 1987; Griffiths & Preston, 1992; Pendley et al., 1994; Peterson & Treagust, 1989a; Peterson & Treagust, 1989b; Treagust, 1988; Zoller, 1990).

According to Zoller (1990), inorganic chemistry is "probably the most problematic traditional science discipline taught," and "Students' misunderstandings and alternative conceptions in school sciences at all levels constitute a major problem of concern to science educators, scientist-researchers, teachers, and, of course, students (Zoller, 1990)." Instructors of chemistry place particular importance on the concepts of atomic and molecular structure, and it is reasonable to assume that a clear grasp of these topics is needed in order to properly understand material on stereochemistry. The history of chemistry relates several well-known anecdotes of famous chemists and their revelations regarding chemical structure. Two of the best known are Friedrich Kekule's vision of snakes grabbing their tails while he gazed into the fire, leading to his speculations on the structure of benzene, and James Watson relating how Francis Crick's idle flipping of cardboard models of nucleotides aided them in the determination of the structure of nucleic acids (Shepard, 1978). Several studies on alternative conceptions in chemistry have either focused on atomic and molecular structure or included these topics as part of a
Griffiths and Preston (1992) investigated alternative conceptions on structure, shape, and compositions of atoms and molecules in grade twelve chemistry students in the Avalon peninsula of Newfoundland, Canada. In this pilot study, students were classified as being enrolled in either an academic science program, an academic non-science program, or a non-academic, non-science program. Material for this study was collected by interviews, which is a commonly used technique for collecting information on alternative conceptions (Peterson & Treagust, 1989a). These interviews were used to identify fifty-two alternative conceptions which were placed into eleven broader categories. Examples of some of the alternative conceptions identified include "Water molecules contain different numbers of atoms," "The shape of a container will affect the shape of a molecule," and "All atoms are alive." The most commonly held alternative conception among the academic science students was that water molecules are composed of two or more solid spheres. Among academic non-science students and nonacademic non-science students, the most common misconception was that water molecules within a phase may have different sizes. All ten of the academic non-science participants held this misconception in addition to nine of ten nonacademic non-science students (Griffiths & Preston).

In their study, Griffiths & Preston (1992) identified several alternative conceptions that may have been caused by a particular instructional treatment. Six participants, most of whom were members of the academic science group, believed that water molecules consisted of three solid spheres. These students had more opportunity to work with ball-and-stick models of molecules. Five participants, four of whom were again members of the academic science group, believed that the size of an atom could change as a result of a collision. The authors speculate that an unidentified instructional method may be the cause of this misconception (Griffiths & Preston, 1992). A related finding is that 24.7%
of a control group of 393 tenth-grade students in Israel believed that an atom of copper was malleable (Ben-Zvi et al., 1986).

Ben-Zvi et al. (1986) used a questionnaire to identify twelve alternative conceptions regarding properties of an isolated metallic atom as compared with properties of metallic wire among Israeli chemistry students in eleven high schools. In an effort to correct these alternative conceptions, a program was developed and integrated into the chemistry curriculum. This program included a general introduction to scientific theories and models, a historical review of events leading to the early nineteenth century model of the atom and the aspects of quantitative chemistry that supported it, and modifications of this Daltonian atom which occurred through time. The program was carried on through several months during which the atomic model was altered as many times as necessary to accommodate new facts. Comparisons were made between an experimental group of 383 students who received this program of instruction and a comparable control group of 393 students who did not.

Ben-Zvi et al. (1986) did not include statistical analysis with their data; however, chi-square analysis of their data done by the author of this study reveals significant differences between the experimental group and the control group in eight of the twelve listed alternative conceptions (Tables 2.1 and 2.2). Table 2.1 lists alternative conceptions regarding individual atoms of a metallic solid, and Table 2.2 lists alternative conceptions regarding individual atoms of the corresponding metallic gas. In each case, the experimental group performed significantly better than the control group. The alternative conceptions not yielding statistically significant differences were, in three of four cases, those which most students in both groups appeared to understand best. The exception is the alternative conception that atoms of the gas of the metal had a brown color; apparently this alternative conception was particularly difficult for the designed program of instruction to overcome.
Especially noteworthy in both Tables 2.1 and 2.2 is the category labeled "none of the above." This category lists students who had none of the listed alternative conceptions. In the control group, 7.6% of students had none of the alternative conceptions regarding solids, and 8.1% had none of the alternative conceptions regarding gases, whereas in the experimental group, 32.3% of the students had none of the alternative conceptions regarding solids and 35.1% of the students had none of the alternative conceptions regarding gases. This may indicate both that the program advocated by the authors was at least partially successful in correcting alternative conceptions and that many of these alternative conceptions are extremely difficult to correct.

Although Ben-Zvi et al. (1986) used a survey in the form of a questionnaire to diagnose alternative conceptions, most work on alternative conceptions has been done by conducting interviews (Peterson & Treagust, 1989). This was the approach used by Griffiths and Preston (1992). However, conducting interviews is perhaps not a reasonable approach for the classroom teacher to use in the identification of alternative conceptions, and thus Treagust (1988) and Peterson and Treagust (1989) have worked to develop multiple choice tests to identify alternative conceptions on covalent bonding and structure. Treagust (1988) lists ten stages in three broad areas that are necessary to develop a diagnostic test. The areas are defining the content, obtaining information about students' alternative conceptions, and developing the diagnostic test.

In order to define their content, thirty-three propositional knowledge statements were identified related to covalent bonding. Sample propositional statements on covalent bonding and structure include "Covalent bonds form between atoms of non-metals," "The shared electron pair is located between the nuclei of the atoms involved in the bond," and "Molecular substances with high melting and boiling points have strong intermolecular forces between molecules (Peterson & Treagust, 1989)." Related literature and unstructured interviews were used to obtain information about students' alternative conceptions. Finally, a two-tiered diagnostic multiple-choice test was developed, which
Table 2.1. Statistical Analysis of Students' Alternative Conceptions Regarding a Single Metallic Atom of a Solid. Raw data are taken from Ben-Zvi, et al. (1986).

<table>
<thead>
<tr>
<th>Property</th>
<th>Percent holding Misconception</th>
<th>Experimental Group (N = 383)</th>
<th>Control Group (N = 393)</th>
<th>$\chi^2$</th>
<th>Level of Significance</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conducts electricity</td>
<td></td>
<td>37.8</td>
<td>69.7</td>
<td>69.7</td>
<td>p &lt; .005</td>
<td>.30</td>
</tr>
<tr>
<td>Brown color</td>
<td></td>
<td>35.2</td>
<td>48.1</td>
<td>13.2</td>
<td>p &lt; .005</td>
<td>.13</td>
</tr>
<tr>
<td>Malleable</td>
<td></td>
<td>11.2</td>
<td>24.7</td>
<td>23.56</td>
<td>p &lt; .005</td>
<td>.17</td>
</tr>
<tr>
<td>Compressible</td>
<td></td>
<td>5.7</td>
<td>6.9</td>
<td>0.35</td>
<td>not significant</td>
<td></td>
</tr>
<tr>
<td>Expands on heating</td>
<td></td>
<td>6.8</td>
<td>10.4</td>
<td>3.2</td>
<td>not significant</td>
<td></td>
</tr>
<tr>
<td>Pungent odor</td>
<td></td>
<td>12.5</td>
<td>11.7</td>
<td>0.19</td>
<td>not significant</td>
<td></td>
</tr>
<tr>
<td>None of the above</td>
<td></td>
<td>32.3</td>
<td>7.6</td>
<td>74.7</td>
<td>p &lt; .005</td>
<td>.31</td>
</tr>
</tbody>
</table>
Table 2.2. Statistical Analysis of Students' Alternative Conceptions Regarding a Single Metallic Atom of a Gas. Raw data are taken from Ben-Zvi, et al. (1986).

<table>
<thead>
<tr>
<th>Property</th>
<th>Experimental Group (N = 383)</th>
<th>Control Group (N = 393)</th>
<th>$\chi^2$</th>
<th>Level of Significance</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conduct electricity</td>
<td>16.6</td>
<td>28.0</td>
<td>14.3</td>
<td>p &lt; .005</td>
<td>.14</td>
</tr>
<tr>
<td>Brown color</td>
<td>17.1</td>
<td>18.1</td>
<td>0.14</td>
<td>not significant</td>
<td></td>
</tr>
<tr>
<td>Malleable</td>
<td>1.8</td>
<td>4.3</td>
<td>23.6</td>
<td>p &lt; .005</td>
<td>.17</td>
</tr>
<tr>
<td>Compressible</td>
<td>16.1</td>
<td>29.8</td>
<td>19.6</td>
<td>p &lt; .005</td>
<td>.16</td>
</tr>
<tr>
<td>Expands on heating</td>
<td>18.7</td>
<td>30.0</td>
<td>13.5</td>
<td>p &lt; .005</td>
<td>.13</td>
</tr>
<tr>
<td>Pungent odor</td>
<td>30.7</td>
<td>48.1</td>
<td>24.9</td>
<td>p &lt; .005</td>
<td>.18</td>
</tr>
<tr>
<td>None of the above</td>
<td>35.1</td>
<td>8.1</td>
<td>82.9</td>
<td>p &lt; .005</td>
<td>.33</td>
</tr>
<tr>
<td>(no alternative conceptions)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
required students to answer questions regarding covalent bonding and then choose among possible explanations for their answers. The question was counted as being correct only if both subparts were answered correctly. Treagust concludes that a diagnostic test of this nature could be used either at the beginning or the end of a unit on atomic and molecular structure and covalent bonding in order to obtain clearer knowledge regarding students' alternative conceptions and ideas about how to remedy the problems (Treagust, 1988).

Peterson and Treagust (1989) administered their test on alternative conceptions of covalent bonding and structure (reliability (α) = .76) to two hundred forty-three high school chemistry students in western Australia. They concluded that overall, students did not acquire a satisfactory understanding of this topic, although grade-12 students apparently had a better understanding than did grade-11 students. Ability to establish the correct polarity of both bonds and molecules was low, perhaps in part because of confusion of the importance of electronegativity and unequal sharing of electron pairs in covalent bonds. Most students had difficulty ascertaining molecular shapes, which was attributed to weakness in the understanding of valence shell electron pair repulsion theory. Finally, most students had at least some alternative conceptions regarding intermolecular forces and physical properties of compounds (Peterson & Treagust, 1989).

**Concept Mapping as a Tool to Assess Alternative Conceptions.** One method that has been successfully used to diagnose students' alternative conceptions about a subject, particularly in the sciences, is concept mapping. Concept maps have been described by Wandersee (1990) as "maps of cognition." Cliburn (1990) describes uses of this technique as encompassing "the full spectrum of educational applications, from curriculum planning through instructing to evaluating the outcomes." Concept mapping was developed from Ausubel's cognitive educational psychology (Ausubel 1968; Ausubel et al., 1978; Cliburn 1990).
Using Ausubel's assimilative theory of cognitive learning (Ausubel, 1968), Novak and his students at Cornell University developed concept mapping as a tool to probe how students' concept meanings changed over time (Novak, 1990; Novak & Musonda, 1991). The following ideas, derived from the work of Ausubel, were central to the development of concept mapping (Ausubel, 1963; Ausubel, 1968; Novak, 1990). First, the cognitive structure is hierarchical. Most learning occurs when new concepts are subsumed under existing concepts or propositional ideas. From this proposition is derived the idea that concepts can be represented in frameworks, later described as "cognitive maps" or "concept maps" (Novak, 1990). Second, the connections between the concepts, or the links that form propositions from concepts, can be labeled. This labeling is essential in order to represent the conceptual and propositional meanings within a hierarchical framework. Labeling was not done in early maps, but longitudinal studies carried out for several years revealed its importance.

Novak (1990) states that recent studies, including work with concept maps (Flavell, 1985) tend to refute the Piagetian idea that cognitive systems of individuals are qualitatively different at different ages. Rather, older individuals (and older minds) have acquired more expertise or more organized knowledge. In areas in which an older individual is a complete novice, his or her mind may operate in a manner so as to appear similar to that of a much younger, inexperienced individual. Thus, it is difficult to identify "cognitive metamorphoses" at any given age (Novak, 1990). Symington and Novak (1982) found that primary-grade children could develop very thoughtful concept maps and could communicate their concepts to others.

Although the concept map may bear a striking similarity to a flowchart, in reality it is quite different, and Wandersee (1990) argues that, for a variety of reasons, the metaphor of the map is quite appropriate in description of the concept map. Unlike a flowchart, a concept map does not represent a sequence of steps to be followed in completion of a procedure. Rather, the concept map seeks to represent the psychological structure of
knowledge that exists in the mind of the mapper (Wandersee). The mapper identifies the key concepts, arranges them in a hierarchy from most general to most specific, and then connects these concepts using labeled links and branches. The completed concept map has been called "a schematic device for representing a set of concept meanings embedded in a framework of propositions (Novak & Gowin, 1984)." Because the theory of meaningful learning set forth by Ausubel et al. (1978) states that the cognitive structure is hierarchical, a properly constructed concept map should also be constructed in a hierarchy, with the most general concept at the top, and becoming progressively more specific towards the lower levels of the map (Novak & Gowin, 1984; Rye & Rubba, 1998)

In order to properly construct a concept map, the mapper must have an understanding of what constitutes a concept. Although Novak (1990) argues that he has yet to encounter a discipline in which the learner could not use concept mapping to diagram his or her psychological structure of knowledge, concept mapping has primarily been used as a tool of science educators. Concepts have been defined as "regularities in objects or events designated by some label, usually a term (Wandersee, 1990)." Thus, concepts generally can be described by nouns, and links can be described by verbs.

Some conventions frequently used in the construction of concept maps follow. Concepts are written using the miniscule case and are enclosed within circles, ellipses, or rectangles. Lines connecting concepts (links and crosslinks) must be labeled with linking words. A link which is not bi-directional may be labeled using an arrowhead. Because the map is hierarchical with the most general concept (the superordinate concept) at the top, each branch of the map can be read from top down. Finally, the examples which anchor the map may be included anywhere in the map. Traditionally, they are placed near the bottom. Despite their deceptively simple appearance, good concept maps are not easy to generate, and a good deal of practice is required before one can be said to have acquired expertise in concept mapping (Wandersee, 1990).
Although concept maps have been used for a wide variety of educational purposes (Cliburn, 1990), they have been particularly effective in the exploration of conceptual change (Wallace & Mintzes, 1990) and in the identification of critical junctures in learning (Trowbridge & Wandersee, 1994). Wallace & Mintzes (1990) used concept maps to explore conceptual change regarding the topic "Life Zones in the Ocean" during an elementary science methods course taught at East Carolina University in Greenville, North Carolina. Ninety-one subjects (ninety females and one male) received training, practice, and review on concept mapping in three sessions. Following this, the entire group was pre-tested on their knowledge of an experimental computer assisted instruction (CAI) program entitled "Life Zones in the Ocean." The testing instrument was supplied by the software publishers, Prentice-Hall Edunetics, with reliability (alpha) of 0.76. Forty two students were randomly assigned to an experimental group that was trained using the CAI program. The other forty nine students comprised a control group that was trained using an unrelated CAI program entitled "Body Defenses (Wallace & Mintzes, 1990)." The last session was devoted to post-testing. Both groups were tested using the same instrument used for pre-testing; in addition, both groups drew concept maps on "Life Zones in the Ocean."

A longitudinal study of science concept learning used concept mapping as a tool to assess both science knowledge and science alternative conceptions; confirming, in the authors' view, "the lasting impact of early instruction in science and the value of concept maps as a representational tool for cognitive development changes (Novak & Musonda, 1991)." These authors suggest the use of concept maps as "a useful alternative to the ubiquitous study sheets where students fill in blanks or respond in other ways, often without any substantial cognitive engagement or learning (Novak & Musonda, 1991)."

Trowbridge and Wandersee (1994) used concept mapping to identify critical junctures in a college course on evolution. They note that, "There seem to be certain points in the unfolding of a science course where students must possess an essential
framework of understanding based upon previously taught concepts in order to grasp the new material." This is the hypothesis of the "critical juncture," and was first suggested by Dr. Joel Mintzes (Trowbridge & Wandersee). In order to identify critical junctures in the learning of evolution, students in the evolution course described above concept mapped each lecture using five seed concepts supplied by the instructor and supplemented with five more concepts supplied by the student. These small concept maps are known as "micromaps." The superordinate concept (the highest concept in the hierarchy) chosen by each student for each lecture period was noted. In most cases, there was good agreement among students as to the appropriate superordinate concept. However, for two class periods, there was a wide divergence in the superordinate concepts chosen. These two points in the course were identified as "critical junctures." Trowbridge and Wandersee (1994) note that the material presented by the instructor during both of these periods was "coherent and organized," and postulate that the divergence in superordinate concepts was due to the fact that these two periods represented critical junctures, or times of peak difficulties for students in understanding the course content. The course instructor agreed that the topics presented during these two weeks were among the most difficult in the course. The results of this study may indicate that concept mapping could be used to identify critical junctures not only in courses on evolution but also in many other biology courses and indeed in other secondary and post-secondary science courses.

The Use of Concept Maps in Chemistry Instruction and Teaching. An excellent introduction to the use of concept maps in chemistry is given by Novak (1984); however, the use of concept maps as diagnostic and teaching tools is perhaps currently not used as much in chemistry as in the biological sciences. Nevertheless, some important work has been done in this area. Pendley et al. (1994) used concept mapping to investigate three factors underlying the problems that students encounter in their learning of chemistry. These factors are that students commonly learn by rote rather than constructing their own meanings, the subject matter remains "conceptually opaque" to students and they do not
recognize key concepts and relationships, and the instruction fails to present these key concepts and relationships. The authors did clinical interviews of six students (two women and four men) who volunteered for their first study of second-year college-level students enrolled in a physical/analytical chemistry course. All of the students were considered to be above average. Prior to instruction on chromatography, each student was interviewed to determine his or her current knowledge on this subject. Using transcripts of these interviews, the authors constructed concept maps representing each student's current knowledge on chromatography. Instruction on chromatography consisted of three fifty-minute lectures and three three-hour laboratory sessions. Following post-instructional interviews with the same students, concept maps were again constructed representing their knowledge of chromatography. An alternative procedure might be to train the students in concept mapping and have them construct their own maps.

In their second study, Pendley et al. (1994) studied five first-year graduate students (four men and a woman) who had not demonstrated competency on the American Chemical Society Graduate Analytical Chemistry Examination, and were therefore attending a set of lectures reviewing fundamentals of analytical chemistry. Prior knowledge of chromatography was again ascertained by clinical interviews and concept maps were prepared illustrating students' concepts. Students attended weekly lectures for three weeks, and six weeks later were given an examination. The post-instructional interview was conducted fourteen weeks after the last chromatography lecture because studies had shown that most information learned by rote is lost in six to eight weeks. Concept maps were again constructed using the post-instructional interviews (Novak, 1977). Analysis of the concept maps in both studies (Pendley et al.) revealed that even if instruction is conceptually complete, this alone does not convey understanding to the learner. In addition, the study indicates that the ability to solve numerical problems does not necessarily indicate conceptual knowledge of material. Finally, the authors conclude
that concept maps can offer a valuable tool to reveal strengths and weaknesses in student understanding in chemistry and can be used to facilitate meaningful learning provided students are taught to use this tool.

In an earlier study on the use of concept maps in chemistry, Ross and Munby (1991) investigated Ontario high-school students' understandings of the topic of acids and base, arguing that this methodological approach "both honours the relatedness of the concepts and depicts students' understandings in a way that models the relationships constructed by students" (Ross & Munby, 1991). The topic of acids and bases was chosen because of its great importance to high school chemistry and because not much was known about students' concepts of acids and bases (Ross & Munby). Concept maps were used both to guide data collection and to depict the results. A "Model Concept Map" designed to represent the acid-base content of the Ontario Ministry of Education Curriculum Guide, Part 13, was constructed by the authors, and key links were numbered with item numbers representing items on a multiple-choice test. This twenty-five item test contained fifteen items taken from the Ontario Assessment Instrument Pool provided by the Ontario Ministry of Education. Students in the study were all enrolled in a grade twelve physics class and had each completed a grade eleven chemistry class. Thirty-four students participated in the quantitative portion of the study, and eight students participated in the qualitative portion. High, medium, and low achievers were represented in the qualitative study, which consisted of two audio-taped interviews, conducted three days and four weeks following administration of the multiple choice test. During the interviews, each student was presented with four tasks, written on cards, regarding acids and bases. Questions regarding these tasks were asked and the answers recorded (Ross & Munby).

Concept maps were constructed for each of the eight students based on the qualitative interviews. Analysis of the multiple-choice test revealed that the students performed best on items dealing with pH and everyday phenomena, and had difficulty with ideas dealing with bases, ions, and balancing chemical equations. This was confirmed by the
qualitative studies and concept maps, which indicated that students did not in general understand that pH is a measure of both basicity and acidity, and that students had difficulty in establishing correct links among ions, pH, and other related concepts (Ross & Munby, 1991). The authors recognize that the small numbers of participants threaten the external validity of the study, but feel that this is less important than their generation of descriptions of students' concepts. They feel that the concept maps generated by students are particularly revealing in the gaps in understanding which they portray (Ross & Munby). However, it is perhaps worth repeating that the actual concept maps were constructed by the authors of the study and not by the participants.

Stensvold and Wilson (1990) investigated the interaction of verbal ability and concept mapping in one hundred and four ninth-grade students studying a set of laboratory activities in a midwestern city. Verbal abilities were measured using the vocabulary subtest scores on the Iowa Test of Educational Development. An experimental group was trained in concept mapping, whereas a control group received no such training. During one week, students in both groups completed a set of six laboratory activities on chemical reactions, and the experimental group concept mapped these activities. Following the activities, a thirty-three item test of comprehension was administered to both groups. Results demonstrated that the number of words on concept maps was not a significant predictor of achievement, but both the number of links and number of links per word were significant predictors (Stensvold & Wilson). From this finding, the authors concluded that "Concept map instruction should focus on relationships between concepts and not be limited to acquiring lists of items (Stensvold & Wilson)." Regression analysis of scores on the comprehension test and the vocabulary subtest of the Iowa Test of Educational Development further revealed that concept mapping appeared to be helpful to students with low verbal ability. However, the non-mappers with high verbal abilities outperformed their counterparts who did concept mapping. The authors suggest that this may indicate that students with good verbal ability...
ability may prefer a rote learning style, and in constructing concept maps they perhaps selected and attended to too little information. The authors conclude that, "High ability students may find concept mapping more useful if an effort is made to reduce possible interference with these students' learning patterns (Stensvold & Wilson). It should also be noted that these students had only a brief introduction to concept mapping, and further training might alter these results.

Another study of the use of concept mapping in the chemistry laboratory was done by Markow and Lonning (1998), who were concerned that first-year college chemistry students "learn little of the conceptual material associated with chemistry experiments they perform. These investigators studied a group of thirty-two non-science majors enrolled in a first-year chemistry course at a small private women's college. The experimental group constructed prelaboratory and postlaboratory concept maps, whereas the control group wrote essays explaining the conceptual chemistry of each laboratory exercise. Both groups took a twenty-five item achievement test one week after each laboratory exercise was completed. These investigators found no significant difference between the control and experimental groups with respect to students' conceptual understanding as determined by the achievement tests; however, students "responded very positively toward the use of concept maps in the laboratory (Markow & Lonning)."

Not all teachers of chemistry are enthusiastic about the use of concept maps. Zoller (1990) feels that students' alternative conceptions that are not interrelated logically or derived from one another are not readily addressed by the concept mapping approach and should be dealt with by an appropriate teaching strategy. For example, in organic chemistry, Zoller (1990) states that problems involving optical isomerism (a field of stereochemistry) are best dealt with using models, but offers no suggestion regarding how to diagnose alternative conceptions in this area. Although Zoller (1990) recognizes that concept mapping is a powerful tool in overcoming alternative conceptions, he advocates the use of specific teaching strategies for addressing specific concepts.
In a rebuttal to Zoller (1990), Cullen (1990) finds that concept mapping is entirely appropriate as a tool for teaching chemistry, and, in particular for teaching specific chemical concepts. Cullen states that a concept map does not need to contain all the concepts of a discipline in order to be valuable, and there is no reason not to draw separate concept maps for separate topics. In his discussion on nucleophilicity, Zoller gives a specific teaching scheme to teach this topic, implying that this specific strategy would be preferable to a concept map. Cullen offers a concept map for this topic and advises that a well-drawn concept map shows that the topic of nucleophilicity is not as "clear cut" as was implied by Zoller.

Problems in the Use of Concept Maps. Several authors in addition to Zoller (1990) have questioned various aspects of the use of concept maps as teaching and research tools. Advantages and disadvantages of concept maps have been reviewed by Ruiz-Primo and Shavelson (1996), who note the value of multiple investigations when drawing inferences regarding performance assessment. These authors note that the wide variety of concept maps can generally be classified into two major types: hierarchic concept maps, which were developed by Novak and Gowin (1984) in accordance with Ausubel's learning theory based on a hierarchical cognitive structure (Ausubel, 1968), and network concept maps, based on associationist theory (Deese, 1965) which characterizes concepts as nodes in a network. Although work with both types of maps continues, concept mapping as used in this study proposes to use hierarchic concept maps.

Ruiz-Primo and Shavelson (1996) also note that the response format used in producing concept maps varies greatly. A fill-in-the-blank format gives the user a framework of nodes and a list of terms and requires only that the appropriate term be placed at the proper node. Students can also be given all of the terms without a framework, some of the terms and no framework, or no framework or terms. The fill-in-the-blank format may be appropriate as a tool to train novice mappers, but it probably is
not appropriate when assessing knowledge structure. The response format is also important when assessing concept maps.

Assessing Concept Maps. Several different scoring rubrics have been developed for concept maps. Perhaps the first of these rubrics was developed by Novak and Gowin (1984) and was used by Wallace and Mintzes (1990) to score their post-test concept maps and more recently by Markow and Lonning (1998) to score both pre- and post-test concept maps. Using this scheme, one point is awarded for each valid proposition, five points for each valid level of hierarchy, one point for each branch, ten points for each valid cross-link, and one point for each valid general-to-specific example.

In the Wallace and Mintzes study (1990), the students with the five highest and the five lowest concept map scores were interviewed regarding their understanding of the material of interest one week after the final training session. Although preliminary analysis of both the pre- and post-test scores revealed statistically significant differences in knowledge of the material in favor of the experimental group, these differences were small, and the authors attribute them as being largely due to "pretest differentials" (Wallace and Mintzes). Analysis of the concept mapping scores revealed that the experimental group achieved substantial and significant gains in all five categories scored, whereas the control group demonstrated a modest gain in only one category (branching), perhaps attributable to a "practice effect." The authors suggest that "substantial and potentially important changes in both the complexity and propositional structure of the knowledge base are revealed in concept maps after only 45 minutes of computer-assisted instruction," and conclude that this technique provides a useful tool for probing changes in cognitive structure (Wallace and Mintzes). They finally note their belief that concept maps complement such techniques as clinical interviews, sorting tasks, and conventional testing instruments without duplicating them (Wallace and Mintzes).

Novak and Musonda (1991) developed a scheme based on ideas of Ausubel's assimilation theory (Ausubel et al., 1978), but nevertheless, they called the scheme
"somewhat arbitrary." Novak and Musonda first determined the number of conceptual levels (the "hierarchy"), and gave a score of ten points for each relevant first-level conception (broad, inclusive concept), with five points given for each second-level conception, two points for each third-level conception, and one point for each fourth-level conception. In addition, interlinkages on maps were scored as follows. Twenty points were given for each first level interlinkage, ten points for each second level interlinkage, and five points for each third level interlinkage. Ten points were deducted for each major misconception and three points for each minor misconception. The total score was determined by adding the points (Ausubel et al.). This scheme is obviously not appropriate when using a fill-in-the-blank format (Ruiz-Primo & Shavelson, 1996).

Trowbridge and Wandersee (1994) used a more subjective scale in their study on critical junctures in the study of evolution, assigning each concept map between one and four points. They then used a concept map performance index based on the scores of up to ten concept maps which attempted to reflect the total map points earned, the difficulty of each map, and the total number of assigned maps submitted. Some of the correlations (Pearson's r) observed by Trowbridge and Wandersee are as follows: course grade with map index, .230; course grade with map average, .323; lab grade with map index, 0.472.

Schreiber and Abegg (1991) developed a quantitative method for scoring concept maps generated by students in introductory college chemistry. Their scheme evaluates concept maps quantitatively by categories, with scores assigned for propositional validity and hierarchical structure. Schreiber and Abegg identified eight map constructs necessary to grade a concept map; these are listed in Table 2.3.

Schreiber and Abegg (1991) then used the following formula to determine total concept map score:

\[ X = [x - n(b + c)] + (b/c) \]

in which \( X \) = total concept map score, \( x \) = tally of points awarded for recognition of hierarchical, propositional, and validity constructs, \( n \) = number of strands on concept
map, b = ratio of sum of vocabulary terms to number of hierarchical levels, and c = summed ratios of number of valid connecting lines to total number of connecting lines drawn. Using this scheme, analysis of variance indicated a significant positive correlation between standardized American Chemical Society tests scores and students' overall concept map scores.

Reliability and Validity of Concept Map Scores. Many schemes used for scoring concept maps have not examined the reliability of the reported scores. Reliability, or the ratio of the (hypothetical) true score variance to the observed score variance, is "the degree to which test scores are consistent, dependable, repeatable, that is, the degree to which they are free of errors of measurement. Reliability has to do with score dependability or precision but not with score meaning, accuracy, or validity (Harvill, 1991, p. 33)." Perhaps reliabilities have not been calculated more frequently for concept map scores because of the difficulty in calculating any type of reliability when each subject does not answer the same set of questions. Reliability is frequently calculated using dichotomously scored items (e.g. KR$_{20}$ or KR$_{21}$ reliabilities), although this is not necessarily so. Several methods have been developed to calculate reliability coefficients when each subject answers the same questions, and an individual score can be determined for each (Crocker & Algina 1986). One way to calculate internal reliability, (e.g., Cronbach's alpha) of concept map scores would be to use the scoring scheme of Novak and Musonda (1991), with scores for relevant first-, second-, third- and fourth-level conceptions, first-, second-, and third-level interlinkages, and major and minor misconception each being counted as one item, for a nine-item test. Liu (1994) instead calculated reliabilities of concept map scores using Item Response Theory (Hambleton, Swaminathan, and Rogers, 1991).

A statewide study of concept mapping in Connecticut found that reliabilities based on both numbers of concepts and numbers of connections were fairly reliable, with reliability coefficients ranging from $r = .62$ to $r = .89$ on the topics of blood transfusion and
Table 2.3. Map Concepts Used in Scoring Concept Maps (Schreiber & Abegg 1991).

1. Total number of vocabulary terms incorporated into map
2. Number of hierarchical levels
3. Ratio of number of vocabulary terms to number of hierarchical levels
4. Number of connecting lines drawn
5. Number of connecting lines validly labelled
6. Ratio of connecting lines validly labelled to number of connecting lines drawn
7. Number of strands recognized within map
8. Number of cross-links between strands

Growing plants (Lomask, Baron, Greig, & Harrison, 1992). In addition, concept maps constructed from student essays on these subjects had reliabilities of .78 and .81, respectively. This study indicates that concept maps can be reliably scored; however, some other investigators have not had these types of results (Liu, 1994). Because most of the scoring schemes used for concept maps rely mainly on the structure of the maps rather than the correctness of the propositions, it can be argued that a key component is missing in determination of reliability.

Liu (1994) has noted that some investigators have found good correlation between concept map scores and student mastery as measured by traditional examination scores, while others have found only a poor correlation. Specifically, Liu (1994) notes that Fraser and Edwards (1985) found good correlation between concept map scores and end-of-unit tests, whereas only low correlation between concept map scores and standardized tests was found by Novak et al. (1983). Similarly, Trigwell and Sleet (1990) found that concept mapping scores correlated poorly with traditional examination scores. Liu (1994) speculates that this may be because different scoring schemes have been used for concept maps. An early scheme by Novak and Gowin (1984) advocated awarding one point for
each valid link, five points for each hierarchy, two points for insignificant cross-links, and ten points for significant cross links.

One possibility for determining reliability when using a scheme such as put forth by Trowbridge and Wandersee (1994) would be to train two or more raters, have each evaluate a set of concept maps, and calculate the inter-rater reliability (Crocker & Algina, 1986). This method was used by McClure, Sonak, and Suen (1999), who compared the reliabilities obtained when six different methods were used to score concept maps generated by students enrolled in an introductory course in educational psychology. Two different scorers rated each set of concept maps generated. Reliabilities in this study ranged from $r = .23$ to $r = .76$. These authors described their six scoring methods as holistic, holistic with master map, relational, relational with master map, structural, and structural with master map (McClure et al., 1999). When using the holistic method, two raters examined each concept map and assigned each map a score ranging from 1 to 10 based on the rater's judgment of the mapper's overall understanding of the concepts in the map. When using the relational method, each proposition within a given concept map was given a value ranging from zero to three, using a scoring scheme that evaluated the correctness of the proposition. The final concept map score was determined by adding the scores of each separate proposition. The structural scoring method was adapted from the scheme of Novak and Gowin (1984).

The holistic, relational, and structural scoring schemes were each modified by providing the scorers with master concept maps to be used as a guide in scoring. Scores generated by each method were analyzed by generalizability analysis using the GENOVA program (Brennan, 1983). "The g-coefficients are an estimate of the score reliability assuming a single rater (McClure et al., 1999)." The g-score for the holistic method without a master map was .67; when using a master map as a guide, the g-score for this method dropped to .36. The g-score for the structural method was .41; when using a master map as a guide, the g-score dropped to .23. Finally, the g-score when using the
relational method was .51; when using the master map as a guide, the g-score rose to .76. Based on these results, the authors recommended using a relational method with master map in order to rate individual concept maps (McClure et al.).

Scoring schemes such as that proposed by Wallace and Mintzes (1990) that rely on parameters such as the number of concepts, links, cross-links, and examples probably would be unreliable in scoring micromaps because the mapper is restricted to a small number of concepts, to be supplemented by a small number of his or her choice. Thus, the variances in some parameters will be small, perhaps artificially small, and the reliabilities as calculated by the proposed scoring schemes will be low. Another legitimate criticism of most of the schemes used to evaluate reliability of concept maps using these parameters is that they do not address whether the concept map actually measures student understanding. In other words, the map score may be reliable but have little use to student, teacher, or researcher. Whether information derived from concept maps is valid is an important issue.

Validity has been defined as "an integrated evaluative judgment of the degree to which empirical evidence and theoretical rationales support the adequacy and appropriateness of inferences and actions based on test scores or other modes of assessment (Messick, 1989)." Messick also notes that validity is a matter of degree, and that multiple lines of evidence should be used to establish validity. Messick lists five traditional types of validity, which are content validity, concurrent validity, criterion-related validity, predictive validity, and construct validity. Ruiz-Primo and Shavelson (1996) note that few studies have been done to evaluate the content validity of concept mapping, or whether the concept map scores accurately measure content. More work perhaps has been done with concurrent validity, a measure of how well the test of interest correlates with other accepted tests of achievement. Results, however, have been mixed. Ruiz-Primo and Shavelson (1996) report "substantial correlation" (ranging from .49 to .74) between concept map scores and science achievement as measured by the Stanford
Science Achievement test. However, others have determined concurrent validities near zero, and conclude that multiple choice tests measure a different type of learning. Novak et al. (1983) concluded that low concurrent validities between concept map scores and scores on multiple choice tests may mean that the former measure meaningful reception learning whereas the latter measure rote reception learning in accordance with Ausubel's learning theory. Clearly, more work is needed to clarify this.

In an effort to improve content validity of concept map scores, Rice, Ryan, & Samson (1998) attempted to link instructional objectives, concept maps, and multiple choice items from state criterion-referenced and national norm-referenced tests in seventh grade life science classes (Rice et al.). Upon completion of a given unit, students were given a set of concepts to map. A three-part scoring rubric for each concept map was developed that was based on the instructional objectives of the corresponding unit. Rubric A assigned points based on the presence or absence of the assigned concepts, rubric B assigned points based on correctness of the links between concepts, and rubric C assessed misinformation incorporated into the concept maps. As the authors state, "It is evident that Category A is mutually exclusive of Category B (Rice et al.)." This appears to place a limit on the variance in concept map scores. Rice et al. obtained reliabilities (KR-20) ranging from .63 to .88 on the seven sets of concept maps in their study. As evidence of content validity using this method, the coursewide correlation (Pearson's r) of total concept map scores (rubric B) to scores on related multiple choice questions was 0.90. Correlation of concept map scores to multiple choice items from each individual unit ranged from .22 to .68 (Rice et al.).

Studies on the other types of validity (criterion-related validity, predictive validity, and construct validity) and concept mapping are few. McClure et al. (1999) evaluated criterion-related validity by comparing individual concept maps to a master map using a set-theoretic method. A map similarity score was calculated for each map as compared to a master map, and the similarity score for each map was correlated to the score obtained
by each of the six scoring methods described above. Statistically significant correlations (as determined by Pearson's $r$) were obtained for five of their six scoring methods. The highest correlation ($r = .608$) was obtained when using their "relational scoring with master map," which also gave the highest reliability (McClure et al.).

Although validity has generally been evaluated in quantitative terms, qualitative researchers are now evaluating what they call "trustworthiness," and ask the question whether the researcher's findings are worthy of consideration (Lincoln & Guba, 1985). It should be asked whether qualitative techniques could be used in studies of the validity of concept maps and whether qualitative studies are of use in determining alternative conceptions.

**Some Alternate Schemes to Evaluate Concept Maps.** Perhaps because any scheme intended to assign a score to an individual concept map has inherent disadvantages, other methods to evaluate concept maps have been proposed. In their study on the use of concept maps as an interview tool for the investigation of students' understanding of global atmospheric change, Rye and Rubba (1998) proposed the use of a Pathfinder network in order to compare student-generated concept maps with the concept map generated by the course instructor (the "teacher-expert" concept map). The Pathfinder technique generates a "similarity index" through measurement of the proximity of concepts from student maps to those in the teacher-expert map. This similarity index has values ranging from zero to one. Use of the Pathfinder technique requires that all students and the "teacher-expert" map an identical set of concepts. In the Rye and Rubba study (1998), eight concepts were supplied (global warming, greenhouse gas, ozone layer, ultraviolet light, coolants, chlorofluorocarbons, depletion, and man made). No additional concepts could be added to the concept maps by the students.

The object of the Rye and Rubba (1998) study was to determine the relative effectiveness of two types of interviews in eliciting students' understanding of global atmospheric change following a unit on this topic. One type of interview required
students to generate concept maps as part of the interview process and the other did not. Although Rye and Rubba found no significant difference in the two interview methods, they did find that "the Pathfinder index was a reliable confirmatory measure of the degree to which students held the ideal postinstructional understanding" (Rye & Rubba). The highest Pathfinder index reported from seventeen concept maps analyzed was 0.786, and the lowest was 0.158, and the authors suggest that visual inspection of the concept maps indicate that there is a great deal of similarity between the teacher-expert concept map and the map of the student with the highest Pathfinder index. Similarly, "considerable dissimilarity appeared to exist in the cognitive structure between the teacher and the student who had the lowest Pathfinder index." Rye and Rubba's measurement of "ideal postinstructional understanding" is limited to comparison of student concept maps with the teacher-expert concept map through use of the Pathfinder index.

Concept maps are hierarchical in structure. The most general, superordinate concept should be placed at the top, and progressively more specific concepts should then be located further down the map (Novak & Gowin, 1984). Each level of a concept map can be considered as an ordinal rank, and each concept can be ranked according to its level within the map. Thus, a set of concept maps can be analyzed using nonparametric methods. The Kendall coefficient of concordance (Kendall's W), a nonparametric correlation coefficient (Leach, 1979), can be calculated to give a measure of how closely a given set of concept maps agree in the relative rankings of their concepts. If students are assigned a set of seed concepts as part of a concept mapping assignment, these seed concepts as a set should be present in every concept map. Because two or more concepts may occur in the same level, a method is needed to accommodate ties. One simple and effective method is to use a midrank technique (Leach). For example, if a concept map contains five seed concepts with one of these being the superordinate concept, two others tied at the second level, one on the third level, and a final seed concept on the fourth level, then the ordinal rank of the superordinate concept is 1, the ordinal ranks of the two seed
concepts that are tied are each 2.5, the ordinal rank of the lone seed concept on the third level is 4, and that of the last seed concept on the fourth level is 5. Review of the science education literature did not reveal any study in which Kendall's $W$ was used in this manner.

Like the well-known Pearson coefficient of correlation (Pearson's $r$) (Gravetter & Wallnau, 1992; Gall, Borg, & Gall, 1996), Kendall's $W$ has a value of 0 when no correlation exists and 1 or -1 when the correlation is perfect (Leach 1979). One difficulty that should be noted when using Kendall's $W$ to evaluate concept maps is that two different concept mappers may construct maps with different but equally valid hierarchies. "At first glance it may appear disturbing to see that the same set of concepts can be represented in two or more valide hierarchies" (Novak and Gowin, 1984, p. 17.).

Qualitative Evaluation of Alternative Conceptions. It appears that there is much about alternative conceptions and evaluation of concept maps that will be difficult to address using quantitative methods. "Because of the problem of idiosyncrasy, however, no research finding and no theory will ever generalize to every setting and to every child (Donmoyer, 1989)." Qualitative methods are finding their own niche in educational research, and mixed research methodologies are finding a new respectability. Howe (1988) asks, "But why should paradigms determine the kind of work one may do with inquiry any more than the amount of illumination should determine where one may conduct a search?" He concludes that "The growing tendency of educational researchers to resist the tyranny of methodological dogma is a good thing. It is high time to close down the quantitative versus qualitative conversation." Two commonly-used qualitative research tools are the interview and the student journal.

The Interview as a Tool in Qualitative Analysis. Several types of interviews have been identified and used in qualitative research. Among these are the informal conversational interview, the interview guide approach, the standardized open-ended interview, and the closed, fixed-response interview (Patton, 1990). When using the
informal conversational interview, the topics of questions or their wording is not
determined in advance. Rather, questions emerge from the immediate context of the
interview. In this type of interview, questions can be tailored to individuals and
circumstances, but different questions and different types of information will be collected
from different people, leading to less systematic data and sometimes causing difficulty in
data organization and analysis (Patton).

When using the interview guide approach, topics to be covered are specified in
advance in outline form, but the interviewer selects the sequence and wording of the
questions. Data collection is more systematic than in the informal conversational
interview, but the interviews remain somewhat informal and conversational. At times,
important topics may be omitted, and it can at times be difficult to compare responses of
different interviewees. The interview guide approach is frequently combined with the
informal conversational interview (Patton, 1990).

When using the standardized open-ended interview, the exact wording and sequence
of questions are determined in advance, but the questions are open-ended in format.
Because interviewees answer the same questions, comparability of responses is
increased. This format tends to reduce interviewer bias and facilitates organization and
analysis of data, but gives little flexibility to the interviewer to adapt to individuals or
circumstances. Because standardized wording of questions offers little flexibility in
tailoring questions to particular individuals and circumstances, the standardized open-
ended interview may "limit naturalness and relevance of questions and answers" (Patton,
1990, p. 289). The standardized open-ended interview is frequently combined with the
interview guide approach. The more structured, basic questions characteristic of the
standardized open-ended interview are generally asked first (Patton, 1990).

When using the closed, fixed response interview, both questions and response
categories are determined in advance, and the respondent must choose from a selection of
fixed responses. When using this interview format, data analysis is relatively simple and
many questions can be asked in a short time. However, respondents are limited in 
expression of both feelings and experiences, and this format can "distort what 
respondents really mean or experience by so completely limiting their response choices 
(Patton, 1990)."

Just as there are different formats for interviews, there are different types of 
interview questions (Patton, 1990). Among these are background and demographic 
questions, sensory questions (that seek information about what was seen, heard, felt, 
etc.) knowledge questions (that explore factual information possessed by the 
interviewee), experience and behavior questions (that elicit information about what an 
interviewee has done), opinion and value questions (aimed at "understanding the 
cognitive and interpretive processes of people", and feeling questions (that question 
emotional responses to experiences or thoughts) (Patton).

The clinical interview is frequently used in the study of alternative conceptions, and 
in fact has been described as the "workhorse" tool in this area (Wandersee et al., 1994). 
When using this technique, subjects are given objects, events, and situations to describe 
and explain (Finley, 1984). A think-aloud protocol is frequently employed (Lythcott, 
1990). Examples of the use of interviews to identify and categorize alternative 
conceptions in science include Treagust's (1988) study of alternative conceptions in 
eleventh and twelfth grade chemistry students, the Griffiths and Preston (1992) study on 
fundamental characteristics of atoms and molecules, the Demastes, Good and Peebles 
(1996) study of conceptual change in evolution, the Boo (1998) study of students' 
understanding of chemical bonds and energetics, and the Haidar (1997) study of 
preservice chemistry teachers' conceptions of conservation of mass. The disadvantage to 
interviews is that it is difficult for classroom teachers to diagnose alternative conceptions 
using this time-intensive technique; however, it is well-suited to research purposes.

Boo (1998) studied grade twelve students' understandings of chemical bonds and 
chemical changes through the use of a semistructured interview protocol. Forty eight
students were interviewed for this study, which asked what kinds of conceptions students have about chemical bonds, what kinds of conception they have about the energy changes involved, and what kinds of conceptions they have about the driving force behind chemical reactions. Boo used five events (hot copper in air, a burning candle, the Bunsen flame, addition of magnesium metal to dilute hydrochloric acid, and the reaction of aqueous lead nitrate with aqueous sodium chloride) and examined four aspects of each event. These aspects were the type of change predicted, the overall energy change predicted, how the process was conceived or imagined, and the driving force for the chemical change. Boo tabulated the results of the interviews and reported that, although students were generally successful in predicting types of chemical change, the majority believed that reactions such as burning a candle were endothermic because energy had to be supplied to initiate the burning. For most of these students, the chemical bond "was seen as a physical entity." In addition, students had little understanding of the relationship between electronegativity and chemical bonds, frequently conceived of a covalent bond as a single shared electron, and had difficulty conceiving the nature of the ionic bond or the three-dimensional nature of the crystal lattice. Half of the students confused the concept of element (sodium) with the concept of ion (sodium chloride) or of atom with ion (Boo).

Problem solving in chemistry has also been studied using interviews. Lythcott (1990) used this technique to study the relationship between high school chemistry students' chemical knowledge and their problem-solving performance, and found a slightly higher percentage of perfectly correct solutions among students who were trained to memorize algorithms than among those students than among students were trained in learning strategies. However, the percentage of totally inadequate solutions (students who had no ideas what to do) was also much higher in the group of students trained to use memorized algorithms (Lythcott, 1990). In conducting the interviews, students were asked to use a think-aloud protocol in which they said aloud the things that they usually
thought silently or muttered to themselves, and the researcher spoke only in order to encourage students to talk aloud during the process.

**Characteristics of Journals and Journal Writing.** According to Fulwiler (1987), the language of journals should be informal, and have many of the qualities that are commonly associated with conversational language. He cites several properties of journals, based on interviews with teachers who successfully use journal writing in the classroom. These are colloquial diction, first person pronouns, informal punctuation, rhythms of everyday speech, and experimentation. Thus, teacher and researcher should not expect the journal to be a formal document. However, certain formal features should be present, including frequent entries, long entries, self-sponsored entries, and chronology and chronological documentation (Fulwiler).

Fulwiler (1987) also lists what he describes as the cognitive modes that can be found in journal writing. Among these are observations, questions posed by the writer, speculations by the writer, self-awareness, digression, synthesis of ideas and finding new relationships, revision of prior entries, and information (which may be collected from lectures, books, articles and other sources).

Among the assumptions regarding the relationship between language and learning, Fulwiler (1987) cites Bruner's assertion that when connections between new learning and what is already known are articulated, new information is learned better, Emig's view that when people learn, all language modes are used (reading, writing, speaking, listening), and each contributes in a unique way, and Britton's (1975) statement that when people write about new information, they learn and understand it better.

Fulwiler (1987) lists several guidelines for assigning journals. Among these are an explanation that journals are neither diaries nor class notebooks, a suggestion that students do short in-class journal entries, and a suggestion that journals be counted in the student's grade but not actually graded. However, although the necessity of positive feedback from journal writing seems almost universal, others have devised more
elaborate grading schemes (Bailey & Markowicz, 1983; Malachowski, 1988; Pyle & Trammell, 1982).

The Use of Student Journals in Science Education Research. Peter Woodford (1967) once wrote, "It is surely no accident that greater lucidity and accuracy in thinking should result from the study of clarity and precision in writing. For writing necessarily uses words and almost all thinking is done with words." Statements like this indicate that appropriate writing could be an important tool in promoting metacognition in students, and journals that are used to promote metacognition have been called "thinking journals (Sullivan, 1994)." Hettich (1993) concluded that journal writing can be used to encourage students to reflect on course content and connect concepts to past and present experiences. In a small study of organic chemistry students, Steiner (1982) concurred, and although his data were largely anecdotal, he concluded that writing about classroom material correlated well with overall class performance.

Several precedents exist for the use of student journals both in science teaching and in science education research. In an introductory geology course at the College of Wooster, students were required to "maintain a regular thoughtful journal (Coles, 1991)." The course instructor concluded that use of this technique strengthened student achievement and provided immediate feedback. In these journals, it was noted that student writing developed in several stages. Initially, students simply restated ideas presented in class, but as the semester progressed, they began to synthesize two or more ideas and finally, late in the semester, applied new ideas. The instructor also found that the journals provided the opportunity to discover "confusion over ideas (Coles)."

The journal entries in this case were designed to cover a wide range of topics covering much of the content of an introductory geology course. Another instance of journal writing covering most of the content of an entire course is Malachowski's project at the University of San Diego (Malachowski, 1988). Malachowski used journal writing in an introductory chemistry course for nonmajors. The format was highly structured,
and students wrote at least two journal entries per day, which accounted for twenty-five percent of the total course grade. Journal entries were based on scientific observations made outside the classroom, in-class prompts, observations of classroom experiments, and response to other students' writing. Grading was based on the number of journal entries, the length of the entries (which were required to be at least one page in length), the detail of the entries, and the insights provided in the entries. Journal entries were graded on the basis of content rather than correctness of grammar. Malachowski stated that many of the entries were "particularly fascinating and showed uncommon insights that led to closer attention on my part." Approximately ten percent of class time (in addition to that spent out of class) was devoted to journal writing, and it was concluded that most students enjoyed writing component of the course, as assessed by their writing and the course evaluations. Malachowski has also incorporated journal writing in chemistry laboratory courses, and has concluded that this type of exercise hones observational skills and finds favor among students.

In contrast with studies on journals and student writing that cover the entire content of a course, Beall (1994) used student essays in his general chemistry class at Worcester Polytechnic Institute to specifically probe misconceptions in thermodynamics in freshmen. During the course of the semester, students were required to write three brief essays during class. Beall concluded that this type of writing was "a powerful means for identifying student problems and misconceptions so that they can be remedied at the time." Beall's study, however, was limited by the small number of essays required and the brief amount of time allotted for their writing, and perhaps the results obtained and the misconceptions identified are all the more remarkable because of this. Beall concluded that these writings, which were informal and ungraded, probed student knowledge in an effective yet unthreatening manner, and like the studies cited above, was pleased with student response.
Beall's (1994) writing assignments were highly structured; each was designed to address some specific point or specific learning difficulty. In another study, Beall and Trimbur (1993) list attributes of student writing assignments that were very successful, successful, and less successful. Some attributes of very successful assignments were that they directed students' interests and caused them to think about the purpose of the course, elicited unexpected answers and helped students realize that most assumptions made in science are not entirely true, and allowed students to express opinions. Successful assignments had no simple answer, allowed students to connect experimental results to model building, and required students to "synthesize a link between theory and observation," or to articulate a new concept. Less successful assignments could easily be written by simple examination of text or lecture. Beall and Trumbull found another unexpected consequence of student writing. Some students "mouthed off" in their writings, and a few refused to participate in any way. A small number found that writing caused them shame and felt that writing was not a proper component of a chemistry course. Beall and Trumbull attributed this to student "underlife," a sociological concept developed by Goffman (1963) referring to "the behaviors students draw upon to resist or reject or hedge on investing themselves completely in the roles and identities ascribed to them by institutions," and note that the concept of underlife has been applied to student writing. It should be noted that examples of "underlife" in student writing were few in number, and though deemed important, did not appear to be particularly useful to the instructors when diagnosing learning difficulties or alternative conceptions.

The use of student writing has not been without its detractors. In what they call "an heretical perspective," Lablanca and Reeves (1985) challenge the use of writing in chemistry, mainly because it requires a great commitment in time both from students and teacher. Atkison (1986) responded to the criticisms of these authors by saying, "If it is made clear to students that writing of a competent standard is essential for earning a respectable grade not just in a writing course but throughout one's major or core (or both)
requirements, it is pleasantly surprising how well they respond," and he concluded that writing can aid students in becoming self-educating.

Although used in an introduction to fiction class rather than a science class, Seshachari's experience with journals seems to be very instructive (Seshachari, 1994). Seshachari emphasizes the value of what are called "instructor-mediated journals," in which the student receives critique from the instructor on a regular basis. Through the use of traditional journals, students merely "lose their fear of writing" However, through instructor mediation, students also enhance their critical thinking skills, and "raise their level of discourse within their discipline (Seshachari)." Seshachari gave students credit no matter what they wrote and gave individuals only positive feedback. Negative comments were never written in the journals but rather were disguised as positive ones and presented to the class as a whole.

Rating Student Journals. Assigning numerical grades to student journals may be even more risky than scoring concept maps. Several authors have concluded that it is best to simply give students credit for their journals (Fulwiler, 1987; Seshachari, 1994; Steiner, 1982). Others have proposed various scoring rubrics, such as that proposed by Malachowski (1988), based on the number of entries, the length of each entry, the detail in each entry, and the kind and amount of insight described in each entry.

Evaluating Qualitative Data. Although qualitative researchers frequently use the term "trustworthiness" instead of validity, both refer to whether either a quantitative researcher's outcome variable or a qualitative researcher's reconstruction is worth paying attention to or is credible (Lincoln & Guba, 1985). Qualitative analysis can be used to triangulate quantitative data in order to achieve a richer and fuller picture. A very common method of analyzing qualitative data such as interviews is the constant comparative method of Lincoln and Guba, in which data are unitized, or broken into units that appear different from one another, and then iteratively categorized into a relatively small number of categories, generally not exceeding ten (Lincoln & Guba). A more
detailed approach to analysis of qualitative data is given by Spradley (1980). Spradley’s six steps include asking descriptive questions, making a domain analysis, asking structural questions, doing a taxonomic analysis, and asking contrast questions and making a componential analysis. Although Spradley’s approach gives a very structured format to the data, it has been this observer’s experience that it does not always answer the questions that need to be answered, and that frequently the method of Lincoln and Guba is to be preferred.

**Analysis of Clinical Interview Data.** The method by which clinical interview data are unitized and categorized is important in analyzing clinical interview data. Student knowledge as analyzed in this manner is frequently described in a manner similar to a description of the components of a concept map; that is, knowledge is organized in memory as networks of propositions composed of concepts and the specific relationships that link them together (Finley, 1984). Analysis of data of this sort is made particularly complex because of at least three factors. First, interview data are obtained serially, and only an approximation of the network of propositions held by the subject can be reconstructed by the interviewer. Second, statements made by subjects may include more than one proposition. And third, different words and sentence structures can be used to express the same meanings (Finley, 1984). Several approaches have been described and successfully implemented in analyzing clinical interview data. Perhaps most common is to write interpretations of subjects’ statements, including careful documentation of these statements, although various methods of constructing map-like representations have also found favor (Finley, 1984).
MATERIALS AND METHODS

Students from a one-semester course in organic chemistry at a Carnegie Research I Level public university in the Deep South participated in this study during the Fall, 1997, and Spring, 1998 academic semesters. Final enrollments in these two classes, both of which were taught by the author of this study, were 140 students and 83 students, respectively. In the university catalog, the course is simply described as consisting of the study of "aliphatic and aromatic compounds; biological aspects of organic chemistry (Louisiana State University, 1997)." Students commonly enrolled in this course have majors in pre-veterinary science, dietetics, agronomy, food science, dairy science, and other agricultural programs, and environmental science and environmental management systems. Chemistry, biochemistry, physics, biology, and microbiology majors generally do not enroll in the course. A summary of the course content and grading scheme is given in Table 3.1.

Interviews. Clinical interviews, described as the "workhorse" tool in alternative conceptions research (Wandersee et al., 1994), were used in this study. Using a think-aloud protocol (Lythcott, 1990), subjects were given objects, events, and situations to describe and explain (Finley, 1984) that were related to the learning of stereochemistry. A combination of the interview guide approach and the standardized open-ended interview was employed as described by Patton (1990), who lists background and demographic questions, sensory questions, knowledge questions, experience and behavior questions, opinion and value questions, and feeling questions as examples of types of questions that can be used in an interview. Examples of each were used in this study. Interview data were unitized, categorized, and analyzed according to the methods described by Lincoln and Guba (1985).

A total of ten students, five male and five female, were chosen from the Fall, 1997 and Spring, 1998, semesters to be interviewed. Twelve students were asked to participate over the course of two semesters. One student was unwilling, and one wished
<table>
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<tr>
<td>B</td>
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<tr>
<td>C</td>
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</tr>
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<td>The Alkanes: Structure and Nomenclature</td>
<td>2</td>
</tr>
<tr>
<td>Alkenes and Alkynes: Structure and Nomenclature</td>
<td>3</td>
</tr>
<tr>
<td>An Introduction to Organic Reactions</td>
<td>4</td>
</tr>
<tr>
<td>Reactions of Alkenes and Alkynes</td>
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</tr>
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<tr>
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<tr>
<td>Alcohols, Phenols, and Ethers</td>
<td>9</td>
</tr>
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</tr>
<tr>
<td>Proteins</td>
<td>17</td>
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</table>

\(^a\)Material covered and chapter numbers are from the course text, Bailey and Bailey (1995).
to participate but was unable to because of personal commitments. Participants were chosen to provide a range of academic abilities as evidenced by performance on the first test. In addition, participants were chosen in order to provide a distribution of majors and career goals that would be somewhat representative of the classes as a whole.

Each student was interviewed four times (with the single exception of one student who was prevented from attending his last interview because of illness), and each student was paid five dollars per session. Interviews were tape-recorded and transcribed, and the written work produced by the interviewees was retained and stored with the written transcripts. Interviews typically required between forty-five minutes and one hour, with some being slightly longer or shorter. The interviewer, who was also the course instructor and author of this study, is indicated throughout by his initials, G. L.

The first interview, consisting of nine questions, was designed to obtain biographical information about each student and probe some of the introductory course material on stereochemical topics, including usefulness of past learning on valence shell electron pair repulsion theory (VSEPR), visualization of the shapes of pi bonds, the nature of conformers, and various methods of representation of geometric and structural isomers. Questions prepared for this interview are given in Table 3.2.

At the time of the second interview (sixteen questions), the participants had not yet studied optical activity. Questions from this interview were designed to probe participants' understanding of the nature of conformers, geometric isomers, and structural isomers in cyclic compounds, particularly substituted cyclopentanes, cyclohexanes, and benzene derivatives. In addition to pencil-and-paper problems, participants were required to build and manipulate models in this and all subsequent sessions. Questions prepared for this interview are given in Table 3.3.

The third interview (sixteen questions) probed students' understanding of the representation of optical isomers. In particular, questions were designed to probe what
Table 3.2. Questions Prepared for the First Interview.

1) Each student was asked to give name, place and date of birth, information about schooling and family background, employment history, and career plans.

2) Did you study VSEPR or ED theory in either high school or your college freshman chemistry course? How has this helped you in C2060 thus far?

3) What difficulties do you have visualizing p-bonds?

4) Draw a picture of a molecule containing a p-bond, describing what you're doing as you go.

5) Draw me a picture of the conformers of this molecule. Describe what you're doing as you go.

\[
\text{Cl-CH}_2\text{-CH}_2\text{-Cl}
\]

6) Give me a name for this molecule. As you work, please describe what you're doing.

\[
\begin{align*}
H & \quad \text{H} \\
\text{H} & \quad \text{C} = \text{C} \\
\text{CH}_3\text{CH}_2 & \quad \text{CH}_2\text{Cl}
\end{align*}
\]

7) Please describe the relationship between these molecules, and describe for me what you're doing.

\[
\begin{align*}
\text{I} & \quad \text{II} \\
\text{ClCH}_2\text{CH}_2 & \quad \text{ClCH}_2\text{CH}_2 \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{C} = \text{C} \\
\text{H} & \quad \text{H} \\
\end{align*}
\]

\[
\begin{align*}
\text{III} & \quad \text{IV} \\
\text{ClCH}_2 & \quad \text{ClCH}_2 \\
\text{C} = \text{C} & \quad \text{C} = \text{C} \\
\text{CH}_3 & \quad \text{CH}_3 \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{C} = \text{C} \\
\text{H} & \quad \text{CH}_3 \\
\end{align*}
\]
Table 3.2 (cont.).

8) Draw the structure of this molecule and give it a name. As you work, describe for me what you are doing.

\[
\begin{tikzpicture}
\node at (0,0) [draw, circle, thick] (c) {};
\node at (-1,-1) [circle, thick, label=above:CH\textsubscript{2}CH\textsubscript{3}] (a) {};
\node at (1,-1) [circle, thick, label=above:CH\textsubscript{3}] (b) {};
\node at (0,1) [circle, thick, label=above:H] (c) {};
\node at (-1,1) [circle, thick, label=above:H] (d) {};
\node at (1,1) [circle, thick, label=above:H] (e) {};
\end{tikzpicture}
\]

9) Give this molecule a name. As you work, describe for me what you are doing.

\[
\begin{tikzpicture}
\node at (0,0) [draw, rectangle, thick] (c) {};
\node at (-1,-1) [rectangle, thick, label=above:Cl] (a) {};
\node at (1,-1) [rectangle, thick, label=above:Cl] (b) {};
\end{tikzpicture}
\]
Table 3.3. Questions Prepared for the Second Interview.

1) Build a model of any dichlorocyclopentane and draw it. Discuss what you are doing as you go. If you are unsure of something, please ask.

2) Can you build a conformer of this molecule? Why or why not?

3) Build all of the models of dichlorocyclopentane that you can. Give each one a name and draw it. Describe what you are doing as you go.

4) On your paper, find the pairs of geometric isomers and the pairs of structural isomers. Describe what you are doing as you go.

5) Build a model of any dichlorocyclohexane and draw it. Discuss what you are doing as you go.

6) Can you build a conformer of this molecule? Why or why not? Please try, using your model.

7) Now build all of the models of dichlorocyclohexane that you can. Give each a structure and name it. Describe what you're doing as you go.

8) On your paper, find the pairs of geometric isomers and the pairs of structural isomers. Describe what you're doing as you go.

9) Please build a model of this, describing what you're doing as you go.

```
\begin{center}
\begin{tikzpicture}
  \node at (0,0) [below left] {H};
  \node at (1,1) [above] {H};
  \node at (2,0) [below left] {Cl};
  \node at (2,-1) [below] {Cl};
  \node at (2,-2) [below] {Cl};
  \node at (2,-3) [below] {Cl};
  \node at (2,-4) [below] {Cl};
\end{tikzpicture}
\end{center}
```

10) Now build a model of this, describing what you're doing as you go.

```
\begin{center}
\begin{tikzpicture}
  \node at (0,0) [below left] {Cl};
  \node at (1,1) [above] {Cl};
  \node at (2,0) [below left] {H};
  \node at (2,-1) [below] {H};
  \node at (2,-2) [below] {H};
\end{tikzpicture}
\end{center}
```

11) What is the relationship between these two structures?

12) How could you convert one to the other? Please do this for me.
Table 3.3 (cont.).

13) Please build a model of this, describing what you're doing as you go.

14) What is the relationship between these three structures?

15) Draw all of the isomers of dichlorobenzene that you can. Give each of them a name. Describe what you're doing as you go.

16) What type of isomers do you have here. Why? Can you make any conformers of this molecule? Why or why not?
strategies the participants utilized in order to determine whether two representations were enantiomers, diastereomers, or different representations of the same molecule, the reluctance or willingness of participants to use molecular models, and the ability of participants to correlate a three-dimensional model with a two-dimensional representation on a piece of paper. Questions prepared for this interview are given in Table 3.4.

The fourth interview consisted of fifteen questions and, because of its length, not every student was able to complete some of the questions. This interview probed student understanding of the importance of stereochemistry to chemical reactions and mechanisms. Questions about first and second order nucleophilic substitution reactions (SN1 and SN2, respectively) and second order elimination reactions (E2) were asked. Questions prepared for this interview are given in Table 3.5.

This fourth interview required students to use two different sets of models to demonstrate what occurs in both first and second order nucleophilic substitution reactions (SN1 and SN2, respectively). As the SN1 reaction proceeds, the leaving group leaves before approach of the nucleophile, forming an intermediate planar carbocation. After this, the nucleophile enters as illustrated in Figure 3.1. Because the intermediate is planar, approach of the nucleophile is equally likely from either side, and if the initial reactant is chiral, the final product will be a racemic mixture consisting of an equimolar mixture of enantiomers.

In the mechanism of the SN2 reaction, the nucleophile enters at the same time that the leaving group departs, simply forming a transition state. This process is illustrated in Figure 3.2. Because the nucleophile must enter from the back side and force the leaving group out, inversion of configuration occurs in this mechanism, and if the reactant is chiral, only one enantiomer forms as the product.

A wooden model designed to illustrate the process of nucleophilic substitution was designed and built for use in this set of interview questions. Use of this model was demonstrated to the entire class before the individual interviews. The model consisted of
Table 3.4. Questions Prepared for the Third Interview.

1) Describe the relationship between compounds A and B. Describe what you are doing as you go.

![Compound A and B](image)

2) Draw a non-three-dimensional (dash) representation of this molecule and name it. Describe what you are doing as you go.

3) Build a model of each structure from question one and show me what they are (same compound, enantiomer, etc., depending on what was said in question 1.)

4) What is the relationship between the following two structures? Tell me what you're doing as you go.

![Compound A and B](image)

5) Build a model and name this compound.

6) What is the relationship between the following two structures? Tell me what you're doing as you go.

![Compound A and B](image)

7) Build models of these compounds and show me what the relationship is.

8) What is the relationship between the following two structures? Tell me what you're doing as you go.

![Compound A and B](image)

9) Build models of these compounds and show me what the relationship is.

10) Give the compound a name.
11) What is the relationship between the following two structures? Tell me what you're doing as you go.

![Diagrams of structures A and B]

12) Build models of these compounds and show me what the relationship is.

13) What is the relationship between the following two structures? Tell me what you're doing as you go. Build models if you wish.

![Diagrams of structures A and B]
Table 3.5. Questions Prepared for the Fourth Interview.

1) Use the wooden model to demonstrate what happens in an SN2 reaction. Describe which atom you choose to be the nucleophile and which atom you choose to be the leaving group. Describe for me what you're doing as you go.

2) Now use the "normal" models to do the same thing and describe the difficulties that you have.

3) Use the wooden model to demonstrate what happens in an SN1 reaction. Describe which atom you choose to be the nucleophile and which atom you choose to be the leaving group.

4) What kind of reaction is this?

\[
\text{HS}^- + \text{CH}_3\text{CH}_2\text{CH}_3\rightarrow \text{SN}_2
\]

5) What is the nucleophile? The leaving group?

6) Does this reaction proceed through a transition state or an intermediate? Why is this important stereochemically?

7) Draw what happens in this reaction in three dimensions.
   a) What difficulty do you have and how can you solve it?
   b) Give the mechanism as well as you can.

8) What kind of reaction is this?

\[
\text{HS}^- + \text{CH}_3\text{CH}_2\text{CH}_3\rightarrow \text{SN}_1
\]

9) What is the nucleophile? The leaving group?

10) Does this reaction proceed through a transition state or an intermediate? Why is this important stereochemically?

11) Draw what happens in this reaction in three dimensions.
    a) What difficulty do you have and how can you solve it?
    b) Give the mechanism as well as you can.
12) What kind of reaction is this?

13) What is the product? Why?

14) Draw the structure of the product.

15) If $H_a$ is anti to the Cl, what is the product? Why? $H_b$? 
Figure 3.1. Mechanism of first order nucleophilic substitution. The symbol Nu is used for the nucleophile, and LG for the leaving group. In this example, both nucleophile and leaving group have a negative charge.

\[ \text{Nu}^- + \text{Nu} \rightarrow \text{Nu} \]

Figure 3.2. Mechanism of second order nucleophilic substitution. The symbol Nu is used for the nucleophile, and LG for the leaving group. In this example, both nucleophile and leaving group have a negative charge.
a wooden hoop connected to a wooden base. Attached inside the hoop were three wooden balls, each of which represented a substituent on a central carbon atom. Attached to each ball was a cup hook capable of holding a rubber band, which represented a sigma bond.

Attached to the base were two wooden posts, each of which could hold a removable wooden ball. These two balls represented nucleophile and leaving group, and each also contained one cup hook capable of holding a rubber band. The wooden ball representing the central carbon atom contained five cup hooks. Figures 3.3 - 3.5 illustrate this model used at various points in the $S_N2$ mechanism.

Figure 3.3 illustrates the configuration of the model when it represents the reactant. In second-order nucleophilic substitution ($S_N2$), the nucleophile, represented by a wooden ball entering from the right, enters and forms a transition state (Figure 3.4). After this, the leaving group departs, forming a product with inverted configuration (Figure 3.5).

Because the central wooden ball representing the chiral center can accommodate up to five bonds and assume trigonal planar, tetrahedral, and trigonal pyramidal shapes, the wooden model shown in Figures 3.3 - 3.6 can be used to demonstrate formation of both the planar $S_N1$ intermediate (Figure 3.6) leading to subsequent racemization, and the trigonal pyramidal $S_N2$ transition state (Figure 3.4) leading to subsequent inversion of configuration. Commercially available models such as the set used in this study (Prentice-Hall Molecular Model Set for Organic Chemistry$^{TM}$) are inflexible at the chiral center and cannot be used as satisfactorily to represent either the mechanism or change in stereochemistry (retention or inversion of configuration) that occurs. These types of inflexible models will be referred to as "static models" in this study.

**Concept Maps.** During each of the three semesters in which this study was performed, a portion of each of the first few lecture periods was devoted to teaching the skills needed to construct concept maps. Twelve sets of seed concepts (containing
Figure 3.3. Wooden model representing the reactant in either $S_N 1$ or $S_N 2$ reaction. The wooden ball on the far left represents the leaving group and the empty peg on the right is capable of holding the ball representing the nucleophile.

Figure 3.4. Wooden model representing the transition state in the $S_N 2$ mechanism.
Figure 3.5. Wooden model representing the product of the SN2 mechanism. The wooden ball on the far right represents the nucleophile, and the empty peg on the left held the leaving group.

Figure 3.6. Wooden model representing the intermediate carbocation of the SN1 mechanism. The wooden pegs on both the left and right are empty because the leaving group is gone and the nucleophile has not yet approached the intermediate.
between four and six seed concepts) were developed, generally dealing with stereochemical topics, and were assigned at the appropriate times during each semester (Table 3.6). Each concept map was designed to cover material that was covered in either one lecture period or two consecutive lecture periods and are listed in the order in which they were assigned (Table 3.6). Concept map 1 covered hydrocarbons and the types of bonds in these molecules, concept map 2 covered conformer, conformer extremes, and the equilibrium between these extremes, and concept map 3 introduced isomers, structural isomers, and geometric isomers. Concept map 6 introduced reaction intermediates and the methods by which they are formed, concept map 7 introduced enantiomers and their properties, and concept map 8 covered the importance of stereochemistry to mechanisms. Concept map 9 related types of stereoisomers to structural isomers, and concept map 10 investigated further the relationships between stereochemistry and mechanism. At times, the organization of the course dictated that some concept maps not dealing primarily with stereochemical material be assigned. These concept maps (Table 3.6, maps 4, 5, 11, and 12) are included in this study.

Each student-generated concept map was analyzed to determine what, if any, difficulties in learning might be expressed in the map. In addition, maps were analyzed to determine to what degree the choice of superordinate concept agreed from map to map. Finally, the agreement in choice of map level for the seed concepts in a set of maps was analyzed using Kendall's W.

Student Journals. Students were required to keep a journal in which they wrote their views on how they learned organic chemistry. A set of directions for writing this journal was given to the students and is reproduced in Table 3.7. Students were required to write a journal entry on each day that they attended class. For most of these days, students could write on any subject that seemed to them to be relevant to the class; however, on eleven days, a topic was assigned that was relevant to their learning of stereochemistry. These topics are given in Table 3.8. Journals were collected four times during the
Table 3.6. Seed concepts for concept maps.

<table>
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<th>Map 1</th>
<th>Map 2</th>
<th>Map 3</th>
<th>Map 4</th>
<th>Map 5</th>
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<td>eclipsed</td>
<td>stereoisomer</td>
<td>elimination</td>
<td>free radical</td>
<td>free radical</td>
<td>chemical properties</td>
<td>mirror image</td>
<td>stereoisomer</td>
<td>alkene</td>
<td>carboxylic acid</td>
<td></td>
</tr>
<tr>
<td>hydrocarbons</td>
<td>staggered</td>
<td>geometric isomer</td>
<td>addition</td>
<td>electrophile</td>
<td>electrophile</td>
<td>plane polarized light</td>
<td>inversion</td>
<td>enantiomer</td>
<td>proton</td>
<td>oxidation</td>
<td></td>
</tr>
<tr>
<td>multiple bonds</td>
<td>rotation</td>
<td>conformer</td>
<td>reaction intermediate</td>
<td>nucleophile</td>
<td>leaving group</td>
<td>racemic mixture</td>
<td>absolute configuration</td>
<td>diastereomer</td>
<td>inversion</td>
<td>elimination</td>
<td>reduction</td>
</tr>
</tbody>
</table>

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Table 3.7. Journal Guidelines

1. The journal must be kept in a sewn, bound composition book. Spiral notebooks are not acceptable.

2. The journal must be written neatly in ink.

3. You must have an entry consisting of at least one page for each day that class meets (except test days). You can have additional entries if you wish.

4. You must answer each of the assigned questions at the appropriate time during the semester. Note that there are only 11 assigned questions. You must, however, write something for every class period.

5. The journal should not be a rehash of the lecture. You should already have a good set of lecture notes! Rather, the journal should give your insights as to how you learn the material, the difficulties you have with the material, the strategies that you employ when you study and learn the material, and the analogies and metaphors that you find useful.

6. It's your journal! You should feel free to be creative with it! If you take the journal seriously, there will be no "right" or "wrong" answers. However, cavalier or frivolous entries will be graded accordingly.

7. It takes some time to produce a good journal entry. You can't do it in five minutes!

8. If you want to use the journal as a means to communicate with me during the semester, please give it to me to read and I'll get it back as soon as possible.
Table 3.8. Assigned Journal Questions

<table>
<thead>
<tr>
<th>Number</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>What do you personally find to be the most difficult and the easiest aspects regarding understanding molecular and electron pair geometries? Explain in detail. In other words, what was difficult and why? What was easy and why?</td>
</tr>
<tr>
<td>2</td>
<td>Compare the difficulties you experience when you are given a structural formula and asked to give the name with the difficulties you experience when you are given a name and asked to draw the structural formula. What is more difficult and why?</td>
</tr>
<tr>
<td>3</td>
<td>Clearly describe in your own words the differences between structural isomers, geometric isomers, and conformers.</td>
</tr>
<tr>
<td>4</td>
<td>We have seen two classes of compounds (alkenes and cyclic alkanes) that demonstrate geometric isomerism. Compare the strategies that you use to determine whether a specific compound in each class can exhibit this type of isomerism. Give an example in each case.</td>
</tr>
<tr>
<td>5</td>
<td>Describe in your own words the relationship between electrophile, nucleophile, carbocation, and carbanion when these species occur in reaction intermediates.</td>
</tr>
<tr>
<td>6</td>
<td>How do you determine what types of compounds may form two different products when Br₂ is added across a double bond? List and discuss as many different factors as you can.</td>
</tr>
</tbody>
</table>
| 7      | What strategies do you use when you look at the structure of an alkene in order to determine:  
   a) whether it is capable of cis-trans- isomerism?  
   b) how highly substituted it is? |
| 8      | Describe the strategies that you find to be the most useful when you identify and distinguish between the following:  
   a) structural isomers  
   b) stereoisomers  
   c) geometric isomers  
   d) enantiomers  
   e) diastereomers |
Table 3.8 (cont.).

Number Assignment

9 You have been given the structures below, both of which represent 2-butanol, and are asked to determine whether they represent the same compound or enantiomers. You decide that you need to prove this to yourself rather than simply following a set of rules regarding the exchange of substituents.

Describe what strategies you employ and the difficulties you encounter.

\[
\text{CH}_3 \quad \text{&} \quad \text{CH}_3
\]

\[
\text{HO-CH}_2\text{CH}_3 \quad \text{&} \quad \text{HO-CH}_2\text{CH}_3
\]

10 What is your opinion of journal writing as a learning tool? Please consider the following points:
   i) What benefits do you feel that you have received from journal writing in this class?
   ii) Does journal writing provide a means for you to monitor how you learn? Please explain.
   iii) Would you consider keeping a journal in classes in which it is not required? Why or why not?
   iv) If you were a teacher, would you consider assigning journal writing as an exercise for your class? Please explain your answer.
   v) What would you do differently if you were to assign journals to this class?

11 What is your opinion of concept mapping as a learning tool? Please consider the following points:
   i) What benefits do you feel that you have received from concept mapping in this class?
   ii) Does concept mapping provide a means for you to monitor how you learn? Please explain.
   iii) Would you consider drawing concept maps in classes in which it is not required? Why or why not?
   iv) If you were a teacher, would you consider using concept mapping in your class? Please explain.
   v) What would you do differently if you were to assign concept maps to this class?
semester, student writings were evaluated, and journals were returned to the students with instructor comments. These journals were collected on final time at the end of the semester and kept by the course instructor. The journals were evaluated as roughly 15% of the course grade.

The Participants. Six students were interviewed for this study during the Fall, 1997, semester, and four additional students were interviewed during the Spring, 1998, semester. It was intended to interview each student four times for a total of forty interviews; however, due to illness, one student was unable to complete the last scheduled interview. Interviewees were chosen by stratified purposeful sampling (Gall et al., 1996) to give a set of students deemed representative of the entire class in terms of college major and gender. Each interviewee was paid five dollars per interview. The typical length of an interview was from forty-five minutes to one hour, with a few interviews lasting a bit longer. A brief biography of each participant follows; names have been altered in order to preserve confidentiality. The six participants from the Fall, 1997, semester are listed first, followed by the four participants from the Spring, 1998, semester.

James was born in New Orleans although his parents currently live in a small town in southern Louisiana. His father is an engineer for an oil company, and his mother has had a variety of part-time jobs and is currently a homemaker. James is currently majoring in wildlife management and would like to combine this with his interest in photography. He graduated from high school in 1994 and was twenty-one years old at the time of the interview. He plans to graduate in 1998.

Tammy is from a small Louisiana town north of Baton Rouge. Her parents are divorced; her father is a factory worker and her mother is a secretary. She attended a small private elementary and high school, and began her postsecondary education at Northwestern Louisiana University in Natchitoches before transferring to Louisiana State University. She is currently majoring in dietetics, but originally was in pre-medicine and for a time
was majoring in nursing. She plans to get both a bachelor's and master's degree in dietetics. She was twenty years old at the time of the interview, and plans to graduate in 1998.

Andrea was born in 1978 and is from a small Louisiana town east of Baton Rouge. Her father was in the navy and is currently disabled; her mother is a counselor. She is in the pre-veterinary program at Louisiana State University and hopes to graduate in 1999.

Anna is from Alexandria, Louisiana, and is thirty-one years old. She has a degree in merchandising from Louisiana State University, and has worked as an assistant buyer and area sales manager for well-known retailers in this area. Although she feels that she is good at this work, she does not feel that she is a businesswoman, and would rather work with animals. She therefore has returned to Louisiana State University to take coursework that would allow her to be admitted to veterinary school.

Michael is from the Houston, Texas area. His father is a dentist and his mother teaches first grade. He is majoring in environmental management systems and is planning on going to graduate school, perhaps at the University of Wisconsin. Although he spent a summer at Austin Community College, most of his college course work has been taken at Louisiana State University. Michael is currently teaching a computer lab for environmental statistics. He has been diagnosed with mild dyslexia.

Brian is from Baton Rouge and his parents run two restaurants in this area. On graduation from high school, he went to school in San Antonio ("to play baseball") and has since returned to Louisiana State University. Brian was twenty-one years of age at the time of the interview and is hoping to graduate in 1999. He is majoring in environmental engineering.

Kathy was raised on her family's Louisiana farm and was twenty years old at the time of the interview. All of her collegiate education has been at Louisiana State University. She is majoring in agronomy and works part time for a wheat breeder. When asked if she wants to go back to the family farm, she said, "I do, but there's not
enough money in it right now." She would like to do agricultural research and perhaps teach at the university level.

David is a dietetics major from a small town south of Baton Rouge. He was twenty-seven years old when interviewed. He currently works at a local book store. All of his college course work has been at Louisiana State University.

Marianne is from Baton Rouge, though both of her parents were born in Bombay, India. Her father is an electrical engineer, and her mother was a medical technologist, although she currently does not work outside the home. Marianne was twenty years old when interviewed and has done all of her college work at Louisiana State University. She currently is employed part-time at the Pennington Biomedical Research Center and is majoring in medical technology. Marianne plans to graduate in 1999 and pursue her medical technology degree at a medical school in New Orleans.

Jason was raised on a family farm southwest of Baton Rouge and was twenty-one years old when interviewed. He attended Louisiana State University at Alexandria for one year, Southwestern Louisiana University for one year, and then returned to LSU-A for another year before coming to Louisiana State University in Baton Rouge. He is majoring in agronomy and plans to return to the family farm on graduation.

A summary of the participants in this study is given in Table 3.9.
Table 3.9. Participants in This Study.

<table>
<thead>
<tr>
<th>Participant</th>
<th>Age&lt;sup&gt;a&lt;/sup&gt;</th>
<th>College Major</th>
<th>Semester&lt;sup&gt;b&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>James</td>
<td>21</td>
<td>wildlife management</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Tammy</td>
<td>20</td>
<td>dietetics</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Andrea</td>
<td>19</td>
<td>pre-veterinary medicine</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Anna</td>
<td>31</td>
<td>pre-veterinary medicine</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Michael</td>
<td>20</td>
<td>environmental management systems</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Brian</td>
<td>21</td>
<td>environmental engineering</td>
<td>Fall, 1997</td>
</tr>
<tr>
<td>Kathy</td>
<td>20</td>
<td>agronomy</td>
<td>Spring, 1998</td>
</tr>
<tr>
<td>David</td>
<td>27</td>
<td>dietetics</td>
<td>Spring, 1998</td>
</tr>
<tr>
<td>Marianne</td>
<td>20</td>
<td>medical technology</td>
<td>Spring, 1998</td>
</tr>
<tr>
<td>Jason</td>
<td>21</td>
<td>agronomy</td>
<td>Spring, 1998</td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents the participant's age at the time of the interview.

<sup>b</sup>Represents the semester in which the participant was interviewed.
INTERVIEW 1 RESULTS

The first interview was conducted approximately one month after the beginning of the course. This interview was designed to investigate the methods used by students to represent pi bonds, conformers, structural isomers, and geometric isomers in three dimensions.

Use of Valence Shell Electron Pair Repulsion Theory. Many students are exposed to ideas regarding the shapes of molecules when they study valence shell electron pair repulsion theory (VSEPR), sometimes known as electron domain theory (ED), which is commonly covered in college-level freshman chemistry textbooks (Bodner, Rickard, & Spencer, 1996; Brown, LeMay, & Bursten, 1997). This theory provides a guide for predicting three-dimensional shapes of molecules. Each student was questioned as to whether he or she had studied VSEPR and whether this material had been helpful in the study of the shapes of organic molecules (Table 3.2, Question 2).

All of the participants, no matter where they took their first year of college chemistry, remembered studying VSEPR; however, most of them did not feel that it was particularly helpful in their study of organic chemistry or learning about the shapes of organic molecules. Some typical responses to the question of whether VSEPR had been helpful were, "Like, I just, I haven't went back to my notes," (Marianne); "Well, it happened so long ago, I kind of don't remember it," (Jason); "Probably if I would go back and look at it, it would. But I'm lending my notes to a friend," (Kathy); and "Mm, I'd say it didn't hurt" (Brian). One student (Tammy) claimed that she'd used VSEPR on the first test, but, "I've already forgotten; I know I've used it. For ... what did we use that for?" Tammy thought that she used VSEPR in the determination of formal charge although this is not properly a part of VSEPR. Only one student, Anna, clearly made use of her knowledge of VSEPR and attempted to correlate what she had learned in her freshman chemistry class with what she learned in organic chemistry. She said, "In fact, when you started going over that, I went back and pulled out those charts that I made that went
over, like, the hybridization, steric numbers, coordination numbers." She felt that learning this material helped her visualize molecules in three dimensions.

**Representing Pi Bonds.** Most of the students said that they had little trouble in visualizing the shapes of pi-bonds (Table 3.2, Questions 3 and 4). A simple "no" was frequently the response when asked if there was any difficulty visualizing pi bonds. One student, Michael, admitted to some difficulties, but "once I saw the illustrations in the book, I got it." However, when asked to draw a molecule containing a pi bond, the responses were very different. Jason asked, "So it'd have to be a ... like a triple bond to have a pi bond?", clearly unsure as to whether a simple double bond would suffice.

Anna, an excellent and conscientious student, was unclear where to start. "Okay, can it be just any molecule? Even one I make up?" Michael was unsure what bonds to include in his drawing. "You want me to draw the sigma bond and everything, too?" And Marianne was unsure where to begin. "I don't even know which one has a pi bond. I just know what it looks like." When prompted to draw a two-carbon alkene, she was able to complete the task. Seven of the students eventually drew some representation of ethene (the simplest hydrocarbon containing a pi bond), and another drew a 1,1-dialkylethene. The last two simply drew a pi bond between two atoms without specifying the composition of the whole molecule.

Each diagram of a pi bond had some type of problem associated with it. Most of these could be described as either problems resulting from drawing the wrong number of bonds to a carbon atom or problems resulting from representation of the geometry of the pi bond. A good example is Tammy's representation of ethene. She had little difficulty describing either what she was doing or the properties of the molecule. "Okay. I'm drawing a double bond between a carbon and a double bond has one sigma bond and one pi bond. So this would be like the sigma bond and this would be like the pi bond. And it looks like two, but it's really not. It's really only one pi bond. It restricts rotation. It sticks out where it can be attacked." Tammy has accurately described the two lobes of
one pi bond and seems to have a good idea of the geometry of the bond. But her drawing appears to show two sigma bonds between the carbon atoms (Figure 4.1). Despite the introduction and use of wedge-and-dash notation in the lecture, Tammy's representation of ethene appears to show the pi bond and the six atoms of ethene in the same plane, although it was emphasized to the class that the two lobes of the pi bond are perpendicular to the plane of the surrounding six atoms.

![Figure 4.1](image)

**Figure 4.1.** Tammy's representation of a molecule containing a pi bond. This drawing appears to show two sigma bonds between the central carbon atom as well as depicting all of the atoms and the pi bond in the same plane.

Jason's representation of a molecule containing a pi bond was very similar to Tammy's, and his explanation, although more terse, was also adequate. As he pointed to both lobes of the pi bond, he said, "That's one bond." And when asked about the shape of the molecule, he turned his flat hand horizontally and said, "The pi bonds ... if you flip it like this, the pi bonds would be on top and bottom." But his molecule, like Tammy's, appears to contain two sigma bonds and one pi bond between two carbon atoms, and the diagram does not appear to show the pi bond perpendicular to the plane of the molecule.

Several students drew only the pi bond, and then when prompted to draw a complete molecule, added the wrong number of atoms. Marianne confirmed that she knew that carbon atoms required four bonds, but initially attached only one hydrogen atom to each of ethene's two carbon atoms.

GL: "Yeah, you've got to have two hydrogens on each carbon."

Marianne: "On each one?"

After this exchange, she then added two additional hydrogen atoms to each carbon. She finally crossed out the extraneous hydrogen atoms.
Andrea also had trouble drawing the proper number of bonds to carbon. It appears that she was attempting to draw a triple bond consisting of a sigma bond and two mutually perpendicular pi bonds, but her diagram also shows two other sigma bonds attached to each carbon atom; a total of five bonds to each carbon (Figure 4.2). Andrea was unable to explain either how many bonds she wished to represent or the exact geometry she wanted to portray.

Figure 4.2. Andrea’s representation of a molecule containing a pi bond. This diagram appears to show a sigma bond and two pi bonds connecting the central carbon atoms, which also contain two additional substituents.

Michael protested that he wasn’t a very good illustrator, but proceeded to draw a fairly good representation of a sigma bond and a pi bond between two carbon atoms. Michael also drew two hydrogen atoms to each carbon, representing them with circles rather than H’s, and attempted to explain the geometry of the molecule because he felt the his diagram was unclear (Figure 4.3). Pointing to the two "hydrogen" circles he had drawn on each carbon, he explained, "This one is supposed to be coming out at you. And the other one is going back."

Figure 4.3. Michael’s representation of a molecule containing a pi bond. The two lobes at each end of the diagram represent sigma bonds attached to other substituents.
Anna drew a diagram with exceptionally long, horseshoe-shaped pi bonds (Figure 4.4), which might be construed as an effort to draw the pi bonds perpendicular to the plane of the molecule.

![Diagram of a molecule containing a pi bond.](image)

**Figure 4.4.** Anna's representation of a molecule containing a pi bond.

GL: "Now, how are the hydrogens that you have drawn there related to related to the pi-bond?

Anna: Well,...

GL: Spatially. Do you understand what I'm asking you?

Anna: "Well, they're going to be ... the pi bond is going to be kind of pushing them away, I believe, because you know, you've got, it's going to have like two electrons, which are negatively charged, um,... in the pi bond. So these two electrons are kind of sticking off into space, as are the hydrogens. Actually, the hydrogens ... let me think about it using a little Lewis dot ... they're really not charged. I'm not sure if I'm drawing it in the right direction. Okay, it doesn't look to me like it's going to affect the hydrogens at all because there's no charge to the hydrogens. They're neutral, because the carbon is kind of completing their shell." Anna never did explain that the pi bond was perpendicular to the plane formed by the neighboring atoms.

Perhaps the most satisfactory diagrams of molecules containing pi bonds were drawn by Kathy (Figure 4.5) and James (Figure 4.6), although even these diagrams did not use...
dash and wedge to illustrate the three dimensional shape of the structure. Both clearly represented all of the relevant sigma and pi bonds, and attempted to show the pi bonds perpendicular to the plane of the molecule. Kathy did this by skewing the pi bonds to one side, and James attempted to add depth to his bonds. Kathy clearly described the geometry of the molecule. James also described the molecule as being flat. He emphasized the position of the sigma bond "in the middle" and the pi bonds as being caused by overlap "over and under, over the C like the clouds that form right there."

\[ \begin{align*}
\text{H} & \quad \text{C} = \text{C} - \text{C} \\
\text{H} & \quad \text{C} \quad \text{C} - \text{C} \
\end{align*} \]

**Figure 4.5.** Kathy's representations of molecules containing pi bonds. The upper representation simply shows two bonds between two carbon atoms but the lower representation attempts to reproduce the actual geometry of the molecule.

**Figure 4.6.** James' representation of a molecule containing a pi bond.

**Representing Conformers.** Each student was asked to draw conformers of 1,2-dichloroethane (Cl-CH₂CH₂-Cl), and to describe what he or she was doing in the process (Table 3.2, Question 5). Difficulties in this exercise seem to be of three types. Participants frequently were unclear on the exact meaning of the word "conformer." When clued with the term "rotation," the meaning of "conformer" usually became clearer. Participants were reluctant to depict conformers in three dimensions, frequently preferring some type of two-dimensional representation that could not distinguish one conformer from another. Finally, some participants were unwilling to abandon the idea that, unlike
geometric isomers, individual conformers cannot be isolated from one another. Most participants were able to describe conformers as species that result from free rotation around a sigma bond. In addition in the previous problem, the pi bond was generally described as restricting rotation. Nevertheless, several students initially were tempted to draw conformers of 1,2-dichloroethane with a double bond between the carbon atoms. Some students used the terms cis and trans to describe conformers, as might be done in the representation of geometric isomers.

Only two students, David and Jason, initially drew Newman projections to represent the conformers of this molecule. David immediately set to work, drew Newman projections of an eclipsed conformer and two staggered conformers (anti and gauche), discussed the free rotation around the sigma bond connecting the two carbon atoms, and described the conformers in terms of equilibrium and interconversion. He was comfortable with this topic, producing a 'textbook' representation of these conformers (Figure 4.7). Initially, Jason was less comfortable with the subject of conformers.

![Figure 4.7. David's representation of the conformers of 1,2-dichloroethane.](image)

GL: "Could you draw me the conformers of that molecule? And as you go, talk. You know, tell me what you're thinking about."

Jason: "Um, the conformers, that's like the structural...? You just want the structural isomers?"
GL: "Well, not structural isomers, because you remember, conformers means, you know, they can rotate freely. Just, you know, the different shapes that that thing can adopt without breaking any bonds."

Jason: "I see... (draws)... so it'd be like, if I had, uh, two carbons, and then, like, staggered like that?"

GL: "Oh, perfect, yeah!"

Jason: "And if they'd rotate like... wait, actually, it'd be... (draws)... like that?"

At this point he drew an eclipsed conformer. He finished by drawing the Newman projection of his initial staggered conformer (Figure 4.8).

![Figure 4.8](image)

**Figure 4.8.** Jason's representation of the conformers of 1,2-dichloroethane. The relative orientations of each atom are clear in these diagrams.

Michael attempted to draw a staggered representation looking down the carbon-carbon bond axis without resorting to Newman projections (Figure 4.9). Although perhaps unorthodox, his diagram along with his explanation made it clear that he was attempting to draw the staggered conformer in the anti configuration.

GL: "Draw me a picture of some conformers of that molecule, and as you're going, describe to me what you're doing, what you're thinking about."
Figure 4.9. Michael's representation of a staggered conformer of 1,2-dichloroethane. Although the drawing is unconventional, Michael could use it to represent conformational isomerism in this molecule.

Michael: (draws) "Like that?"

GL: "Yeah, now, there's..."

Michael: (pointing to the two central carbon atoms) "This should be behind that."

When asked if he was trying to draw a Newman projection, he responded, "Oh, yeah!" and proceeded to draw an acceptable diagram. He was then asked to draw a different conformer and asked, "You want me to rotate it?"

GL: Whatever you want; that would be fine.

Michael: Okay. So I'd rotate one of these.

GL: Okay

Michael: (draws)

GL: Oh, that's good! Now, would you call those staggered or eclipsed?

Michael: These are ... staggered.

GL: Okay, could you draw that eclipsed as well?

Michael: Sure (draws)
Each of the other seven participants was reluctant to draw Newman projections to illustrate these conformers. In general, they attempted to draw two-dimensional structural formulas (called "dash formulas" in their lecture) to represent conformers. An example is the set of drawings done by Andrea (Figure 4.10). Although these structures appear different, it is not possible to use them to represent different conformers. Several students used the terms cis and trans in describing conformers. These terms are appropriate in describing geometric isomers, many of which can easily be drawn in two dimensions on a flat surface, but cannot be used to distinguish between various conformers.

\[
\begin{align*}
\text{C} & \text{L} \quad \text{C} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{C} \\
\text{H} & \quad \text{C} \\
\text{C} & \quad \text{H}
\end{align*}
\]

*Figure 4.10. Andrea's representation of the conformers of 1,2-dichloroethane. This set of drawings cannot be used to distinguish the staggered and eclipsed conformers of the molecule.*

The term "conformer" presented a problem, and elicited comments such as "You might have to refresh me on this" (Kathy), "I can pick it out of a lineup, but I'm not sure I can draw it out here" (Anna), and "I wouldn't think that one could have conformers" (Tammy). The last comment was made after Tammy had drawn the chair and boat conformers of cyclohexane.

GL: Okay, let me ask you... Tell me what a conformer is in your way of thinking."
Tammy: "I really, I probably didn't understand as much as I should have about conformers. But I basically just knew about the chair and the boat. The way I picture a conformer is just like it could ... I'm thinking this one isn't a conformer because no matter what you do to it, it's going to stay the same. Except maybe I could put a chlorine up here and bring hydrogen ... would that be considered to be a conformer?" Like Andrea, Tammy then drew a set of dash formulas that cannot be used to distinguish between the conformational isomers of 1,2-dichloroethane. Her diagrams are shown in Figure 4.11.

Kathy and Marianne attempted to put a double bond between the two carbon atoms of 1,2-dichloroethane. Kathy cleared up her own confusion on this point.

GL: "Do remember conformers means that there's free rotation around a bond, so, you know, how can you draw that to show that there's different shapes that that thing can adopt?"

Kathy: "Okay. Uh, to me the easiest one is going to be this, because you have all single bonds here."

GL: "Okay, very good. You sure do."

Kathy: "And then you could double bond it here."

GL: "Oh?"
Kathy: "Oh, no, no. You've got to single bond it. And you could double bond it here. Put one H, one H, oh, I'm missing two H's."

Kathy quickly abandoned the use of double bonds, but instead draw the common, two-dimensional "dash" formula similar to Andrea's described above (Figure 4.12). Only on prompting did she decide to draw a Newman projection of the staggered conformer (Figure 4.13).

![Figure 4.12](image1.png)

**Figure 4.12.** Kathy's initial representation of the conformers of 1,2-dichloroethane. The first representation cannot be used to distinguish between the actual conformers of the molecule, the second contains double bonds that would restrict rotation in the molecule, and the third has incorrect bonding between the atoms.

![Figure 4.13](image2.png)

**Figure 4.13.** Kathy's final representation of the conformers of 1,2-dichloroethane. Kathy was able to use these Newman projections to explain conformational isomerism in 1,2-dichloroethane.
GL: "Okay, now, now, that thing that looks like the middle of the Mercedes-Benz symbol. Right there. What does that represent?"

Kathy: "This?"

GL: "Right"

Kathy: "That's the center of your axis."

GL: "Is there an atom there?"

Kathy: "Um, yes."

GL: Okay, what kind of atom is that?

Kathy: "Um, it's going to be a ... carbon?"

GL: "Right. Okay, what does that circle represent in the back?"

Kathy: "This circle, that's like the back side of that atom.

GL: Is the same atom or a different atom as that point."

Kathy: "It's, uh, the other carbon, right there."

Kathy then finished drawing the staggered conformer, saying "'Cause it's the most stable way."

GL: "I would agree with that entirely. Now, can you draw me any other conformers?"

Kathy: "I could do it the eclipsed way, but that's the same thing. You could do..."

GL: Go ahead!

With this encouragement, Kathy completed drawing the eclipsed conformer (Figure 4.13).

Marianne also discovered that she could not use double bonds in her conformers, but was unsure where to place the chlorine atoms given the formula $\text{ClCH}_2\text{CH}_2\text{Cl}$. "Can I just put them anywhere?" She initially placed both chlorine atoms on the same carbon atom (she drew the Newman projection of 1,1-dichloroethane). She was questioned about this and responded, "Oh, they're on the same one. They have to be on different..."
ones." Nevertheless, a short while later she did the same thing, and when questioned she said, "Oh, I keep doing that!"

Anna also drew Newman projections after prompting, having first drawn typical two-dimensional "dash" formulas similar to those drawn by Andrea and Tammy (Figure 4.14). She described both the dash formulas and the Newman projections as representing different conformers. Apparently she did not want to give up the idea that conformers could be represented using the flat "dash" representation. James did this as well. He described his initial drawing of the conformers as follows.

\[
\begin{array}{c}
\text{Figure 4.14. Anna's representation of the conformers of 1,2-dichloroethane. This set of drawings cannot be used to distinguish the staggered and eclipsed conformers of the molecule.}
\end{array}
\]

James: "Okay, first I'm going to start off by just drawing the C's, on the carbon-to-carbon chain, and then I'm going to add the hydrogens in. Well, let's see. I'm going to add the chlorines to the top right here and the bottom, like catty-corner towards each other...And that'll give me trans uh, whatever this molecule is... this is the trans form of it. If I put both chlorines like together, like above or below the sigma bond between the
two carbons, then I'm going to get like a cis. So I'll draw that. This is trans, and that's cis."

GL: Okay. Now, let me ask you another question. Are those distinctly different molecules, or are they the same?

James: "Mmm, golly, that's tough. I would say that they're different. Different properties, they're the same because they're isomers, but they have different chemical properties."

James used the terms cis and trans to describe conformers, although these terms should instead be used to describe geometric isomers. In contrast to the conformers represented in this exercise, geometric isomers are distinctly different molecules. James' use of these terms to describe conformers may have been part of the source of his difficulty. After drawing Newman projections of the structures, he correctly concluded that they represented the same molecules. James initially described his Newman projections using the terms cis and trans, but ended by using the correct terms, eclipsed and staggered. The conversation proceeded as follows.

GL: "Okay. Could you draw a Newman projection of that?"

James: "Uh, I'm trying to think of it."

GL: "I'll give you a hint. Draw a circle."

James: "Oh, yeah, I gotcha. Which one do you want, the trans, or both of them?"

GL: "Don't care."

James: "Okay, for the Newman projection, when you're drawing a trans bond, you want the chlorine, the two chlorine atoms as far apart as possible. So, really, it's going to be like staggered. And I drew it in the most stable form, because that's how I can remember it. Because they're the farthest apart from each other. And then the eclipsed form is like when they're being eclipsed by each other, I mean, like that."

GL: "Okay. Now, let me ask you a question. Is there any rotation that goes on there?"
James: "Yes, there is, because there's a single bond between the two carbons."

GL: "Okay, so are they the same or are they different?"

James: "Hmm, same, this right here?"

GL: "Yeah."

James: "Same molecule, same isomer, same...."

GL: "Yes, are they the same molecule?"

James: "Same molecule, but different forms of it."

Marianne's experience was similar to that of James. After drawing Newman projections of 1,2-dichloroethane, she explained rotation around the single bond. When finally asked if she could "just get a bottle of the staggered," she replied, "No, you can't just pick and choose."

**Nomenclature of an Alkene.** Each participant was asked to provide a name for the structure shown in Figure 3.1, question 6 (cis-1-chloro-2-pentene). This question was intended to elicit information regarding how the participant determined whether geometric isomerism was possible in a molecule exhibiting hindered rotation caused by the presence of a pi bond. However, the question was more difficult than originally anticipated for two reasons. First, many participants concluded that the molecule was a substituted ethene rather than a pentene. Second, none of the participants acknowledged in their names that the molecule was capable of geometric isomerism.

Each participant initially focused on either the presence of the double bond or the total number of carbon atoms in the molecule. Michael mixed these concepts together.

"Michael: Okay, the first thing I'd do is I'd count the carbons, alright. So the longest carbon chain."

GL: "Okay"

Michael: "So, this is what I sometimes get confused about. Do you count ... sometimes ... the alkyl groups?"

GL: "I'm not going to tell you right now."
Michael: 'Cause I mean, that's part of the ...Okay, okay, that's why it takes me a
long time."

Michael then focused on the double bond, concluding that the molecule was a
substituted ethene. "It has a double bond. And it's got two carbons in it. In the chain."
But then he encountered a problem with how to name the rest of the molecule. "And it's
got another ethane over here, and ethyl ... it's got ... I'm trying to figure out what this is
right here (NB: the CH₂Cl)."

GL: "What's the longest chain?"

Michael: "The way it did it, I put down that this was the longest chain (NB: the two
carbons bearing the double bond)."

GL: "Could you find one that's longer?"

Michael: "Well, if you attached all the carbons all the way through."

GL: "Why don't you try it and see what happens?"

Michael: "You know what helps me out a lot, actually? If I actually draw out each
individual molecule (NB: 'atom'). Like this. I draw it like this. (Figure 4.15). That
helps. Then I can see the chain easier." After this, Michael named the molecule 1-chloro-
2-pentene.

\[
\begin{align*}
\text{-} & \quad \text{C} \quad \text{-} \quad \text{C} \quad \text{=} \quad \text{-} \quad \text{C} \quad \text{-} \quad \text{C} \\
\text{!} & \quad \text{!} \\
\end{align*}
\]

Figure 4.15. Michael’s representation of cis-1-chloro-2-pentene. Michael has drawn a
'dash' representation in which each individual carbon atom is clearly delineated. The
only hydrogen atom shown in this structure is misplaced.

James initially focused on the double bond, describing it as an alkene with the suffix
"-ene."

GL: "Ask yourself this, how many carbons are in that thing."

James: "Two."
GL: "How many carbons total are in that thing?"

James: "Oh, oh, oh, I didn't see that. Oh, oh, I see it now. I gotcha. Okay, so I'm going to start again, back up, and count the rest of these carbons. And there's five of them in this straight chain. So it'd be ... pentene, and ... let's see, 1,2 ... 2-pentene."

From this point he easily got the name 1-chloro-2-pentene.

Tammy also had difficulties identifying the longest chain of carbon atoms. She initially described the molecule in the following conversation.

Tammy: "Okay, this would be ethene, because it has a double bond on the longest carbon chain, and this would be ... okay that'd be 1-propyl-2- ..."

GL: "What's the longest chain?"

Tammy: "Could this be a chain? It could! Okay, so I'd have these four carbons in a row, and that would be the longest chain. And then that would change everything!"

Almost immediately, she recognized that the longest chain actually has five carbon atoms, and she then wrote down the name 1-chloro-2-pentene.

Most of the participants who eventually named the molecule correctly stumbled at the beginning. Marianne provided a good example.

GL: "What's the first thing your eye catches?"

Mariane: "The double bond. So it's an alkene ... oh, wait, is that what you call it?"

GL: "Yeah! What else does your eye catch?"

Marianne: "... um, the two carbons. It's going to be di ... wait, okay. I have to name this stuff, too."

GL: "Right, you've got to name everything!"

Marianne: "Okay, oh no! I didn't study!"

GL: "That's alright. You weren't supposed to study."

Marianne: "(laugh) Um, I have no idea. I need some help.

GL: Okay, fine. Okay, how many carbons are in it?"
Marianne: "Two. Oh, altogether, there's one, two, three, four, five, six... five, five."

GL: "Okay, what are you going to do with that five?... with the fact that there's five carbons?"

Marianne: "Um... oh, okay, it's pentene. Okay, I know what I'm doing now."

Anna didn't take too long to name the compound, and called it 1-chloro-3-ethyl-2-pentene. She was asked if she "needed to put the ethyl in there," and responded, "...No, because it's all one chain."

Brian immediately identified the longest chain and called it a pentene. He had no difficulty with the name 2-pentene and realized that he needed to do something with the chlorine. Like Anna, he wanted to include extraneous methyl groups (methyl and propyl). Kathy gave what might be called a "textbook procedure" for naming the molecule. She first identified the molecule as a pentane by counting the carbon atoms, added the name chloro, and then modified her suffix to "-ene." "Pentene because it has a double bond in it." She finally called it 1-chloropent-2-ene, and then said "Pent-diene; oh no, it's just regular ene. Diene would be if there would have been two sets of double bonds in there."

After obtaining the name 1-chloro-2-pentene, none of the participants identified the structure as one of a pair of geometric isomers, or attempted to add the prefix "cis-" to the name. However, with encouragement, most participants recognized that they were dealing with the cis isomer. Upon being told that she needed to consider whether isomers were possible, Anna immediately said "Oh, okay! It's, um, it's, uh, cis."

GL: "Okay, how did you know that?"

Anna: "Because the two groups coming off the two carbons of the double bond are both on the same side."

GL: "And how did you determine that it was the same side? What strategy did you use to say, oh, they're on the same side."
Anna: "Okay, well, the way I've been viewing cis- isomers is, either they're going to be above the carbon bond or both are going to be below the carbon bond. I don't know if there's a more technical name to say that."

When Marianne was asked if it was possible for the compound to have a geometric isomer, she responded in the affirmative, and was then asked if there was anything else she wanted to say about the double bond.

Marianne: "... Oh, okay, I know, I know! It's, um ... cis."

GL: "Okay, good! How did you know that?"

Marianne: "Okay, because the two hydrogens are together and not on the opposite side. 'Cause trans means opposite sides."

Marianne's strategy of looking at the hydrogen atoms was unusual; most of the other participants focused on the alkyl group and the chlorine atom. James was one of these, and he was uncomfortable with the presence of the chlorine. "I mean, can you have a trans-cis isomer ... without it being, like, one chlorine?" But James agreed that this was the cis isomer. Only Brian was determined that geometric isomerism was not possible in 1-chloro-2-pentene. Brian was asked if the molecule could exhibit geometric isomerism?

Brian: "cis- and trans-?"

GL: "Okay."

Brian: "cis? Well, there is..."

GL: "Can you make a cis-trans isomer of that?"

Brian: "No, actually, you can't. These are identical, right?" (NB: the two hydrogen atoms attached to the doubly bonded carbon atoms)

GL: "Does that matter?"

BF: "Yes."

For Brian, geometric isomerism was not possible if each carbon bearing the double bond was connected to a hydrogen atom.
Identifying Pairs of Isomers. Each participant was asked to identify the relationships between pairs of their choice chosen from among five structures (Table 3.2, Question 7). Structures I and II are two representations of the same molecule, rotated 180° around the C=C axis. Structures III & IV are geometric (cis-trans) isomers. Any other pair of structures from this set represent structural isomers. The course text describes all of these structural isomers as "positional isomers" because they "differ in the location of a noncarbon group or a double or triple bond (Bailey & Bailey, 1995. p. 46)."

Most of the difficulties in this problem arose from one of two sources. The nature of rotation and the significance of rotation around a bond compared with rotation of an entire molecule confused some students. And the correlation of structural elements with structural isomers was a difficulty for almost everyone.

Three students noticed that structures I and II were identical. Despite being slightly dyslexic, Michael immediately chose these two structures and said, "I mean, it's just flipped around. So it's still the same molecule, it's just at a different angle." Tammy also picked these two structures first and said, "Um, they're really the same thing, because all you did, you still have three hydrogens, and all you did was rotate this ClCH₂CH₂ from the top to the bottom. I'm thinking that ... I'm going to stick with that." One other student, James, stumbled a bit, but also identified this pair as being the same. "One and two are the same, right here. They're isomers, structural isomers I'm guessing? No, geometric isomers, I say, anyway, because ... now I'm confused here.... Uh .... actually, they look the same. One and two are the same thing. If you start counting, like I like to start doing it that way, anyway. Yes, they're the same. One and two are the same."

The rest of the participants had a great deal of difficulty with this pair, and many of them attempted to avoid it. In general, structures I & II (Table 3.2, Question 7) were identified as a pair of structural or positional isomers. Anna’s experience was typical.
Anna: "Um, let's see. 1 and 2 look similar. Um, you really couldn't call them cis-trans, because you only have one alkyl group coming off of it."

GL: "Okay, what could you call them?"

Anna: "Mmm, you mean like name them again?"

GL: "No, I mean, what's the relationship? You can name them if you want to, if that helps you."

Anna: "Oh, the relationship, let's see..."

GL: "What are you looking at right now?"

Anna: "I just glanced down at number 5. I was thinking there's got to be an easier way on this."

She went on to another set of structures, eventually returned to I and II, and said, "They would be structural isomers as well. "You really couldn't call them cis-trans, because you only have one alkyl group coming off it."

GL: Okay, why do you say that they're structural isomers?

Anna: Well, it's just that they have the same formula right now, um, they've got the same number of hydrogens, the same number of carbons, same number of chlorines. Again, the hydrogens are just in a group... No, I'm sorry, the hydrogens, they're really in the same orientation around the carbons, it's just looks like it's maybe somehow rotated?

GL: "Ahh!"

Anna: "Um, is that the key?"

GL: "I don't know, is it?"

Anna: "You're not answering questions, are you? (laugh) It's like the flip side, almost. It's like the flip side of one. Just kind of flip it over. It's like, it's rotated, but then again, (sigh), you can't really get much rotation around a double bond. That shouldn't be. Um, I know you can rotate well around a single bond, but on a double bond, you're kind of held in place by that pi bond."
GL: "Well, let me ask you a question. Can you rotate an entire molecule?"

Anna: "I guess so. If I dropped it!"

GL: "(laugh) Yeah, okay, fair enough! Exactly. What would happen if I rotated that entire molecule?"

Anna: "You'd get the same thing. The exact same thing. So, would it be considered to be a structural..."

GL: "Would it?"

Anna: "Would it be a conformer? Oh, no, they're the same thing!"

Brian identified structures I and II as positional isomers, but when questioned as to what would happen if structure I were flipped over, he recognized, "It'd be two. That's why I'm thinking it's not positional any more." He never volunteered that they were the same, but agreed that this might be the case when this was offered to him as an option. Jason identified I and II as structural isomers, but when asked what would happen if number one were picked up off the page and turned over, he immediately laughed and said, "They'd be the same!"

Kathy initially recognized that structures I and II could not be geometric isomers because, "You don't have another group on this side to make it a cis or a trans. It's just hydrogens."

GL: "I see, okay, now let me ask you a question. What would happen if I took number 1 and I completely flipped it over? Rotated it, you know, this way ... turned it around that double bond. What would happen to it?"

Kathy: "It would be like number 2."

GL: "So are they structural isomers?"

Kathy: "No"

At this point, Kathy realized that she was not dealing with structural isomers, but she did not yet conclude that these two structures actually represented the same molecule.

GL: "What are they?"
Kathy: "Mmm ... geometric isomers."

Kathy finally realized that the two structures were the same when it was pointed out that no bonds were broken when turning one structure over to form the other.

GL: "Okay, now, why would they be geometric isomers? If I could take number 1 and totally pick it up and turn it over, and it becomes number 2, did I have to break any bonds to do that?"

Kathy: "No. So it's the same atom."

GL: "So what are 1 and 2?"

Kathy: "Same atoms. The same."

Identification of structures III and IV as a pair of geometric isomers was not difficult for most of the participants. Marianne, Anna, and Jason immediately focused on this pair, correctly identifying which was the cis isomer and which was the trans. Anna's response regarding how she could tell that these were geometric isomers was typical. "Well, they both have the same... the carbon-carbon double bond ... both of them have the same groups coming off of them, but in three, the two groups, alkyl groups are going upwards, above the double bond, and in four there is one going above the double bond and one going below the double bond. so they are definitely cis-trans." Kathy's response was more succinct. "Number three is a cis, because they're both on top. Number four is a trans; you have one on top and one on the bottom." Michael described the relationship as follows. "'Cause this, one of them is flipped onto the other side of the atom ... of the molecule."

Only two students, Brian and Tammy, had difficulties with structures III and IV. Brian identified this as a pair of positional isomers, and when pressed, had little further comment. Tammy's comment was, "Um... Three and four, I think, are ... I don't know if they'd be geometric isomers or not. Because all I did was switch places, right there, but ...".

GL: "Okay, let me ask you a question. Can three and four be conformers?"
Tammy: "Yes."

GL: "You don't have to answer 'yes.' The answer might be 'no,' okay? I'm just asking."

Tammy: "Okay."

GL: "Okay, if they're conformers, why do you think they're conformers?"

Tammy: "...Um, I was just thinking because they switched places, but I'm realizing that's not right!"

GL: "Okay, so if they're not conformers then, what do you think the relationship might be?"

Tammy: "...I'd say they were geometric isomers."

GL: Okay. Um, if they're geometric isomers, then which is which?

Tammy: "This would be cis- and this would be trans- because the hydrogen is in opposite directions. I'm talking about three and four."

GL: "Okay"

Tammy: "And I think these would have to be the same group to be able to be considered cis or trans, right? So this would be trans, four is trans and three is cis."

Correctly identifying pairs of structural isomers gave many students difficulty. Structure V is a structural isomer of each of the other four. Many participants were uncomfortable with structure V. When asked about it, they initially described various structural features and differences between this structure and the others, but were unwilling to describe structure V as a structural isomer of any of the others. Anna's difficulties were typical:

Anna "I just glanced down at number five. I was thinking there's got to be an easier way on this.... Number five doesn't look like any of the other four. Um, it is a cis isomer of something, because it has two methyl groups above the double bond. But you could almost say it is a trans isomer as well, because there is a chlorine going below the double bond and a methyl going above the double bond... Um, it doesn't look like it
really relates to anything above it, though... I just realized it does relate to these above here. Because here I've got like, in three there's um, ClCH₂, and in five there's a CH₃, and it’s like the Cl and the H have switched places... Um, could have been some sort of a substitution reaction ... No, not really, no, I wouldn't classify it as a reaction. I'm sorry, that was silly. Um, so I guess you would call those structural isomers, because it's the same formula, it's the same compound, but they're just drawn out different ways."

It is interesting to note that, in her discussion, Anna discovered a point that was not explained in class. This compound does have a geometric isomer (not shown), but the two cannot adequately be differentiated using the terms cis and trans.

Michael initially focused on the chlorine atom in structure V, saying, "And the chlorine is individual there." But he didn't want to describe structure V as a structural isomer of any of the others. When asked if there were any pairs of structural isomers, he said, "Um, yeah, the carbons are moved around. So if you're talking about structural, the carbons ..." He was initially unwilling to concede that structural isomers could form in any other way than by breaking and making bonds between two carbon atoms. In the conversation that followed, Michael finally identified structures IV and V as structural isomers.

GL: "Okay, that's what I wanted to know. How about 4 and 5, what's the relationship there?"

Michael: "Everything's split up...."

GL: "What are you thinking about right now?"

Michael: "I'm just trying to visualize the molecule. The way I would draw it."

GL: "Go ahead and do that. If you want to draw it out and give it a dash formula, go right ahead." Despite this encouragement, Michael did not draw a dash formula.

Michael: "The carbon, the double bond's on the second carbon. "The double bond's on the same carbon there. Okay. The chlorine's attached to a different carbon."

GL: "Okay, the chlorine's attached to a different carbon."
Michael: "Right. Here the chlorine's attached to the end of the molecule. And here it's attached to the second carbon."

GL: "Okay. Does that make them structural or geometric?"

Michael. "That would make them ... geometric."

GL: "Okay, well, why would that make it geometric?"

Michael: "... It would ... be structural, because you're actually moving the chlorine."

**Using Newman Projections.** Each participant was asked to draw a 'dash' or condensed formula of the Newman projection of 2-chloropentane given in Table 3.2, question 8. Difficulties in this problem generally appeared to be of two types. Some participants had difficulty discerning the meaning of the symbols denoting the two central carbon atoms in the Newman projection. In addition, many participants had difficulty connecting the various structural elements in the proper order, frequently drawing the incorrect number of bonds to carbon atoms.

Many subjects began by first drawing the ethyl group (-CH\(_2\)CH\(_3\)) located at the back of the structure and were then unsure how to proceed. Marianne's difficulties were instructive.

Marianne: "I'm just going to take the first one, and make it CH\(_2\)CH\(_3\), and then have a hydrogen..."

GL: "Okay, what hydrogen is that?"

Marianne: "This is the one right here."

GL: "That's that, okay."

Marianne realized that there were two hydrogens and an ethyl group attached to the same carbon atom, but was unsure what to do with them. She wrote "H-CH\(_2\)-CH\(_3\)-H,"

Marianne: "And I need to add this one on. So I can just put it like that? Or not?"

She was then asked what the CH\(_2\) was attached to.

Marianne: "That CH\(_3\)."

GL: "And what else is it attached to? Going the other direction."
Marianne: "Um, like this?"

Marianne pointed to the terminal hydrogen. In order to determine if she knew the meaning of the large circle drawn in the Newman projection, she was then asked what was "right in the middle." She responded, "I don't know."

GL: "Okay, isn't that a carbon in the middle there?"

Marianne: "Okay."

GL: "Okay, try it that way."

When it was suggested that she make this large circle into a carbon atom, she said, "See, I don't know how to attach these hydrogens on here." Marianne finally realized that there must be two carbon atoms in the central portion of the Newman diagram, and wrote "CH2CH3CH2-CHCH3Cl." With a great deal of coaching, she finally produced the diagram given in Figure 4.16. Marianne named this molecule "2-hydrochloropentane"; when asked about the "hydro," she quickly responded "No, okay, just 2-chloropentane." When asked why she had used the "hydro" prefix, she responded, "Oh, just because I had put the chloro in, and I felt bad for the hydrogen!"

![Figure 4.16. Marianne's final representation of 2-chloropentane. Unlike Marianne's initial drawings, this representation is properly drawn with the methyl and methylene carbon atoms in the correct order.](image)

Jason also began by drawing the ethyl group at the back of the structure and attempted to add two hydrogens to it. He was asked "And what's this thing right here in the middle?" He responded, "It's a carbon. So it'd be 'C,'" and concluded that it was attached to another carbon. A problem for Jason, as well as several others, was whether he should place a dash in his condensed formula to represent the bond between the two central carbon atoms (CH3CH2CH2CHClCH3 vs. CH3CH2CH2-CHClCH3); however,
he and most of the others readily accepted the idea that it really didn't matter. Once Jason
determined that the central portion of the Newman projection represented two carbon
atoms, one in the front and one in the back, he was still unsure what to put on the front
carbon atom. He concluded that there must be "The CH$_3$ and ... and a hydrogen and a
chlorine." He asked, "So just put all that together?" When he did so, he produced the
drawing given in Figure 4.17. Jason needed some encouragement to keep track of what
groups were attached to the central carbon atoms.

![Figure 4.17](image)

Figure 4.17. Jason’s initial representation of 2-chloropentane. In this drawing, Jason
has simply attached onto the end of the structure the substituents that should be attached
to the second carbon atom from the viewer’s right.

GL: "There’s three things attached to it. Could you put three lines, three dashes
there, to indicate three other things attached to it? Yeah, one up, one down, and one out
to the side?

Jason: "Okay"

GL: "Yeah! Okay, now, what’s attached onto there?"

Jason: "The H, CH$_3$, and Cl."

GL: "Yeah! Where are you going to put those? It doesn’t really matter, I don’t
suppose."

Jason: "This is Cl at the bottom, ’cause it’s at the bottom." (NB: at the bottom of the
Newman projection)

He ultimately produced the diagram shown in Figure 4.18, and had little difficulty
determining the name once he had drawn a condensed formula, concluding "One, two,
three, four, five. It’s a pentane. Pentane, and you have one chloro to it. It’s on the
second ... second carbon? So it’d be 2-.... chloropentane."

Like most of the others, Anna began by drawing the ethyl group, and then had
difficulty with the hydrogen atoms attached to the central carbons.
Anna: "There's three H's written by themselves, and I know that those are going to be attached to, um, carbons."

GL: "Are they all attached to the same carbon?"

Anna: "Not necessarily."

GL: "How could you tell?"

Anna: "Ooh! I'm having a lot of trouble with this one." She produced the drawings given in Figure 4.19, and realized that none of her structures could be correct.

Once she was told the proper meaning of the symbols representing the central carbon atoms in the Newman projection, she had little further trouble. "So, coming off this first carbon, the one with the peace sign, um, we've got a methyl group, a hydrogen, and a chlorine, which completes the octet, and we've got the other carbon attached to it, and coming off the other carbon is going to be a ... okay, coming off the other carbon is
going to be the ethyl group and two hydrogens." She drew a condensed formula and was asked to name it.

Anna: "Um, and I'm going to put the 1-ethyl first, so it's going to be 1-ethyl-2-methyl... oops... that kind of blows that rule... out of the water, because I've got the chlorine in there, so it's got to be... I don't know if that makes a difference... or not... but I've got 2-chloro-1-ethyl-2-methylethane."

GL: "What's the longest chain?"

Anna: "Oh! I missed that! Okay, yeah, it should be a... it's not an ethane, it's a butane. No, actually, it's a pentane! Yeah, just take that whole numbering system out of there. Okay, let's see, we're going to go, um... and it also gets rid of the methyl part and the ethyl part, so we've got pentane, um... and I'm going to want to start... I'm going to want to get that chlorine with the lowest number possible, so actually, ..., no, it's still 2-chloro. 2-chloropentane."

Brian had little trouble with the meaning of the symbols representing the central carbon atoms of the Newman projection. "And I would assume that it would be a... it's going to be a single bond." Once he assured himself of this, he had no difficulty putting the structure together, and it took him only a moment to give the name "2-chloropentane."

Because Brian had difficulty with the previous question on conformers (Table 3.2, Question 5), he was asked if he could now answer this question. With confidence, he produced the drawings given in Figure 4.20, and correctly identified the staggered and eclipsed conformers.

Neither Kathy nor David had much trouble drawing the condensed formula or giving it a name. David initially produced the two structures given in Figure 4.21. When asked if he could draw it in a linear fashion, he produced the first drawing in Figure 4.22, with the chlorine atom on the terminal carbon atom, and then quickly changed it to the correct drawing in Figure 4.22.

Kathy originally determined the condensed formula to be CH₂CH₃CH₂CHCH₃Cl.
Figure 4.20. Brian's representations of the conformers of 1,2-dichloroethane.

Figure 4.21. David's initial representations of 2-chloropentane.

Figure 4.22. David's final representations of 2-chloropentane. The upper drawing does not show the proper number of bonds to two carbon atoms. David has corrected this in the bottom drawing.
GL: "Which one of those carbons is connected to the carbon at the middle point there? The CH₂ or the CH₃?

Kathy: "I would say the CH₂."

She then altered her subscripts to reflect this. Without prompting, she moved the chlorine to the second carbon atom, producing the drawing shown in Figure 4.23. When asked for a name, she said, "Okay, I'm going to start numbering from here. If I don't do this, I'll never get it." She numbered from the right, "because your chlorine's closest if you number it from the right. It's a 1-chloro ... uh, 2-chloro... A 2-chloropentane." In addition, Kathy had the same question as Jason on the presence of dashes. "Um, this, the C right here, could you just connect all those together instead of me putting a dash right there?" When she was told that the dashes were unnecessary, she replied, "Okay. It kind of helps me to separate them, but I just wanted to know."

Figure 4.23. Kathy's representation of the structure of 2-chloropentane. Without prompting, Kathy moved the chlorine atom twice to produce a correct drawing.

**Geometric Isomerism in Cyclic Molecules.** The last question of the first interview (Table 3.2, Question 9) asked participants to give the name of the structure shown, *trans-*1,2-dichlorocyclobutane. The original intent was to determine how the subject determined whether geometric isomerism was possible in a molecule exhibiting hindered rotation caused by the presence of a ring. In this regard, it is similar to question 6 that asks about hindered rotation around a double bond (Table 3.2). Unexpected problems arose with this exercise when many participants did not name this structure as a cyclic compound. Several participants also had difficulty numbering the carbons, being unsure which carbon atom was the first.
James and Anna performed this exercise well. James worked this problem as follows. "Well, I see it's a cycloalkane, and there's no double bonds in it. So, what I do is, it's got four carbons in it. It's a four-carbon ring. So, that would be cyclo... I hope... butane, yeah. And I'll go and count the chlorines in it, like in order to where I get the number, the chlorines have the smallest number possible. So, I go, 1,2-dichlorocyclobutane. And it's trans because they're pointing in opposite directions. Or, you've go one, nope, I don't know. The whole thing about the axial and equatorial bonds kind of confused me, because you've got one up, down, up, down. Does that only work for hexane, or does that work? ... You can't say! Oh, man, that's my answer; I'll stay with that."

Anna reasoned this out in a similar manner. "Okay, well, it's a cyclobutane. It's going to be the -ane because there's no double bonds. Cyclo because there's, well, I guess you'd call it a parallelogram. My geometry was many years ago. Um, I've got two chloros, so it's going to be a dichloro, but I also need to number, and give the chlorines the lowest two numbers possible, so it's going to be, really, 1,2-chloro... oops! ... 1,2-dichlorocyclobutane. And it's also trans, and I admit, I don't remember, do I put the trans at the very beginning or right before the cyclobutane?"

In order to determine if Anna realized that the molecule was drawn in a manner that emphasized the positions of the substituents, she was asked why it was drawn as a parallelogram (instead of a square).

GL: "Why did I draw this structure as a parallelogram?"

Anna: "Um, because, well, the molecule itself is not flat. There's a bond angle to it. I can't remember right off hand what the bond angle is, but ... And I'm not really sure if that applies, but it's not flat. Your molecules normally are not flat."

GL: "What would happen if the molecule were drawn as a square?"

Anna: "Well, for one thing, it would be harder to detect the trans chlorines. 'Cause your, uh, vertical lines on one of those chlorines would be part of the wall."
Both Jason and Marianne named this molecule "dichlorobutane." When asked if there was something special about the way the four carbon atoms were arranged, Jason also used a geometric analogy, calling the molecule a rhombus. But neither he nor Marianne were able to recall the "cyclo" prefix, although both recognized it when told. However, both immediately recognized it as a trans isomer.

Kathy also named this molecule "1,2-chlorobutane," omitting the "cyclo" prefix. When asked if there was anything unusual about the arrangement of the four carbons, she replied, "Mmm ... besides they're in a square shape?" She was asked if she were given the name "1,2-dichlorobutane," would she put the carbon atoms in a square, and replied, "No, I wouldn't connect them." So how would she indicate that they were in a ring? "So it would be cyclobutane. 1,2-di... chloro... cyclobutane."

Only David immediately wrote "trans-1,2-dichlorocyclobutane" with no prompting. No one else added the prefix "trans." However, when asked if the molecule was a geometric isomer, each participant immediately replied that it was the trans isomer, without further comment.

**Summary of Results from First Interview.** Seven broad classes of difficulties and strategies relating to representations pi bonds, conformers, structural isomers, and geometric isomers in three dimensions among beginning organic chemistry students emerged from this interview. These were titled "use of VSEPR," "representations of pi bonds", "representations of conformers", "nomenclature of alkenes", "recognizing isomer types", "using Newman projections", and "geometric isomerism in cyclic molecules." The category "use of VSEPR" relates to students' potential application of valence shell electron pair repulsion theory to organic structures. The category "representations of pi bonds" involves difficulties drawing pi bonds and relating the shapes of these bonds to the geometry of an entire molecule. The category "representations of conformers" describes difficulties in depicting conformers, rotating around sigma bonds, and distinguishing conformers from structural and geometric
isomers. The category "nomenclature of alkenes" discusses difficulties in naming alkenes, particularly in identification of the longest carbon chain and recognition of the possibility for geometric isomerism. The category "recognition of isomer types" relates to difficulties in recognizing types of isomers and orienting entire structures. The category "drawing Newman projections" describes difficulties in recognizing the meanings of the symbols in a Newman projection, reluctance to use these types of diagrams, and properly orienting substituents on a Newman projection. Finally, the category "geometric isomerism in cyclic molecules" involves difficulties in recognizing, drawing, and naming cyclic structures and their geometric isomers.

The categories of difficulties derived from the first interview are summarized in Table 4.1.
Table 4.1. Difficulties in Learning Derived From the First Interview.

I) Use of VSEPR
   Students interviewed claimed to be familiar with VSEPR, but did not associate
   what they had learned with any conclusions that they could make about the shapes
   of organic molecules.

II) Representations of pi bonds
   A) Students could draw the shape of a pi bond, but frequently could not include
      this shape in a representation of a molecule.
   B) Students could describe the shape of a pi bond in isolation but were less
      successful describing its shape within a molecule.
   C) Students were generally unsuccessful when describing what types of
      molecules contain pi bonds.
   D) Students frequently did not represent the pi bond of an alkene as being
      perpendicular to the plane of the atoms in its vicinity.

III) Representations of conformers
   A) Students frequently represented conformers as a type of structural isomer.
   B) Conformers were frequently drawn in only two dimensions through the use of
      dash formulas.
   C) Although conformers were described in terms of free rotation around a sigma
      bond, students often stated that individual conformers could be isolated.
   D) Students generally did not associate Newman projections with representations
      of conformers and were reluctant to use them until specifically asked.
   E) Discussions of the term "conformer" were sometimes restricted to mentioning
      the chair and boat forms of cyclohexane.
   F) The terms "cis" and "trans" were occasionally used to describe conformers,
      when their use is properly restricted to geometric isomers. Use of the terms "cis"
      and "trans" was most common when students attempted to use dash formulas to
      draw conformers.

IV) Nomenclature of alkenes.
   A) Students who focused on the double bond instead of the longest chain of
      carbon atoms frequently named alkenes as substituted ethene molecules.
   B) Students frequently failed to recognize whether a simple alkene could exhibit
      geometric isomerism.

V) Recognizing isomer types
   A) Rotating an entire molecule was frequently not differentiated from rotation
      around a sigma bond.
   B) The presence of the same structural elements in different structures was not
      correlated with the presence of structural isomers.

VI) Using Newman projections
   A) Students were generally unaware of the meaning of the symbols representing
      the two central carbon atoms in a Newman projection.
   B) Students frequently were unable to connect the structural elements to a
      Newman projection in the proper order.
   C) Students frequently placed the wrong number of bonds to a given atom when
      using Newman projections. Especially common was inverting the positions of
      "CH₃" with that of "CH₂," giving five bonds to the methyl carbon and three to
      the methylene carbon.
   D) Students were reluctant to use Newman projections to represent conformers,
      instead frequently attempting to do this using two-dimensional dash formulas
      instead.

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Table 4.1 (cont.).

VII) Geometric isomerism in cyclic molecules.

A) Students frequently failed to recognize a molecule as cyclic when given its structural formula.
B) Students attempted to describe substituents in essentially planar cyclic molecules as being "axial" and "equatorial."
C) Students ascribed the use of a parallelogram to represent cyclobutane to it being nonplanar rather than as an effort to bring the ring substituents into proper perspective.
INTERVIEW 2 RESULTS

The second interview was conducted six to seven weeks into the course. This interview was designed to probe student learning, understanding, and difficulties regarding conformers, geometric isomers, and structural isomers of cyclic hydrocarbons and their derivatives.

Isomers of Dichlorocyclopentane. The first four questions from the second interview session (Table 3.3, Questions 1 - 4) asked about conformers and isomers of cyclopentane. Because the cyclopentane ring is rigid and almost flat it does not form conformers; its structural and geometric isomers are given in Figure 5.1. Each participant was asked to build a model of any dichlorocyclopentane and was then questioned about the possibility of making conformers of this molecule. Finally, each participant was required to build, draw, and name all possible isomers of this compound and to identify the individual pairs of geometric and structural isomers. Difficulties in properly numbering the carbon atoms in the cyclopentane ring and difficulties in representing and visualizing cyclic structures emerged from this set of exercises.

![Diagrams of dichlorocyclopentane isomers](image)

(a) 1,1-dichlorocyclopentane  
(b) α,α'-1,2-dichlorocyclopentane  
(c) γ,γ'-1,2-dichlorocyclopentane  
(d) α,α'-1,3-dichlorocyclopentane  
(e) γ,γ'-1,3-dichlorocyclopentane

Figure 5.1. Structural and geometric isomers of dichlorocyclopentane.
Anna's experience with dichlorocyclopentane was representative of that of many of the students. When she built the carbon framework of dichlorocyclopentane she discovered, "Okay, it's relatively flat." After adding the chlorines to form cis-1,3-dichlorocyclopentane she drew its structure (Figure 5.2) and said, "And now the molecule is no longer flat ... I guess it could have ... I've got them both sticking off in the same direction; I guess it could have gone in opposite directions." By this statement, Anna was indicating that she could have constructed a model of the trans-isomer instead of the cis-isomer.

![Figure 5.2. Anna's representation of dichlorocyclopentane. Although it is not clear from the drawing, Anna attempted to draw the cis isomer.](image)

GL: "Could you make a conformer of that structure?"

Anna (confidently): "No. Because it's a pentagon, and if I remember right, conformers work only with hexagons."

GL: "What if you didn't remember this? What else could you do?"

Anna: "Well, you couldn't, because it's flat ... I think it's going to have to do with the bond angle. I think we're looking at about a 109.5 as the bond angle, which is closest to the ideal ..."

Because Anna was looking at her structure without handling it, she was asked to pick it up.

GL: "Can you rotate it?"

Anna (picking up the model): "Well, you ... you can rotate it a little bit, but .. it's not very flexible."
Anna readily recognized that 1,4-dichlorocyclopentane was identical to 1,3-dichlorocyclopentane, and 1,5-dichlorocyclopentane was the same as 1,2-dichlorocyclopentane. "There's no such thing as a 1,4- or a 1,5-, because, um ... well, you're just ... you would just be going in the opposite direction." She also quickly identified 1,1-dichlorocyclopentane as a structural isomer. However, even though she recognized that the 1,2- and 1,5- isomers were identical, when asked if there was more than one possible isomer of 1,2-dichlorocyclopentane, she initially said, "Well, yes, okay. I could go in the other direction. I could go, from the top, um, put the first chlorine on the top and the second chlorine to the left point."

GL: "But aren't those the same?"

Anna: "Yes they are."

GL: "Okay, now I want you to look at the structure that you have in your hand. And don't look at what you've drawn. And tell me if there's more than one 1,2-dichlorocyclopentane that you could build."

Anna: "Well, I guess there ... okay!"

Anna laughed and said, "Okay, I'm in a flat world! All right, we'll get into a three-dimensional world now." At this point she identified the cis and trans-isomers of 1,2-dichlorocyclopentane, but said, "Um, ooh, I'm not quite sure how to draw this!" Anna attempted to use dash-and-wedge drawings to represent cis-1,2-dichlorocyclopentane, and then was unsure whether this represented one structure or two. In order to distinguish between geometric isomers, Anna resorted to using a "little dotted line" and a wedge. Although she thought that "they could both go back, or both go forward," she showed her concern.

Anna: "There might be something wrong with that, as I think about it, sterically (Figure 5.3)."

GL: "Just play with the model that you have in your hands, and see if you can do those things."
Figure 5.3. Anna's representation of 1,1-dichlorocyclopentane and her first representation of cis-1,2-dichlorocyclopentane. Anna has attempted to add some three-dimensional perspective to her diagrams.

Anna: "Okay. Well, I can do it with the model, so I guess it's okay to do it!" At this point, it seemed that Anna realized that her two drawings simply represented two different orientations of the same structure. To test this, Anna was asked to describe the difference between her two diagrams of cis-1,2-dichlorocyclopentane (Figure 5.3), and responded, "Hmm. I'm thinking about cis-trans, but I don't know if that's right."

GL: "What's the easiest way to take the first one (this one with two wedges) and turn it into the one with the two dashes?"

Anna: "The easiest thing would be to rotate."

But when she tried to demonstrate this, she began pulling the model apart.

GL: "Wait, wait. You just said to rotate it, but you're pulling it apart!"

Anna (laughing): "Oh, okay, well, that won't happen!"

GL: "Could you just turn it over?"

Anna: "Well, if I turn it, okay. Well, mentally ... they, they'd have to be the same molecule, because if I'm just turning it over ... it's like, um, a molecule that's just falling to the ground, and just flipping every which way. See what I'm saying?"

Anna then built a model and drew the structure of trans-1,2-dichlorocyclopentane (Figure 5.4). When asked to describe the relationship between the cis and trans isomers
of 1,2-dichlorocyclopentane, she said, "I'm still thinking about cis-trans isomers, but then again I don't think that the stipulation applies."

![cis-trans isomers diagram](image)

Figure 5.4. Anna's representation of trans-1,2-dichlorocyclopentane. This diagram uses dash and wedge to accurately depict the geometry of the structure.

GL: "Well, tell me what cis-trans isomers are."

Anna: "Okay, well, with cis isomers, your molec ... your alkyl groups, or your halogens, or whatever your attachment is, are going in the same direction, pointing in the same direction. And with, um, trans isomers, they're pointing in opposite directions. Which is what it looks like here. And I don't know why I have it in the back of my mind that this doesn't apply."

Anna decided that it was important to emphasize that the molecule was flat, and in order to do this, moved the two chlorine atoms to the bottom of the structure. But she found this unsatisfactory as well.

Anna: "Oh, no, no, that's going to be flat. Drawing it flat makes it look like it sticks up!" (NB: In a proper drawing, the chlorine atoms should appear to stick up.)

GL: "How could you draw the pentagon differently?"

Anna: "More of a flattened pentagon. Like if you were looking at a ... more of a diamond. With some kind of a correction. See, in that way, the two chlorines here ... ."

Anna then produced the structure shown in Figure 5.5, and had no further trouble describing which structures were cis and trans.

However, Anna hesitated when describing the relationship between cis-1,2-dichlorocyclopentane and cis-1,3-dichlorocyclopentane (Figure 5.6).

Anna: "Hmm, I'm not sure what you're wanting."
Figure 5.5. Anna's second representation of the isomers of 1,2-dichlorocyclopentane. Anna has resisted drawing the cyclopentane ring perpendicular to the plane of the paper to emphasize the orientation of the halogen substituents.

Figure 5.6. Anna's representation of the isomers of 1,3-dichlorocyclopentane. Anna has drawn the cyclopentane ring perpendicular to the plane of the paper to emphasize the orientation of the halogen substituents.

GL: "Are they isomers?"

Anna (laughing): "Oh! They would be structural isomers ... because they're ... different spatial orientation for the attachments."

When asked whether the cis- 1,2- and cis- 1,3-dichlorocyclopentanes could be geometric isomers, she finally decided that, "Well, the chloro group is coming off a different carbon altogether. And when you're thinking geometric, you're thinking more of, I want to say, symmetrical appearance. Um, but there's a totally different carbon involved, so it can't be."
In many ways, Anna's experience with the isomers of dichlorocyclopentane mirrored that of several other students. However, each was unique. Most participants were uncomfortable with use of the term "conformer" in conjunction with a cyclic molecule. In this regard, Marianne was typical. When asked if she could make any conformers of dichlorocyclopentane, she asked "A conformer?" And when asked if she knew what a conformer was, she said "Okay, um ... can you refresh my memory?" In order to refresh her memory, she was asked to build a model of ethane (CH$_3$CH$_3$).

Marianne: "Conformers are just like, you rotate it like this, right?"

GL: "Yeah, yeah, okay!"

Marianne: "I remember now!"

Once she built the ethane model, it was easy for her to conclude that there were no conformers of dichlorocyclopentane, "because of the ring."

Only two participants, David and Kathy, were initially comfortable with the term conformer. When asked if she could make conformers of dichlorocyclopentane, Kathy said, "Um, no. Because it's a circle. 'Cause they're all attached to each other."

GL: "What would happen if you tried?"

Kathy: "You would break a bond."

Kathy defined 'conformer' as follows. "A conformer means it can rotate around a single bond without breaking any bonds." David also said that this molecule does not have conformers. "Because it's restricted ... um... you can't rotate them; you'd have to break bonds to do that. And that doesn't fit the definition of conformer."

Several subjects had difficulty properly numbering substituents on the ring. Sometimes this difficulty was ephemeral. Brian build isomers of 1,2- and 1,3-dichlorocyclopentane, and then said that he could also build the 1,4- isomer. As soon as he was asked to build it, he said, "Actually, that's the 1,3- also. I don't know what I was thinking." Michael, Kathy, and Tammy had very similar experiences.
David initially built a model of \textit{trans}-1,2-dichlorocyclopentane and then said, "Uh, this is 2,3-dichlorocyclopentane."

GL: "Why do you call it "2,3-"?

David: "Because I'm not really sure this is right, but ... I think you would start numbering the carbons from the top and go clockwise."

GL: "But what if you rotated it and put one of the chlorines at the top?"

David (laughing): "1,2-." David never had this problem again.

In contrast, Andrea struggled with ring numbering, and insisted that she could make 2,4- and 3,4-dichlorocyclopentane.

GL: "Does it have to be 3,4-?

Andrea: "Well, no, because you could turn it this way, I guess, you don't need to ... It could be 1,2-.

Andrea finally agreed that there was no '3,4-dichlorocyclopentane', but later, regarding another isomer, she said, "This one is 2 and 5." When she placed both chlorines on the same carbon (1,1-dichlorocyclopentane, Figure 5.7), she said, "Oh, it'd be 2,2-, like this one would be 2,2-dichloro..."

\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{figure5_7.png}
\caption{Andrea's representation of 1,1-dichlorocyclopentane. All of the atoms appear to be depicted in the plane of the paper.}
\end{figure}

GL: "What's the difference between '2,2' and '1,1' ?

Andrea: "There isn't."

Although she could visualize and state that there was no difference between '1,1-dichlorocyclopentane' and '2,2-dichlorocyclopentane,' Andrea continued to have trouble
numbering any cyclic compound that did not have a substituent at the 'top' of the ring. Tammy had a similar problem when she held the model she had previously identified as 1,1-dichlorocyclopentane and said, "Okay, I'll just rotate it. There, it's 'three.'" However, when she was asked, "Is it?", she replied, "No, it's still 'one,' actually, 'cause you just label it from where it is."

After identifying the cis and trans isomers of both 1,2-dichlorocyclopentane and 1,3-dichlorocyclopentane, many of the participants had difficulty finding the 1,1-dichloro isomer (Figure 5.1). However, this was the first isomer drawn by Kathy and Marianne, both of whom named this isomer "dichlorocyclopentane." When asked to clarify which isomer it was, Kathy immediately said, "1,1-;" whereas Marianne said it was "1-dichlorocyclopentane."

Except for Anna, none of the other students identified the 1,1-dichloro isomer as a possibility unless prompted. Some of the students were queried about the difficulty. Sometimes the prompting was subtle. James was simply asked, "Okay, are there any more?", to which he responded, "There's this. Which is 1,1-dichlorocyclopentane." At times, more forceful suggestions were needed. When Tammy was asked if there was another isomer in addition to the cis- and trans- 1,2-dichloro and 1,3-dichlorocyclopentanes, she said, "There must be, because you wouldn't be asking me if there wasn't! I'm just trying to think what!"

GL: "You're doing really good, really good!"

Tammy: "Okay, if I do this...it moves like. If I move it anywhere else, it would be 1,3-, because...."

GL: "My question is, what happens if I put both of them on the same carbon?"

Tammy (laughing): "Oh yeah! Okay, then it would just be 1,1-.

Two of the subjects were asked why it was difficult to spot the 1,1-dichloro isomer. James said, "Cause you're looking ... 'cause when you first do like this, 1,2- and then you switch them and get 1,3-, you never think about, uh, the same one. Putting them
both on the same one. You just don't think about it." He agreed that he would probably
not miss that type of problem again. David explained his difficulty in this way.
"Probably because, when you draw these, you typically don't show the hydrogens. And
if the hydrogens were there, then it would be very obvious."

The isomers of dichlorocyclopentane were commonly drawn using bond-line
formulas, with the carbon atoms represented as the vertices of a regular pentagon drawn
in the plane of the paper. Anna's representation of cis-1,2-dichlorocyclopentane is typical
(Figure 5.3). James described this type of representation as being "looking at it from like
aerial view, you could say," and then concurred that it was "from the top." His
representation of the cis-1,3-isomer is given in Figure 5.8. Two students, Tammy and
Marianne, put symbols for each individual carbon atom in their diagrams; Marianne's
representations of cis- and trans-1,2-dichlorocyclopentane are given in Figure 5.9.
Despite seeing diagrams of cyclopentane isomers in their lecture in which the carbon
framework had been rotated out of the plane of the paper in order to give some
perspective to the drawings and facilitate viewing the geometric isomers, only Anna's
final drawings were done using this type of representation (Figure 5.6).

\[ C_1 \]

\[ C_2 \]

\[ C_3 \]

\[ C_4 \]

\[ C_5 \]

Figure 5.8. James' representation of cis-1,3-dichlorocyclopentane. This diagram is
drawn to give the viewer an accurate view of the geometry of the molecule.

Conformers of Dichlorocyclohexane. In contrast to cyclopentane, cyclohexane and
its derivatives readily form conformers because they are not flat, and some rotation
around the sigma bonds is possible. Each participant was questioned about these "chair"
and "boat" conformers (Table 3.3, Questions 5 and 6).
Figure 5.9. Marianne's representations of trans-1,2-dichlorocyclopentane, 1,1-dichlorocyclopentane, and cis-1,2-dichlorocyclopentane. Because each atomic symbol appears to be depicted in the plane of the paper, the correct orientation of the atoms in space is unclear.

Only one subject expressed surprise that the carbon skeleton of cyclohexane was not flat. Brian asked, "Shouldn't this be flat?", and when he was asked, "Should it?", he responded, "Benzene's flat."

GL: "Is that benzene?"
Brian: "Oh, that's right. Benzene's got double bonds."

When asked if he could make any conformers of this molecule, Brian was unsure.
Brian: "Um ... ."
GL: "By rotating around bonds, is what I'm saying."

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Brian: "Yeah, you can do the chair. That's not the chair. No, I'm trying to look at it."

After a short time, he came up with the term "boat." When pressed whether he could make conformers, Brian said, "Yeah, let's see, you've got to rotate it, in some sort ... I'm trying to rotate it like ... The answer is 'yes,' you can make it." Even though he realized that he should be able to convert the boat conformer to the chair, Brian found this manipulation difficult. Part of Brian's difficulty may have been that he didn't think the chair conformation really looked like a chair.

Brian: "Is that it?"

GL: "Yeah! Doesn't that look like a chair?"

Brian (hesitating): "Kind of. The boat looks so much better!"

Three participants (Kathy, Andrea, and Jason) initially said that it wasn't possible to make conformers of cyclohexane. Andrea said, "I have to look closer ... I don't think, I don't think there is."

GL: "If I said to you, 'Is that a chair or is that a boat?', what would you tell me?"

Andrea: "It's a boat! Oh, you can make conformers! 'Cause it's in the boat shape; the chair is like folded." She tried to make the chair conformer, had some difficulty, but finally succeeded.

When asked if she could make conformers of this molecule, Kathy replied "Mm, nope..."

GL: "Why don't you try?"

Kathy: "Oh, you can do the boat and the chair! Yes you can!"

Kathy had no difficulty interconverting the chair and boat conformers. She explained, "Um, you rotate it, a carbon. You didn't break any bonds. It's just a rotation, is what you did."

Jason tried to explain why there were not conformers of 1,1-dichlorocyclohexane by showing that he couldn't bend the model, and stopped abruptly when he converted the
boat conformer to the chair. He concluded that he really only needed to move one carbon atom when converting from the boat to the chair conformer and back.

Anna made a model of the chair conformer cis-1,3-dichlorocyclohexane, and when questioned whether she could make a conformer of this structure, she said, "All right, I can. I can make the boat. That's the boat." She had no difficulty forming the boat conformation.

GL: "Why do you call these conformers?"

Anna: "Well, before, when we had the chair, the two chloros were both in the axial position. In the boat formation, they're in the equatorial position. Um, so I don't know how to describe it without using the word 'conform,' but they're the same molecule, but just conforming different..."

GL: "What can you do with a molecule when you make a conformer?"

At this point Anna simply hesitated. She was further prodded.

GL: "If it were not in a ring, what would you be able to do to make a conformer? It doesn't matter if it's a ring or not."

Anna: (hesitating)

GL: "What are you doing when you do this? (NB: convert one conformer of dichlorocyclohexane to the other)."

Anna: "I'm rotating the bond! Okay, I'm sorry! I think my brain is fried a little bit."

Despite his dyslexia, Michael immediately recognized that he could make conformers of this molecule. On building his model, he said, "Just made it to the chair. I had the boat." Marianne, Tammy, and David also clearly stated what conformer they had made as they were building the model; only David had difficulty converting one conformer to the other.

Isomers of Dichlorocyclohexane. Participants were requested to build and describe all possible isomers of dichlorocyclohexane (Table 3.3, Questions 7 and 8). After having
previously constructed all of the isomers of dichlorocyclopentane, it was less difficult for the subjects to find the 1,1-dichloro isomer of dichlorocyclohexane. All of them found it without prompting. However, Marianne later attempted to make "3,3-dichlorocyclohexane."

Many of Brian's experiences with dichlorocyclohexane were typical. He drew all of the cis isomers first (1,2-dichlorocyclohexane, followed by the 1,3- and 1,4-isomers). He then drew 1,1-dichlorocyclohexane, saying "And it's neither cis nor trans." The next isomer that he built was the trans-1,3-isomer, about which he said, "I don't think that's cis or trans either. It doesn't look like trans."

GL: "What should you look at in order to determine if an isomer is cis or trans?"

Brian: "You have your axial and equatorial... Yeah, this could be trans."

He then finished drawing the trans isomers and went back to review the 1,1-dichlorocyclohexane, saying, "And ... let me look at this one. 1,1- is neither cis nor trans.

Brian successfully identified all of the pairs of geometric isomers. When asked how he could tell which pairs were geometric isomers, he said, "Um ... you can pretty much ... the geometric isomers are also cis-trans isomers, and you have the relationship between cis and trans."

GL: "What makes an isomer cis as opposed to trans?"

Brian: "The chlorine is on the same side, it would be, uh, cis, and on the opposite side, it'd be trans.

GL: "What do you mean, 'on the same side'?"

Brian: "Like both of the up or both of them down."

Brian had no difficulty identifying the cis isomer; however, identifying the trans isomer was more troublesome.

GL: "What do you look at to tell whether the isomer is trans?"
Brian: "These are ... perpendicular to each other," referring to the halogens on the *trans*-1,3-dichlorocyclohexane.

Brian initially said that there were no pairs of structural isomers, but when questioned about the relationship between the *cis*-1,3- and *cis*-1,4-dichlorocyclohexanes, he said, "Oh, yeah, yeah. They would be positional isomers, right? Okay, yeah. Yeah, the attachment of the chlorine to different carbons would make it positional. So the 1,3- and 1,4- isomers would be positional isomers." Most of the other subjects successfully identified all of the structural and geometric isomers, and many of them noted that 1,1-dichlorocyclohexane was somehow special. Andrea was asked what would happen if she put both chlorines on the same carbon atom. She initially said she would have "1,1-," and then quickly added, "Wait, 1,1-, I think," and then correctly added, "But it can't be cis or trans. Because they're the same. If you change them, you know, there's like a chlorine here and a chlorine here, and if you change it, they're the same." In contrast, Tammy initially said that she had built *trans*-1,1-dichlorocyclohexane.

GL: "Why is it trans?"

Tammy: ""It looks like they're going opposite."

GL: "Could you make *cis*-1,1-dichlorocyclohexane?"

Tammy (hesitating): "...No."

After successfully making all of the other isomers, she returned to this idea, saying, "I could make a ... I could make a *cis*-1,1-." When encouraged to try this using the models, she concluded, "Okay, I couldn't." However, she never abandoned the idea that she could make a *trans*-1,1-dichlorocyclohexane.

Several subjects worried about whether there was a need to use the qualifiers "chair" and "boat" when naming the isomers of cyclohexane. James' experience exemplifies this.

James: "And ... when you're naming them, do you have to say 'boat' or 'chair'?"

GL: "Why would you do this?"
James: "I have no idea."

GL: "Could you isolate either the boat or chair conformer?"

James: "Mmm, don't remember."

However, he did remember that they could flip back and forth and convert one to the other. When he reflected on this, he correctly concluded that he did not need to use the terms 'boat' and 'chair' in naming the isomers of dichlorocyclohexane. Marianne attempted to distinguish between the cis and trans isomers of 1,2-dichlorocyclohexane by using the term 'chair' to describe the cis isomer; however, she quickly abandoned this idea without prompting.

Two participants attempted to accurately draw the entire molecule in three dimensions. Michael and James both drew their isomers in the chair conformation. In contrast, David drew a flat hexagon "on it's side," giving perspective to the chlorine atoms (Figure 5.10). Most of the other subjects used a regular hexagon to represent the cyclohexane skeleton, and had varying degrees of success in representing the geometric isomers. For example, Andrea's representation of cis-1,3-dichlorocyclohexane is probably more aesthetically pleasing, less ambiguous, and more conventional than Jason's, although neither accurately depicts the actual geometry of the molecule (Figures 5.11 and 5.12, respectively).

![Figure 5.10. David's representations of the isomers of dichlorocyclohexane. Because the cyclohexane ring is drawn as if it is perpendicular to the plane of the paper, the orientation of the halogen substituents is clear. The conformation of the carbon atoms cannot be distinguished.](image-url)
When asked how to distinguish the cis from the trans isomers, several participants initially attempted to do this using the terms axial and equatorial. Michael built a model of cis-1,2-dichlorocyclohexane, correctly identifying it as cis. When asked how he could tell it was the cis isomer, he said, "The two chlorines are ... axial? No, no, no, this one is axial right here."

GL: "How can tell that it's the cis isomer?"

Michael: "It's 'cause they're both on the upper part of the carbon atom."

Although he correctly identified each cis or trans isomer, Brian was unable to clearly state how he did so. He simply said, "You have your axial and your equatorial ... ." Anna also used the terms 'axial' and 'equatorial' in her description of trans-1,3-dichlorocyclohexane, although everything she said was perfectly correct. "I have one in the axial position pointing upward, and one in the equatorial position pointing downward. And that's why I'm calling it trans."

GL: "How can you tell that one is 'up' and the other one is 'down'?"
Anna: "Okay, well, the way I'm holding it, my axial chloro is perpendicular to the ring. And I've got it above the ring, versus below. And my equatorial is on the down, it's on the down side of the ring. Pointing downward; they're pointing in opposite directions."

Marianne described \textit{trans}-1,3-dichlorocyclohexane in similar terms. "Ooh, wait a minute. Wait, wait. I think it would be trans. 'Cause one's going down (NB: the axial chlorine on her left) and one's going out (NB: the equatorial chlorine on her right)."

Because she had omitted the hydrogen atoms from her model and included only the carbons and chlorines, it was suggested that she add the hydrogens at positions one and three. After adding the hydrogen atoms, she still described the axial chlorine as "up," with the equatorial hydrogen at the same position described as "down" rather than "out."

When asked to describe the equatorial hydrogen and axial chlorine at the other carbon atom, she said, "'The opposite, so that is \textit{trans}-.."

David initially built a model of \textit{trans}-1,3-dichlorocyclohexane.

GL: "Now, the other question that I have, then, is are there any geometric isomers of 1,3-dichlorocyclohexane, and if so, which one do you have?"

David (hesitating): "...I'm trying to remember if you have geometric isomers with the cyclohexane."

GL: "Well, why don't you try it out? Move one of those chlorines and see if you think you do."

David built his model, but did not add any hydrogen atoms to the structure.

GL: "Would it be easier if you had some hydrogens on there to see that? You don't need put them on every carbon, but maybe the 1 and the 3. " David then added hydrogen atoms to carbons 1 and 3. "Beautiful. Okay, now, which one do you have there? Which geometric isomer do you have right there?"

David: "This is trans."

GL: "You're right. How can you tell?"
David: "Um, ..., um, because, uh, the chlorines are pointed in different directions."

GL: "Okay, which one is pointed in which direction?"

David: "Uh, the one on the number 1 is pointed down, and the one on the number 3 is pointed up."

GL: "Okay, that's fine. That's fine. And which is the toughest one to see the way you have it right there. The one that's pointed up or the one that's pointed down."

David: "The one that's pointed down." David was implying that it was more difficult to visualize the trans-1,2-isomer when both chlorine atoms were oriented in the equatorial conformation.

GL: "Okay, and why is that?"

David: (laughing) Because it's really pointed more out to the side.

GL: "It's only down in relation to what?"

David: "This one." (NB: One chlorine atom is down relative to the other chlorine atom.)

GL: "And in relation to..."

David: "The hydrogen."

Kathy built a model of trans-1,2-dichlorocyclohexane, placing the chlorine atoms in the equatorial position. When asked why they were trans, she gave an excellent description. "I remember this because they're going ... this one's going in the up position and this one's going in the down position." When it was pointed out to her that they were really close to each other, she said, "Right. But they're not going in the same direction. They're going in opposite directions."

Conformers and Geometric Isomerism in 1,2-Dichlorocyclohexane. The next questions (Table 3.3, Questions 9 - 12) required students to analyze the geometric isomers and conformers of 1,2-dichlorocyclohexane. In order to avoid unnecessary clutter while building models, each subject was asked to include only those hydrogen atoms that were specifically shown in the diagrams. Question 9 had participants build...
and name a model of trans-1,2-dichlorocyclohexane in which the halogens were
equatorial and the 1,2-hydrogens were axial. Question 10 required building and naming
the conformer of the previous structure in which the halogens were axial and the 1,2-
hydrogens were equatorial. The subjects were then required to describe the relationship
between these two conformers (question 11) before building, naming, and describing the
relationships in the geometric isomer, cis-1,2-dichlorocyclohexane (Table 3.3, Question
12). Because optical isomerism had not as yet been covered, the participants were not
asked to describe the trans-1,2-isomer as a pair of enantiomers (Table 3.3, Questions 9 -
11). Only the (1S,2S)-isomer was depicted and used in this exercise. The cis-1,2-
isomer is a meso compound; this point was not emphasized in question 12.

Many of the troubles encountered during these questions resulted from difficulties in
classifying equatorial substituents as either cis or trans, in part because of confusion in
the difference in the terms cis-trans and the terms axial and equatorial. In addition,
conformers were consistently confused with geometric isomers.

Most of the participants had difficulty with these questions, although Michael and
Kathy did very well. Michael readily built both conformers of the trans isomer. He
initially described both structures as having one axial chlorine and one equatorial chlorine,
but quickly corrected himself, describing both chlorines from question 9 as equatorial,
and those from question 10 as axial. He correctly noted that both were trans isomers,
saying, "It's just because one's on the equatorial, and on the other, both are axial."

GL: "Can I turn number 10 into number 9 without breaking any bonds?"

Michael (confidently): "Yes."

Michael demonstrated this manipulation and correctly said that the two structures
were conformers. When he built the cis isomer (Table 3.3, Question 12), he correctly
identified it as cis-1,2-dichlorocyclohexane. However, he had some trouble describing
the differences between the geometric isomers (Table 3.3, Questions 10 and 12)
GL: "Now what's the relationship between that one and the one that we call number 10 there?"

Michael: "... It's just that the one chlorine over here ... is on the inside."

GL: "Okay, so are those isomers?"

Michael (hesitating): "... Yes."

GL: "How can you tell?"

Michael: "It's cause this one is on a different carbon bond. The inside of the carbon."

GL: "Can I take number 12 and turn it into number 10 simply by rotating around bonds? Like I did with number 10 and number 9?"

Michael: "No."

GL: "Do you want to try?"

Michael: "Yeah"

GL: "Okay."

Michael: (manipulating the model): "They're not the same."

Kathy readily identified the structure from question 9, in which the halogens are both equatorial, as "trans-1,2-dichlorocyclohexane."

GL: "Why do you call this one trans-?"

Kathy: "Uh ... I remember because they're going ... this one's going in the up position and this one's going in the down position."

GL: "Okay, because they look like they're really close to each other, right?"

Kathy: "Right. But they're not going in the same direction. They're going in opposite directions."

GL: "Oh, that's perfect! Now, do you look at the chlorines or at the hydrogens?"

Kathy: "The chlorines."

GL: "Okay. Why don't you look at the hydrogens?"

Kathy: "Because there's hydrogens all over it."
Kathy agreed that she could have used the axial hydrogens to identify this trans isomer. She then built the conformer with the two halogens in the axial position (Table 3.3, Question 10), and named it "1,2-cis- ... uh, trans-1,2-dichlorocyclohexane. Same thing."

GL: "Okay, now, that one, number 10, doesn't look like number 9!"

Kathy: "No."

GL: "What's the difference? I mean, first of all, why do you call that one trans? You're right. Why is that one trans?"

Kathy: "This one is trans because, well, you could do either the hydrogens or the chlorines. Let's look at the chlorines. They're in opposite directions."

Kathy was then asked why these two types of trans-1,2-dichlorocyclohexane didn't look like one another.

GL: "Okay. Well, what's the difference between number 9 and number 10?"

Kathy: "The difference that I see between number 9 and number 10 is if you do this, it's on the bottom portion of the boat ...I mean the chair, sorry. Whereas number 10, it's on the upside of the chair. But other than that, they're the same thing. And the chloros ... are in different position. And here they're on the axial position..."

GL: "Ah, okay."

Kathy: "But here they're on the equal ... equa..."

GL: "Equatorial?"

Kathy: "Equatorial!"

Describing the difference between the axial and equatorial positions, she said, "Axial runs perpendicular to your carbons, where the equatorial, they don't run perpendicular. They don't run parallel either; I'm not sure what you'd call that!"

When asked if these two structures could be converted one to the other, she said, "Yeah! I think ... you ... try to move the bottom portion of the boat ... my chair! ... take
my upper portion and drop it down," and completed the manipulation of converting one conformer to the other. She concluded that they were the same thing.

GL: "But they're different structures, so what do we call those?"
Kathy: "Um ... structural isomers ... no, no, no ... different structures."
GL: "They're the same, because they can interconvert, right?"
Kathy: "Right."
GL: "What do we call that? You already answered this question."
Kathy (laughing): "Great! Hmm, chair ... conformers."
GL: "Perfect! Now why are they conformers?"
Kathy: "Because you don't break the bonds. You're just rotating them around the bonds."

She explained that they didn't look like conformers because, "I'm used to the Newman... ." When Kathy built the cis isomer (Table 3.3, Question 12), she had no difficulty naming it or identifying it as a geometric isomer of the two trans conformers.

Performance by the others on these questions stood in contrast to that of Michael and Kathy. Andrea continued to have difficulty numbering the positions within the ring. Describing the positions of the chlorine atoms on the ring (Table 3.3, Question 9), she said, "That'll be on carbon three. And on carbon four, the chlorine is down, and the hydrogen pointing up."

GL: "Let me ask you a question. Why did you call that carbon 3 and carbon 4?"
Andrea: "I just started from here."
GL: "Okay, is there any reason for that?"
Andrea: "Not really."
GL: "It just sounded like a good place to start?"
Andrea: "Yes, it just looks kind of good to keep it there."
GL: "Okay, okay, but it doesn't have to be?"
Andrea: "No."
She continued to describe the halogen-bearing carbons with the labels "three" and "four." "So I put a chlorine sticking up on, I guess that's on number three, carbon three. And a hydrogen going down. And the next one, carbon four, put a chlorine down and a hydrogen ..." Later, when asked to name this structure, she asked, "Does it matter that I call this '3'?") Everyone else correctly labeled the halogen-bearing carbon atoms as numbers '1' and '2'.

Many participants had difficulty describing the substituents on the two conformers (Table 3.3, Questions 9 and 10) as being in the trans position. Jason built the conformer with both chlorines in the equatorial position (Table 3.3, Question 9) and named it "1,2-dichlorocyclohexane," but when asked whether it was cis or trans, he said, "... It's neither." However, he then built the conformer with the chlorines in the axial position (Table 3.3, Question 10), and correctly named it "trans-1,2-dichlorocyclohexane."

GL: Okay, now, let me look at this. That looks good! Okay, what's the name of that?

Jason: "... 1, uh, trans-1,2-dichloro... cyclohexane."

GL: "Why do you call it trans? I mean, what is clear to you that made that trans?

Jason: They're on opposite sides."

GL: "Okay, okay. Can you take number ten, and without breaking any bonds, can you turn it into number nine?"

Jason easily converted his model to the other chair conformer.

GL: "What happened?"

Jason: "It's the same."

GL: "So what's the name of number nine? Number ten you told me was trans 1,2-dichlorocyclohexane. And it's the same as number nine."

Jason: "It's the same." (NB: the same name)

GL: "Okay, what is it about that one that makes it hard to tell that it's trans? 'Cause it is trans, right?"
Jason: "Yeah. It's just the, uh, the way the chlorines are."

GL: "What about the hydrogens. Don't they look ...?"

Jason: (hesitantly): "Well, yeah, the hydrogens..."

GL: "Okay, now, what is it that makes it trans?"

Jason: "... The different arrangement of the chlorines."

In regards to the equatorial chlorines, he finally said, "It's not straight up and down, but it's going down." He then reasoned that the next structure (Table 3.3, Question 12) could not be converted either of the previous structures "'Cause one's cis and one's trans," describing them as geometric isomers.

Marianne built the first structure (Table 3.3, Question 9), but described both chlorines as axial and the corresponding hydrogens as equatorial. "Um, just 'cause I know that equatorial means up-and-down, and axial means, like, going out to the sides."

GL: "Okay, if there were an axis to that molecule, where would it be?"

Marianne: "Like right through the middle."

GL: "If that's the axis, which ones are axial?"

Marianne: "The hydrogens. Oh, wait, I had it backwards, huh? Okay! Wait, does equatorial really mean out to the side way?"

When she built the conformer with both chlorines in the axial position, she named it "cis-1,2-dichlorocyclohexane," and then said, "This one's, oh, that's right, it's trans." She identified the first conformer as being trans as well, noting that "they don't look the same." She then checked to make sure they were both 1,2-isomers.

Marianne: "How can you distinguish both of these? Um... I don't remember."

GL: "I don't know that you've forgotten anything. 'Cause we haven't distinguished between those. We haven't tried to name those. Does it seem bizarre to you that those are both the same?"

Marianne: "Yep!"
Marianne said that they differed in that, "Like, one of them, the first chlorine is equatorial, and this one has axial (NB: the corresponding hydrogen atom), and it's the opposite on the other two." And could she convert one to the other? "Um... you could make it into a boat and then make it into a chair. Oh, somehow you can do it, though! Okay, like this, maybe? Yeah!"

GL: "Now, what's the relationship between number nine and number ten?"
Marianne: "They're the same thing."

GL: "Well, they're not pointing the same way ... they're kind of the same thing. But here's number nine, right? This is number nine?"
Marianne: "Uh huh"
GL: "And here's number ten? They're not exactly the same thing, are they?"
Marianne (surprised): "They're conformers!"

Marianne then built a model of cis-1,2-dichlorocyclohexane (Table 3.3, Question 12), immediately identified it as the cis isomer, and was asked, "Can you take number twelve and turn it into number nine there without breaking any bonds?" She responded "I don't think so. Okay ... No, because they're always going to be cis." Having read ahead in the text, she initially described these isomers as enantiomers, but, agreeing that they weren't mirror images, sought for another term.

Marianne: "Are they conformers then? I don't think so."
GL: "Are they isomers"
Marianne: "Yes, they're structural isomers. No, they're geometric isomers!"
GL: "What's the difference?"
Marianne: "Structural means like, it's the same thing, just in a different order. And geometric means they have a different orientation in space." Because she had just built and described several structural isomers of dichlorocyclohexane in the previous questions (Table 3.3, Questions 5-8), Marianne was asked to build a structural isomer. She replied "I don't think you can."
While manipulating his models, Brian said, "I mean, like I told you when you read my journal, I'm not that great with geometric 3-D," although he thought working with the models was "pretty neat. It does help you understand it a little better, though." He built the structures from questions 9 and 10 (Table 3.3), naming the second one trans-1,2-dichlorocyclohexane, but incorrectly concluding that the first one was cis. Because he had included the two hydrogen atoms in his structures, he was told to pick up the model he had described as cis, and describe the position of the hydrogens on the chlorine-bearing carbon atoms.

Brian: "Oh, wow! From there they look trans!"

GL: "Can you convert number 9 to number 10 without breaking any bonds?

Brian: "I don't think so."

GL: "Why don't you try?"

He picked up his model, looked at it, and said, "It's in the boat now. There's got to be a way (NB: to get it back into the chair conformation). I know you can flip ... You can flip them and make them turn around, I think."

When he finished his manipulation, he was asked whether he hadn't made the other structure. "I sure did!" And regarding the names of the two, he said, "Same thing, it'd be trans-1,2-. Can I change that (NB: his previous answer)?" Brian then built a model of cis-1,2-dichlorocyclohexane (Table 3.3, Question 12), but concluded that it was "trans-1,2-dichlorocyclohexane."

Brian returned to the trans conformers (Table 3.3, Questions 9 and 10). When both chlorine atoms were axial (Table 3.3, Question 10), he concluded this isomer was trans because "one is up and one is down."

GL: "What about the hydrogens?"

Brian: "You don't even look at it."

GL: "Okay, that's fine. How about on that one (NB: number 9), that we also decided was trans?"
Brian: "Um, ... the hydrogens are the ones that are pointing down and up."

GL: "Okay, what about the chlorines? Is one up and one down there?"

Brian: "No."

GL: "No?... One of them is axial and one is equatorial, right?"

Brian: "Right."

GL: "But is one of them pointing down and one of them pointing up, but just not as much?"

Brian: "Mm hmm."

It was pointed out that he had decided that the conformer with two equatorial chlorine atoms (Table 3.3, Question 9) was also the trans isomer. What did he look at? "Um, ... the hydrogens are the ones that are pointing down and up." What about the chlorines? Was one down and one up? "No." He described the cis isomer of 1,2-dichlorocyclohexane as follows. "One's down and one's off to the side." He was challenged with this question. "Is that one down or up? If you had to call that one down, down or up, what would you call it?" He said, "Down. If they're both down, then it would be cis."

After struggling to recognize the two trans conformers of 1,2-dichlorocyclohexane, Brian continued to have difficulty with the cis isomer as well. After building a model (Table 3.3, Question 13), he was asked, "Is it cis or trans?"

Brian: "Trans."

GL: "What are you looking at?"

Brian: "The angle that's perpendicular?" (NB: the axial chlorine)

GL: "Okay. When you say they're trans, what does 'trans' mean?"

Brian: "On opposite sides."

GL: "What's on opposite sides?"

Brian: "See, this is down, right? (NB: the axial chlorine) This is not up. (NB: the equatorial chlorine) So it wouldn't be trans."
Having concluded that the structure was did not represent the trans isomer, Brian was still unwilling to state that it represented the cis isomer. He finally concluded that this was the only other possibility, but was clearly not pleased by this. He continued to struggle with this issue, and when finally asked to justify why the model he was holding represented the cis isomer, he finally pointed to the chlorines and said, "One's down and one's to the side."

GL: "Okay, is that one (NB: the chlorine) that's pointing to the side, is that one down or up? If you had to call that one down, down or up, would you call it?"

Brian: "Down. If they're both down, then it would be cis."

Tammy had no difficulty building the first two structures (Table 3.3, Questions 9 and 10), but described the structure from question 9 as being cis. But on comparing this structure with its geometric isomer (Table 3.3, Question 13) she discovered that something was "strange."

GL: "Okay, is that cis or trans?"

Tammy: "Number 9 looks like it would be cis."

GL: "Okay, tell me, why do you call that one cis?"

Tammy: "Because this one looks like the same... This one doesn't look like it's going in the same direction (NB: the equatorial chlorine atoms, Table 3.3, Question 9), but this one really doesn't look its going in the same direction (NB: the axial chhlorine atoms, Table 3.3, Question 10). To me, this looks like the closest one to cis."

GL: "Okay, I'm not arguing with you now. What would you get if you took this one and changed it with that one?"

Tammy: "That's strange."

GL: "What do you think that one is?"

Tammy: "This one looks like it is cis (NB: Table 3.3, Question 12)."

After converting the two trans conformers (Table 3.3, Questions 9 and 10) into one another, she correctly reasoned that both of these represented trans isomers. David had a
similar experience, classifying the first structure (Table 3.3, Question 9) as a cis isomer, because "both of the chlorines are equatorial." He had less difficulty when both chlorines were axial; the second structure (Table 3.3, Question 10) was given the name trans-1,2-dichlorocyclohexane. He was asked to describe the relationship between the hydrogens on this molecule, and said, "They have to be trans."

GL: "That's right. So what's going on in number 9?"

David: "So those are trans- as well. Okay, one's up, one's down, okay."

GL: "Okay, one's up... but they don't look like it, do they?"

David: Unh uh."

GL: "What are they up and down in relation to, the chlorines?"

David: "Um, to the hydrogens."

When asked if he could convert the structure from question ten into that from question nine without breaking any bonds, he hesitated. He laughed and finally said, "How the hell to do this?!"

GL: "Are there any conformers of the molecule?"

David: "Of course! You could make the boat!"

Although he had a little difficulty manipulating the model, David successfully completed this chair-boat-chair conversion. He then built the cis-1,2-isomer (Table 3.3, Question 13), and concluded, "They're both pointing down."

GL: "Is there any way you can make them both point up?"

David (laughing): "Real easily!"

He then flipped the molecule over. He correctly concluded that the structures from Questions 9 and 12 (Table 3.3) were geometric isomers, "because you can't convert cis to trans."

Structural Isomers of Dichlorobenzene. The last questions from this set (Table 3.3, Questions 15 and 16) had participants draw and name all possible isomers of dichlorobenzene and describe what type of isomers they had made. Because
dichlorobenzene a flat molecule that can only have one substituent on each carbon atom, only structural isomerism is possible. These two questions were much easier for the participants than the others. Nobody said that benzene could have any geometric isomers, and everyone thought that the flat nature of benzene was somehow important. Anna’s responses to these questions were typical. She drew the three structural isomers of benzene, naming them o-, m-, and p- dichlorobenzene (Figure 5.13). She was then asked if these structures were isomers.

![Figure 5.13. Anna's representations of the structural isomers of dichlorobenzene. The positions of the substituents and the planar nature of the entire structure are both accurately depicted.](image)

Anna: "Um, these are structural isomers."

GL: "Very good. Why do you call them structural isomers."

Anna: "Because the carbon, the numbered carbon that the chlorine's are on changes for at least one of them."

Anna was then asked if she could make any geometric isomers of dichlorobenzene.

Anna: "Um, there are no geometric isomers of any of these."

GL: "Why is that?"

Anna: "Um, it’s flat."

GL: "It's flat, okay! Anything else? Not that I have anything against that; that's exactly what I would have said, too!"
Anna hesitated, and was told, "Okay, let me put it to you this way. Cyclopentane is flat, and you can make geometric isomers of cyclopentane." She said, "Yeah ... " and still hesitated. At this point, she was asked to build a model of cyclopentane.

GL: "Okay, why can I make geometric isomers in cyclopentane, and it's flat, but I can't make geometric isomers in benzene?"

Anna: "Well, it's really not flat. Completely flat. It's like, um, let's see, it's the bond angles. There's a degree of rotation, because they're all single bonds..."

GL: "Okay, what's not flat? What isn't flat in cyclopentane? I mean, the carbons are all flat, right?

Anna: Right."

GL: "Well, what's not flat in cyclopentane?"

Anna: "The attachments. The substituents!"

GL: "Okay, and how many substituents can I put at each carbon in a cyclopentane."

Anna: "Oh, two. On benzene, you can only put one."

Anna was then asked if she could make any conformers in benzene. She said, "I don't think so, but I'm not quite sure how to explain that."

GL: "Let me ask you a question. Can I rotate around any of those bonds at all?"

Anna: "No."

GL: "Why not?"

Anna: "Um, because double bonds restrict rotation."

GL: "Okay."

Anna: "And I know that's not quite the answer...Um, you can have resonance, but...you can't really rotate anything."

**Summary of Results from Second Interview.** Six broad categories of difficulties relating to conformers, geometric isomers, and structural isomers of cyclic hydrocarbons and their derivatives among beginning organic chemistry students emerged from this interview. These categories are "conformers and flexibility of bonds", "rotation around
bonds and rotation of molecules", "living in a flat world", "focus on only one type of isomer", "structures of structural isomers, geometric isomers and conformers", and "Looking at models without physically handling them". The first category refers to lack of association between conformational isomers and rotation around sigma bonds. The second category discusses difficulties students have when they fail to differentiate between rotation around a bond and rotation of an entire structure. The category "living in a flat world" is derived from a phrase coined by one of the student participants, and refers to a variety of difficulties that students have when they apparently visualize a chemical structure in only two dimensions. The category "focus on only one type of isomer" describes difficulties that students have when they either look exclusively for geometric isomers or exclusively at structural isomers. The category "structures of structural isomers, geometric isomers, and conformers" refers to difficulties in drawing, describing and naming different types of isomers. Finally, the category "looking at models without physically handling them" describes the reluctance of some students to actually pick up models, rotate the entire structure, view it from different angles, and rotate around its bonds.

These categories of difficulties are summarized in Table 5.1
Table 5.1. Difficulties in Learning Derived from the Second Interview.

I) Conformers and flexibility of bonds
   A) Students do not observe that lack of flexibility causes lack of conformers. This isn't accepted until students actually handle the models.
   B) Students simply memorize that molecules in six-membered rings may form conformers, whereas molecules with smaller rings do not.
   C) Students say that the chair and boat forms of cyclohexane represent different molecules.
      1) They may state that you can convert one to the other.
      2) They can become convinced that the two structures represent structures in equilibrium after handling models.

II) Rotation around bonds and rotation of molecules.
   A) A molecule drawn "upside down" is seen as being a different structure. Student fail to distinguish between rotating around a bond and rotating an entire molecule.
   B) Students tend to disassemble models (instead of rotating around bonds) when converting from one conformer to another, just as they must do when converting structural and geometric isomers.
   C) Students tend to insist that the carbon atom labeled "1" must be drawn at the top of the page, and are reluctant to rotate the structure.
   D) Rotation around a bond is not associated with the interconversion of the chair and boat forms of cyclohexane.

III) "Living in a flat world"
   A) Students are reluctant to draw a ring perpendicular to the plane of their paper in order to emphasize the orientation of the attached substituents.
   B) Students tend to state that cyclohexane must be flat because benzene is flat.
   C) Some students state that they can't make conformers of cyclohexane because it is cyclic.
   D) The 'chair' conformation of cyclohexane does not appear to be a chair to some students.
   E) Students fail to describe the lack of geometric isomers in benzene as being caused by the planar nature of the ring and its substituents.

IV) Focus on only one type of isomer.
   A) Students tend to build only structural isomers until prodded.
   B) When asked to build a set of geometric isomers, students then have difficulty identifying structural isomers.
   C) Given a set of structures, students recognize and identify geometric isomers more easily than structural isomers.

V) Structures of structural isomers, geometric isomers and conformers.
   A) The terms 'axial' and 'equatorial' are frequently used in naming geometric isomers, and are associated with the terms 'cis' and 'trans'.
   B) Problems associated with substituents that are perpendicular to the ring.
      1) A 1,1-disubstituted cycloalkane is often described as a trans-isomer.
      2)trans-1,2-disubstituted cycloalkanes in which both substituents are equatorial difficult to attribute. They may be described as "neither cis nor trans"
      3) Equatorial substituents are not qualified using the terms 'up' and 'down' whereas these terms are readily used for axial substituents.
   C) Lack of geometric isomerism in benzene derivatives is not attributed to the presence of only one substituent per ring carbon atom.
   D) Students "number from both ends," and tend to duplicate structural isomers.

VI) Looking at models without physically handling them.

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INTERVIEW 3 RESULTS

The third interview was conducted nine to ten weeks after the beginning of the course, and was designed to probe student learning, understanding, and conceptions regarding the nature of optical isomers and their relationships to structural and geometric isomers. By this point in the semester, students had been introduced to the concepts of chiral centers, enantiomers, diastereomers, and meso compounds. In addition, subjects had been shown that by exchanging the positions of any two substituents on a chiral center, the enantiomer (mirror image) of the original structure was obtained.

Three-dimensional Representations of a Single Molecule. The first three questions of the third interview (Table 3.4, Questions 1 - 3) asked participants to describe the relationships between two three-dimensional representations of the same molecule, (S)-1-bromo-1-chloroethane (Table 3.4, Question 1). The chiral carbon atom in both structures is depicted with two substituents in the plane of the paper, a third substituent above this plane, and the fourth substituent below the plane. The only difference between the two structures as drawn is that the second has been rotated around the vertical carbon-chlorine bond; an observer from above would see that the second structure has been rotated sixty degrees counterclockwise. The type of three-dimensional representation shown here is commonly used to represent optical isomers (or the portions of molecules containing chiral centers).

Several students assumed that these two structures must represent isomers because they do not look identical. Jason confidently stated, "Yeah, they're not mirror images, so they'd be stereoisomers." However, he was unable to explain why they were not mirror images, and asked if he could draw them. He drew structure 'A' and its mirror image (Figure 6.1). At this point he correctly concluded that the mirror image of 'A' was not the same as 'B'. However, from this information he still did not conclude that the structures of 'A' and 'B' were identical.
GL: "What's the relationship between 'A' and 'B'?"
Jason: "They're, uh, ... structural isomers?"
GL: "Are they?"
Jason: "You know, their atoms are just in different orders."

Because Jason incorrectly concluded that these two diagrams represented structural isomers, he was asked to build models of each of them. He readily built a model representing structure 'A' and concluded, "It doesn't line up with 'B'." Although the dash-and-wedge representation of 'A' did not seem to trouble Jason, when lining his model up with structure 'B', he had a question.

Jason: "Well, isn't the hydrogen going down?"
GL: "No, the hydrogen's coming up."
Jason (hesitating): "The wedges mean up?"

At this point, he concurred that his model of structure 'A' also represented structure 'B'.

GL: "So how could you convert 'A' to 'B'?"
Jason (hesitating): "... Would you just rotate them?"

This was certainly correct, but he had difficulty choosing a bond (or an axis) around which to rotate.

Jason: "You'd rotate around the carbon bond."
GL: "All of them are connected to the carbon."

Jason: "Yeah"

GL: "Which bond? Which one would be the easiest one to see, do you think?"

Jason: "The bromine and hydrogen?"

Using the model he had just built, Jason was then shown how to rotate around a bond. At this point, he again was asked which bond he would rotate around, and he said "the chlorine" while rotating the carbon-chlorine bond with his hands. Rotating representation 'A' sixty degrees about the carbon-chlorine bond does yield representation 'B'.

Jason drew a "flat" (dash formula) representation of 1-bromo-1-chloroethane without problems, but when asked to name the structure, he had difficulty.

Jason: "It has one carbon, so it's a methane."

GL: "How many carbons does it have?"

Jason: "One. Two? (laughing) So it's a ... it's ethane. And it'd be a ... I'm not sure."

GL: "That's okay. What's on it?"

Jason: "They're all on the ... the first carbon. So it'd be a 1-chloro-1-bromide ethane."

After writing the name, he corrected it to 1-chloro-1-bromoethane. Because the names of the substituents ('bromo' and 'chloro') should be placed alphabetically, Jason was asked what he might change about his name and was told, "It's pretty trivial." He may have still been unsure about the proper number of carbon atoms in the structure, because he responded, "... Well, I have a methyl." After being asked, "What order are you going to put the chloro and the bromo on there?", he laughed and said, "You put them in alphabetical order."
Like Jason, Marianne also initially classified structures 1A and 1B (Table 3.4) incorrectly. On being shown the drawings of these structures, she immediately said, "They have different orientations in space, so I guess they're geometrical isomers."

GL: "Why do you call them geometric isomers?"

Marianne: "'Cause they have the same elements, just in a different order."

GL: "What do you have to have for it to be a geometric isomer?"

Marianne: "They just have to have a different orientation in space."

She did not know what to say when she was asked what kinds of compounds can have geometric isomers, so she was then asked, "Can you have geometric isomers in alkenes?" Realizing that the structures she was using did not represent an alkene, she responded, "Oh, okay. It's an alkane."

GL: "Are you sure?"

Marianne (hesitantly): "I think it is. An alkane has just single bonds."

GL: "Can an alkane have halogens?"

Marianne: "Oh, I don't think it can," but she was unable to give the term 'alkyl halide' to describe the given structures.

Marianne was then asked to draw the structure of any alkene "that could have geometric isomers. I don't care which one."

Marianne: "Um, an alkene?"

GL: "Just any alkene that can have geometric isomers."

Marianne: "Oh, God!"

To make this question even simpler, Marianne was asked to draw any alkene. She drew a diagram consisting of two carbon atoms connected by a triple bond and having two hydrogens attached to each carbon.

GL: "So how many bonds to carbon do you have?"

Marianne: "Four. Each one has ... no, each one has five!"

GL: "So maybe you shouldn't have a triple bond there?"
Marianne: "Okay, let's have a double bond."

She crossed out a bond to give the structure of ethene. Because ethene does not exhibit geometric isomerism, Marianne was asked to draw any compound capable of geometric isomerism.

GL: "Okay, put something on there so that it can have geometric isomers. Anything, in place of hydrogens."

Marianne: "In place of hydrogens?" She was unsure what to do, and finally chose to replace two hydrogens with two chlorines, giving trans-1,2-dichloroethene (Figure 6.2). On being asked to draw the other geometric isomer, she drew a structure that could be produced by rotating her original diagram 180 degrees around the C=C axis, and said, "Like that?"

\[
\begin{align*}
\text{trans} & \quad \text{C} \quad \text{C} \\
& \quad \text{H} \quad \text{H} \\
& \quad \text{Cl} \quad \text{Cl}
\end{align*}
\]

Figure 6.2. Marianne's representation of a structure that can exhibit cis-trans isomerism (1,2-dichloroethane). This is the trans isomer; Marianne's representation of the cis isomer was just the mirror image of that shown here.

GL: "Okay, are those isomers?... If I flipped them over, wouldn't the first one be the same as the second one?"

Marianne: "Oh, yeah, they would! Okay, um...,"

She crossed out both hydrogens and both chlorines from her second structure. She laughed when asked if she was going to start again, and then said, "I can't think right
now." At this point, she was given a clue. "What if I said 'cis-trans?" She responded, "Oh, okay," and drew the initial trans isomer again.

GL: "Okay, I think those are the same ... I think you want to make it, but aren't those the same thing?"

Marianne: "Oh, they are! Okay, okay, I know what I'm doing now; I'm sorry!"

She then drew the cis isomer and correctly labeled each.

GL: "Okay, now, why is it that you can have cis-trans isomers there? What is the property of that alkene that lets you have cis-trans isomers there?"

Marianne: "Rotation around the double bond."

GL: "Okay, what about the rotation?"

Marianne: "It can't..."

Returning to the original structures (Table 3.4, Question 1), Marianne was asked, "Okay, is that same thing possible here, is there any rotation, is there any restriction on the rotation here?" She thought there was.

Marianne: "I think because it has the halogens attached to it..."

GL: "Why don't you build models of these structures?"

Even after building models, Marianne attempted to show that rotation was not possible around the carbon-carbon bond.

GL: "That can't rotate? It looks like you're rotating it right now!"

Marianne (laughing): "No, okay, it can, right? I don't know."

She finally concluded that there was no hindered rotation in the molecule. She then built both structures (Table 3.4, Question 1), and said, "... Um, they're like mirror images of each other?"

GL: "Are you sure?"

Marianne: "Actually, they're not. Because 'B' is ..."

Marianne was reluctant to conclude that these two structures were the same thing, even with models of both in her hands. She said that they could be isomers of some sort,
because they both contained the same number and same kinds of atoms. She was again asked what these two structures represented

Marianne: "Um ... what's that new thing we learned? Enantiomers or something?"

GL: "Okay, well, if they're not mirror images, then maybe they're the same."

Marianne: "I think they are the same! I don't know."

GL: "I don't know, are they?"

At this point, Marianne's difficulty emerged. She was unwilling to reorient an entire structure in space.

Marianne: "If you turn it around."

GL: "Okay, well, why wouldn't you want to turn it around?"

Marianne: "Okay, it's the same thing, then."

Marianne had little difficulty drawing a flat, two-dimensional structure of this molecule (Table 3.4, Question 2), but when asked for a name, she called it "bromohydrochloromethane."

GL: "Okay, now let me ask you a question. How many carbons are in it?"

Marianne: "Oh, it's two. So it's ... ethane."

GL: "Okay, now, have you ever seen us use "hydro"?"

Marianne: "No"

GL: "Do we need that?"

Marianne: "Oh, we don't even need that, that's right!"

GL: (laugh) "Okay! So, what do you call it?"

Marianne named the structure "bromochloroethane," and was told, "Okay, let me draw you a picture here." Because Marianne had not numbered the positions of the halogen substituents in her name, she was given the structure of a different compound, 1-bromo-2-chloroethane, and asked to name it. The only difference in these two structures is that in the second compound, the halogens are not attached to the same carbon atom,
and in order to distinguish between these two structures, the positions of the halogen atoms within the molecule must be specified.

When asked to name the new structure, Marianne said, "Um ... same thing."

GL: "But are they the same?"

Marianne: "No"

GL: "How could you distinguish between the one that you drew and the one that I drew?"

Marianne: ..."You need to put, like, numbers on it."

GL: "Okay, good! Why don't you do that?"

At this point, she named the initial structure "1,2-bromochloroethane" (Table 3.4, Question 1).

GL: "Okay, why did you call it ... which one is 1,2-bromochloroethane?"

Marianne: "This one." (NB: Table 3.4, Question 1)

GL: "Why do you call it 1,2-?"

Marianne: "Because, like, it's alphabetical order."

GL: "Okay."

Marianne: "Bromo is first."

Although Marianne was correct that the substituents should be named in alphabetical order, she did not number them correctly. Because both the bromine and chlorine atoms are attached to the first carbon atom, the correct name is '1-bromo-1-chloroethane'.

GL: "But what do the '1' and the '2' mean?"

Marianne: "Oh, it's on the '1' and '2' ... no, it's on the second carbon. So it'd just be 2-bromochloro"  

GL: "Okay, why is it on the second carbon?"

Marianne: "Because this is the first one. Oh, you could have done it on the first one! Okay, actually, it should be like this." (NB: Marianne implies that she could have instead
assumed that both halogen substituents were located on the first carbon atom instead of the second.)

Marianne wrote the name '1-bromochloroethane.'

GL: "Now, does the '1' go with the bromo or with the chloro?"

Marianne: "... with both of them. It's on the same carbon."

GL: "Okay, they're on the same carbon, but how do you know that that '1' goes with the bromo or with the chloro? What's the name of the other one?"

Marianne: "You've got to have a '1' for each one."

Only one subject, James, initially chose to build models to solve this problem (Table 3.4, Question 1). He did this because "It's hard to picture in 3-D." James built a model of both structures, holding them parallel with the plane of the paper to assure himself that he had indeed built correct models. While he built them, he said, "You're going to get me this week!" He then completed his models.

James: "Okay, now this should be easy. Okay, let me line them up as ... let me put the models in the arrangement that they are in the paper. And let's see, I have 'A' like this, and 'B' like this. And they're the same."

GL: "How can you tell?"

James: "'Cause all I had to do was rotate. See, if I have my chlorine pinched in my fingers, see ... and where was I? ... like this ... if I rotate it, like, what is this, forty, no, this is twenty-five? I don't know. Rotate about sixty degrees, they all line up and you can put them on top of each other."

Similarly, only one person, Anna, initially attempted to solve this problem (Table 3.4, Question 1) by rotating the structure 'in her mind's eye'.

Anna: "Okay, at first glance, looking at it on paper, I want to say they are the same. Because it looks like everything is just ... the molecule has just turned around a little bit. Like it has been rotated. About sixty degrees."

GL: "Okay, rotated where?"
Anna: "Um..."

GL: "On what axis?"

Anna: "... Um, I'm not sure I understand."

GL: "If you were going to rotate it ... when you rotate something, you think about
an axis..."

Anna: "Mm hmm"

GL: "Between what atoms would you rotate?"

Anna: "Um, oh,... well, they're rotating off of the carbon. Okay, the hydrogen, the
methyl, and the bromine look like they're just... rotating."

GL: "So if you were going to draw a little arrow to show where the rotation
occurred, where would you draw it? Just point for me."

She pointed to the bond connecting the carbon and chlorine atoms. Anna checked
herself by building models of both structures. Like James, she held each model parallel
with the plane of the paper to assure herself that she had indeed built correct models, and
when both were built, she said, "And now I can see that they definitely are the same.
Because I can put them on top and everything matches on all four corners here."

Tammy adopted an interesting strategy to solve this problem, but it gave her some
problems. She redrew structure 'A' and then drew its mirror image. This gave her no
difficulty. She then decided to rotate the mirror image, and drew the arrow in Figure 6.3
to show this, saying, "Okay, now I'm going to rotate it to the right" (Figure 6.3). When
she finished, she said, "I just moved everything and shifted it around." However, from
her diagram she concluded that structures 'A' and 'B' (Table 3.4, Question 1) were
enantiomers, although it was not clear how she did this. She was therefore asked to
make models of these two structures. Although she had no difficulty rotating the
structure she had previously drawn in two dimensions (Figure 6.3), she had more
difficulty rotating the three dimensional models and lining them up with the respective
drawings. When she finished building structure 'A', she asked to align her model with her drawing.

![Drawing of molecules](image)

**Figure 6.3.** Tammy's representation of (S)-1-bromo-1-chloroethane and its enantiomer, showing rotation of the enantiomer. The second structure is drawn as if it were a reflection of the first, and the third structure is drawn from the second by rotating around the carbon-chlorine bond.

GL: "Convince yourself of that by putting it on the paper. Does that seem reasonable?"

Tammy: "Like this?"

GL: "Well, you can rotate it any direction you want."

She had not oriented her model correctly with any drawing, and was asked, "What atom are 'flat' in the diagram?" (NB: This question asks what atoms are aligned in the same plane as the paper.)

Tammy: "The hyd... No, wait. The bromine and the chlorine?"

GL: "An what other atom is flat?"

Tammy: "The carbon."

Having established what atoms should be aligned parallel to the plane of the paper, Tammy still had difficulty actually holding the model in that position.

GL: "Now, can you hold that molecule so that those are flat?"

Tammy: "Okay. Oh, I guess I need to leave it this way."

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"I think what you have is right, but you need to hold it so that... Can you hold it so that the... Can you hold it so that the carbon and the chlorine and the bromine are parallel with the plane of the paper? Do you see what I'm asking you to do?

She eventually was shown how to hold her diagram so that the carbon, chlorine, and bromine atoms were parallel with the plane of the paper, and in this way verify that she had built structure 'A'. Building structure 'B' was much easier for her, and she then readily lined up the two models and said that "They're the same."

Most of the other participants all chose some type of strategy involving the successive drawing of enantiomers to solve this problem (Table 3.4, Question 1). Kathy initially converted both structures into Fischer representations (Figure 6.4). She first converted structure 'A' (Table 3.4, Question 1) to its corresponding Fischer representation, saying, "I'll put my 'Cl' right here. And I'm going to pull these two around (NB: the methyl and the bromine)." This method, which had been demonstrated in class (Figure 6.5), worked well for Kathy. She converted structure 'B' to its Fischer representation in a similar manner. However, she inverted the positions of the hydrogen and methyl groups when she did this, and was asked what she did.

Kathy: "Okay, I pulled the 'H' and the 'C,' the methyl."

GL: "Then why was is hydrogen on the right and the methyl on the left?"

Kathy: (laughing): "Oh! I told you my brain wasn't functioning this morning! Hoo!"

![Figure 6.4](image-url)

Figure 6.4. Kathy's Fischer projections of (S)-1-bromo-1-chloroethane. These structure were drawn from the structures shown in Table 3.4, Question 1A using the rotational strategy shown in Figure 6.5.
Figure 6.5. First commonly-employed rotational strategy. This strategy was frequently used by students to convert dash-and-wedge formulas into Fischer projections.

Once Kathy had drawn the Fischer projections (Figure 6.4), she began to work on them. She used the idea that any time two substituents at a chiral atom are switched, the mirror image is formed. This had previously been demonstrated in class. Beginning with her Fischer representation of structure 'B', she first changed the positions of the methyl group and the bromine atom, and then switched the positions of the methyl group and the hydrogen atom.

Kathy: "Well, now my model 'A' looks just like my model 'B'. And since it took me two turns to get to it, which is an even number, it means that they're the same thing."

GL: "Okay, so tell me again. I mean, you already did. What's the relationship between 'A' and 'B'?"

Kathy: "They are the same."

GL: "Oh, very good."

Kathy (laughing): "It took me forty minutes to get there!"

Brian used a method very similar to Kathy's. He also initially drew the Fischer representations, and performed successive exchanges of methyl group and bromine atom followed by methyl group and hydrogen atom. Brian had previously stated that he had difficulties with exercises in three dimensions, and he was more comfortable using the rote method discussed in class (employing a strategy of successively exchanging substituents) that with the use of three-dimensional models. David drew structure 'A,' exchanged the bromine atom and hydrogen atom to obtain his structure 'T', and then said..."
that structure 'T' was "structure 'B' with one inversion," (Figure 6.6) concluding that 'A' and 'B' were therefore the same thing. Michael and Andrea used similar strategies.

Figure 6.6. David's representations of (S)-1-bromo-1-chloroethane and its enantiomer. David used a strategy of successively switching the positions of pairs of substituents on a chiral atom to produce these drawings.

Most of the subjects had no difficulty drawing flat representations of the 1-bromo-1-chloroethane; however, there were some difficulties in naming the molecule. Anna called the molecule "bromochloroethane," but, like Marianne, did not number the halogens. The next few questions probed whether Anna could see that two structural isomers of bromochloroethane could be built and named.

GL: "Is there was any other way to draw a bromochloroethane?
Anna: "Yeah! Okay, 'cause, well ... are we thinking cis-trans?"
GL: "Is cis-trans isomerism possible in this molecule?
Anna: "Not the way this is drawn."
GL: "Why not?
Anna: "Okay, well, because I've got ... everything is pointing in opposite directions, north, east, south, and west ... um ... there's a way I can draw them the same."
GL: "Would the molecule be different if the positions of the hydrogen and chlorine were switched?"
Anna: "If I switched the chlorine and the hydrogen, I would get the enantiomer of this compound. Because when you switch it once, you get the enantiomer; if you switch it twice, you get the same."
Although this was correct, Anna still hadn't said anything about the relationship between structural isomerism and nomenclature. To test this, she was asked to draw a 'dash' formula of the molecule. She did this correctly.

GL: "Okay, now. Is there any way you can rearrange those atoms that wouldn't give you that particular structure?"

Anna: "Um, again, I'm thinking cis-trans, where, if I would switch the chlorine and the hydrogen on my middle carbon, I would get ... I would get, ooh!"

She then recognized that she really wouldn't get a different compound (geometric isomerism was not possible) and finally realized that she needed to worry about numbering the halogens (and the possibility of structural isomers) when she was asked to exchange the positions of the bromine atom and one of the methyl hydrogens.

Anna: "That would be a different compound."

GL: "But wouldn't it still be a bromochloroethane?"

Anna: "It would be bromochloroethane, but you would have ... it would be a bromo-2-chloroethane."

Anna said that she assumed that the bromine would automatically be at carbon '1', and when she was asked to number each halogen, she correctly named her initial structure as "1-bromo-1-chloroethane." Many of the subjects had a similar problem, and did not see the necessity of numbering the halogens until it was pointed out that two structural isomers of this molecule were possible.

Brian had difficulty distinguishing which atoms were part of the parent chain and which atoms would be considered as substituents. He began by saying "Okay. Um ... okay, um, it's an alkane for sure, because it only has single bonds. Um, so ... I can say ... 1-chloro- ... 1-bromo-2-chloro-3-methyl-... I've got to name the two ... Is it ethane?"

He was told to write on his paper what he thought the name should be.

Brian initially wrote "1-bromo-2-chloro-3-methylethane," and was asked, "Okay, what carbon is the bromine on?"
Brian: ....

GL: "You have it on carbon one, and that's fine. I don't disagree with that. Maybe I should ask, what carbon is the chlorine on?"

Brian: "It's also on one."

GL: "But you have it written as 2-chloro."

Brian: "Right."

Brian changed the name to '1-bromo-1-chloro-1-methylethane', and said, "Which means that the methyl would be on the ... also on it." Brian was indicating that his methyl was also attached to the first carbon atom. At this point he was asked, "Okay, but why would you call it methylethane?" When he hesitated, he was asked "Aren't there just two carbons on it?"

Brian: "Mm hmm."

GL: "Do you need that methyl?"

Brian: "No." At this point, he wrote the correct name, 1-bromo-1-chloroethane.

Three-Dimensional Representations of an Achiral Molecule. Questions 4 and 5 of the third interview (Table 3.4) ask students about the structure of the achiral molecule 2-chloropropane. Although the molecule does not contain a chiral atom, two different three-dimensional representations of the structure were given. Of the ten interviewees, only Michael initially identified this structure as being achiral. On seeing this structure, Michael said, "Okay. Um, they've got the same molecules on them. They must be chiral." But on moving the paper around, he corrected himself. "Okay, and everything's the same. They both have two methanes on them, so they're not chiral." Michael stopped here, and so he was prodded further.

GL: "So are they ... if they don't have a chiral atom, then what are they?"

Michael: "They're ... the same."

Unlike Michael, Tammy initially identified structures 'A' and 'B' as enantiomers (Table 3.4, Question 4). However, Tammy quickly discovered and explained why they
were not, being one of the few subjects who readily identified the molecule as achiral. Tammy initially said, "I'd say those were enantiomers. Those are mirror images because you switched them." Because she had identified the structures as enantiomers, she was asked, "Okay, what do you have to have for them to be enantiomers?" She correctly responded, "Left-handedness and right-handedness."

GL: "Right. What has to be true of the carbon that you're looking at?"

TB: "Oh, it has to be a chiral carbon. Oh, and it's not, because it has two of the same functional groups." She concluded, "They're not enantiomers."

Although Anna recognized that the structures were not chiral, she wondered nonetheless whether they were identical. Like everyone except Michael and Tammy, she was ultimately forced to build models to resolve this question. She began by saying, "Okay, well, they can't be enantiomers. Because there's not a chiral carbon. Because you have two methyl groups on each." But when asked if they would be the same, she said, "Um, let's see. Switching ... I think they would be the same." Anna was apparently not sure whether these structures could be the same, although she knew they couldn't be enantiomers. She built a model of each. Only after seeing these models was she sure that they were the same.

GL: "Okay, are they the same or different?"

Anna: "They're the same."

GL: "Okay, now, would you have had to build models to do that? Because you noticed that there was no chiral carbon."

Anna: "Right. I shouldn't have had to build models!"

All of the other subjects had to build models to convince themselves that these two structures (Table 3.4, Question 4) did not represent enantiomers. None recognized that the central atom was achiral. Jason immediately chose to build models of the structures, saying, "I think I'll build models. I kind of enjoy doing that." He built a model of structure 'A', (Table 3.4, Question 4), and then said, "Can I build two models?" After
building models of both structures, he said, "They're the same. If you rotate on the hydrogen bond, you're going to eventually get the... same thing." When asked why this was difficult to see on the paper, he replied, "I guess just because they're in a different order. But once you get to see them on the model, you can see that if it rotates..." Like many others, James was unsure if the central atom was chiral or whether this was important.

David initially said that these two structures (Table 3.4, Question 4) were isomers, "because they would have the same, um, same molecular formula. I mean, you have all the same atoms in 'A' that you have in 'B'. Um, oh, I believe they are geometric isomers."

GL: "Why?"

David: "Because, um, ... I can see it better if I switch it this way ... but, um, here, ooh, you know what? Well, I'm just thinking, you don't have geometric isomers in alkanes."

David was right about this, but then said, "So they... structural isomers?"

However, once having built models, he said without much conviction, "They're the same?"

GL: "You don't say that with a great deal of conviction in your voice. Are they the same?"

David: "They are the same."

GL: "Okay, they're the same?"

David: (laughing): "They are the same!"

GL: "Okay, now could you make the enantiomer of 'A'?"

David: "No, you can't have an enantiomer, because there's no chiral carbon."

GL: "I agree! (laugh) Now, that question is tough. And everybody stubs their toe on it. And what I want to know from you is, why is that tough?"
David: "It's tough because there's so many isomers to keep straight in your head when you're faced with a question like this, and you don't have choices A, B, C, and D, you just kind of have to go through each possibility until you eliminate."

David later added, "Yeah, when you draw it in three dimensions, it sort of adds another dimension, if you will."

Initially, it appeared that Marianne recognized that these two structures were achiral (Table 3.4, Question 4), and that she would not need to use models to solve this problem. However, this was not the case. Marianne initially said, "They're the same thing," and when asked how she could tell, she said, "Because it had the same things on each one. And they're just rotated differently." Because these statements are correct, she was asked if the structures as drawn could represent mirror images.

In response, Marianne said, "No. Because if you flip this, the carbon would be on top, and the one right here is on the bottom." By this statement, Marianne was indicating that structure 'B' (Table 3.4, Question 4) is not drawn as it would be if structure 'A' were reflected in a mirror (although she had confused carbon with chlorine). However, she still did not indicate that the structures were achiral.

GL: "The carbon or the chlorine?"

Marianne: "I mean the chlorine. All right, the chlorine."

When asked why it was important that her mirror image of structure 'A', as drawn, did not align with structure 'B', Marianne said, "Because you want to keep the same ... the same structure."

GL: "I don't understand what you mean, you want to keep the same structure. I'm not trying to be mean here."

Marianne: "That's fine! ... Actually, I think they are ... like, you can, it's free to rotate, so, it's the same thing, yeah, it's the same thing."

But when asked to confirm that the structures were really the same, Marianne said, "They could be mirror images." It was then suggested that she build models of these..."
structures. After she finished building them, she concluded, "They're different," and
was asked, "Why are they different?" She replied, "Um, the chlorine on one is going up
and on the other one it's going down."

Marianne was then asked if there was any way to manipulate structure 'B' to "make
the chlorine go up," and she immediately began to take the model apart. She was told,
"No, you can't break any bonds! Can you somehow make that chlorine go up? How
could you make that chlorine go up?"

Marianne: "I don't think you can."

GL: "Why don't you try?"

Marianne: "I can't rotate it, right?"

Once she was told that she could indeed rotate the molecule, she said, "Oh, okay,
well, that's what I was thinking. Sure, like that." Marianne was then able to show that
the two structures were indeed the same. However, she was still confused about the
relation between either structure and its mirror image.

GL: "Could you make a mirror image of 'A' that's different from it?"

Marianne: "I think we just did. Because you see how this one has one right here? Is
that what you mean?"

GL (Holding the models of structures 'A' and 'B'): "I mean, isn't this the same as
this? These are the same, aren't they?"

Marianne: "Uh huh."

GL: "I want to know, if I make the mirror image of this, is it different, or is it still
the same?"

Marianne: "It's still the same."

GL: "Okay. Why is it still the same? I mean, it looks like it ought to be different.
You're right, it's the same. I'll tell you."

Marianne: "I don't know why."
At this point, Marianne was asked if the central atom was chiral. She said, "... chiral. Hold it a second. Um ... there's a carbon. What's the definition of chiral?"

After some thought, she concluded that the central atom was chiral, "because it has ... stuff attached to the central carbon."

GL: "Okay, it has stuff attached to the central carbon. But what kind of stuff has to be attached to the central carbon? You're right, it has to do with what stuff's attached to the central carbon."

Marianne: "Hydrogens."

Marianne did not remember that a chiral atom must contain four different substituents, but when reminded of this, she said, "Oh, that's right. That's right!"

However, when asked if the central carbon actually contained four different substituents, she initially said that it did.

GL: "Are you sure?"

Marianne: "No, no, no. Actually, these two are the same."

She finally stated that the molecule was not chiral and that this explained why the two structures were in reality the same.

Like most of her peers, Kathy initially struggled with this problem, solving it only after she had built models. When asked why it was difficult, she laughed and said, "Well, if I would have looked at the paper, I could have figured it out real easy. If I would have sat and thought about it for a little bit. 'Cause you had two carbons. And that means ..." At this point, she was asked, "You mean, you had the two methyls?"

She continued, "Yeah, sorry. Two methyls, which are connected to that one carbon. And the two methyls are the same thing. So that's two of the same group. So automatically you know it's achiral. It doesn't have four different groups on it."

GL: "You're exactly right. But it didn't jump right out at you, did it?"

Kathy: "'Cause I wasn't thinking on those lines."

GL: "What caused you to not think on those lines?"
Kathy: "The previous problem! I was sitting there, okay, what kind of trick do they got for this one?"

Most of the subjects had few difficulties drawing this compound as a dash formula or giving it a name (Table 3.4, Question 5). Marianne's diagram (Figure 6.7) is typical. Although it is correct, a more conventional representation would orient the three carbon atoms in a linear fashion. Once having drawn her diagram, Marianne named the compound "1-chloropropane," and asked why she gave the molecule this particular name, quickly corrected herself. "I'm sorry, it's 2-!" Marianne was indicating that the actual name of the structure is 2-chloropropane, which is correct. Like Marianne, Michael also gave the name "1-chloropropane," and when questioned about it, he quickly said, "Oh, it's 2-." Kathy initially named this molecule as a butane, and James called it a pentane; both readily recognized that the root name was actually propane.

\[
\begin{align*}
\text{Cl} &- \text{C}-\text{CH}_3 \\
\text{H} &
\end{align*}
\]

Figure 6.7. Marianne's representation of the structure of 2-chloropropane. This diagram is typical of the type of 'dash' formula produced by students.

Andrea attempted to name the molecule "1,1-chloropropane," but then changed it, saying, "No, 1-chloro, because there's only one chlorine." She was then asked, "Okay, what carbon is that on?", and she responded, "Two. So it'd be 2-chloro." The worst difficulties in naming were experienced by Brian. "Um ... 1- ... let's see ... 1,2-dimethyl ... 1,1-dimethyl-1-chloro ... propane."

GL: "Okay, it's a propane, I agree. It's a propane. But is it a dimethylpropane?"

Brian ...
GL: If I call it a "dimethylpropane," doesn't that imply that I have a three-carbon propane with two more methyls on it?"

Brian: "Say that again."

GL: "Okay, write down your name."

Brian wrote "1,1-dimethyl-1-chloropropane" on his paper.

GL: "Okay, '1,1-dimethyl-1-chloropropane.' Okay, now, how many carbons in a propane?"

Brian: "Three."

GL: "Okay, well, do I have to say 'dimethyl?'"

Brian: "Nope."

After realizing this, Brian, like the others, had little difficulty correcting his name to "2-chloropropane."

**Representations of Enantiomers.** The next two questions (Table 3.4, Questions 6 - 7) dealt with representations of the enantiomers of 2-butanol. The structure on the left in question 6 is (R)-2-butanol and that on the right is its mirror image, (S)-2-butanol; both are written using a configuration described to the class using the term "bow-tie configuration," meaning that the chiral atom is represented with two substituents above the plane of the paper and two others below this plane. When placed side-by-side, it is not immediately apparent that these two structures represent mirror images.

Two distinct strategies emerged in solving this set of questions. David, Kathy, Brian, and Andrea correctly determined that these two structures were enantiomers though the use of pencil and paper without making use of models. The other six subjects used models; of these, Marianne, Tammy, and Michael initially attempted to solve this problem without the use of models, but were unable to do so. James, Jason, and Anna initially began with the models. Everyone who used models eventually concluded correctly that the structures were enantiomers.
David used the operation he was taught in class, which says that if the positions of any two substituents are switched, the enantiomer (mirror image) is formed. On being given these structures, he said, "Okay. Um, let's see. Each of them has a chiral carbon. So there's a possibility that they're enantiomers. Um ... okay, if you switch, on compound 'A,' the hydroxyl group and the ethyl group, you'll have compound 'B,' so they're enantiomers. One inversion."

Kathy, Brian, and Andrea each used a strategy similar to that used by David. Kathy explained it more thoroughly, immediately saying that the structures were enantiomers.

GL: "How can you tell?"

Kathy: "I switched on 'A'. I have a OH group on the top, and I have a methyl, an ethyl group on the right side. And on 'B', my methyl group's on top, and my -OH is on the left side. So I switched my -OH on structure 'B'; put the -OH to the top and put the ethyl group to the right side."

GL: "Good!"

Kathy: "Which gives you the same thing. And since there was only one change, it's the enantiomer."

Although it appeared that Kathy understood this perfectly, something surprising occurred when she was asked to show this using models. Kathy correctly built both models and could have shown that they were enantiomers by holding them next to each other, showing that there is no plane of symmetry between the two structures and that they are nonsuperimposable mirror images (Figure 6.8). Kathy instead wished to use the same strategy she used on her paper. She decided to exchange two substituents on structure 'B', and then show that the resulting structure was identical to 'A'. This would prove that 'A' and 'B' were enantiomers. However, Kathy had difficulty deciding which two substituents to choose. As Kathy was to discover to her surprise, the choice of which substituents to switch is unimportant.

GL: "Okay, you said 'A' and 'B' were enantiomers, aren't they?"
Figure 6.8. Enantiomers of 2-butanol depicted as nonsuperimposable mirror images.

Kathy: "So I just have to switch one. I have to switch my ... OH ..."

GL: "Does it matter?"

Kathy: "Well, I wouldn't want to switch my hydrogen around, that's for sure."

GL: "Try it. Switch your hydrogen around. Switch your hydrogen with something else."

Kathy: "How about I switch it with my -OH?"

GL: "Fine."

Kathy: "Okay. Mmm, -OH, hydrogen, methyl, oh! It does!" (NB: The models match up.)

GL: "It does! It doesn't matter, does it?"

Kathy: "No way!"

GL: "I'm glad we did that! Okay, could you name that thing?"

Kathy: "Uh, um ... yeah!"

GL: Okay, how would you name that?"

Kathy: (laughing): "I'm still in amazement by it!

GL: "Oh, you're still in amazement by it? Well, I'm glad you're in amazement by it! You proved it to yourself!"

Kathy: "Wow! I thought you couldn't ... you see it on paper, it looks totally different than when you use models."
Kathy was so surprised by this result that she later came back to this same idea, saying, "I'm just, I'm still trying ... 'cause like, if you switch the hydrogen, if I switched the hydrogen and -OH around right? If I switch these two around, it's not the same molecule." Kathy finally proved to herself that by exchanging the position of any two substituents attached to the chiral atom of 2-butanol, she could form the enantiomer, and she concluded, "Wow, that's pretty neat!"

Like Kathy, Tammy explicitly checked for the presence of a chiral atom, and then laughed when she confirmed this, saying, "I know now!" She initially decided not to use models "'cause on the test I'm not going to have a model." Quickly she decided, "Okay, they're mirror images. I switched two substituents." She chose to exchange the hydroxyl and ethyl groups on the second structure (Table 3.4, Question 6) "because if you switched, flipped these two it becomes that." (NB: The second structure becomes the first one.) When Tammy began building models of these structures, she was tempted to change her mind. Looking at the models, she thought they were the same structure rather than enantiomers. However, she finally convinced herself that they were indeed enantiomers when she could not lay one structure on top of the other. She then explained why she thought these structures might be the same.

Tammy: "Um, whenever I saw it on paper, I didn't think they were going to be; I thought they were going to be the mirror image, but then at first when I looked at the models, I thought they would be (NB: the same structure)."

GL: "But what happened?"

Tammy: "But now they're enantiomers."

GL: "Okay, you're right, but ..."

Tammy: "They didn't fit on top of one another; the colors didn't match up with one another."

Brian began by explicitly stating that the structure contained a chiral atom (Table 3.4, Question 6). After struggling with the achiral structure in the previous set of questions
(Table 3.4, Question 4), he laughed and said, "All right. First of all, I'll make sure they're chiral!" Brian also switched the positions of the hydroxyl and ethyl groups to show that these structures were enantiomers (Table 3.4, Question 6), saying, "Okay, I'm looking at it, and right off hand, I can't tell, so I'm going to switch the alcohol, the -OH, with the ethyl. Okay, so that would mean that the alcohol would be up top, and now it's the same as 'A,' so it's the mirror image."

Marianne and Michael attempted unsuccessfully to solve this problem (Table 3.4, Question 6) without the use of models. Michael attempted to rotate and flip the first structure, which he labeled 'A,' saying, "Okay. I'm just going to draw 'A', ... Okay. And there's two different ways to do it, right? You can rotate it ninety degrees counterclockwise or flip it over? (NB: Figure 6.9, Structure 'C')"

![Figure 6.9. Michael's attempt to examine enantiomers. Each structure is correctly drawn using one of the rules Michael learned from his textbook, but they did not allow Michael to come to a conclusion about the relative configurations of his structures.](image-url)
GL: "What happens if you flip it ninety degrees?"

Michael: "It becomes the ... enantiomer?"

GL: "That's correct."

Michael: "Right. And you flip it over, and if it's the same, then they're identical
(NB: Figure 6.9, Structure 'D')."

This method was suggested in the students' textbook (Bailey & Bailey, 1995). As Michael was about to discover, it doesn't always allow for a decision to be made. He worked at his drawings for awhile, and then said, "So now, if I flip it over and it's the same as this one, then they're the same. Then 'A' and 'B' are the same. (NB: Michael labeled the initial structures 'A' and 'B'.) And just looking at it, it doesn't look like that's going to happen... I get ahead of myself sometimes ... okay."

Michael correctly concluded that structures 'A' and 'C' were enantiomers, and structures 'A' and 'D' were the same compound, but he then said that because 'A' and 'D' were the same, that "'A' and 'B' must be the same." When asked if this meant that 'B' and 'D' were the same, he said, "Oh, if 'A' and 'D' are the same, then 'A' and 'B' must be enantiomers."

GL: "What's the relation between 'D' and 'B'?"

Michael: "'D' and 'B' are ... not the same."

GL: "That's my question. I don't know how you can conclude about 'B'."

Michael: "Well, the-OH and the methyl on the same plane here, and the -OH is with the hydrogen here ... hmm ..."

GL: "Okay."

Michael: "I don't know."

Although he knew some rules for manipulating structures and was able to apply them correctly, Michael never did adopt the simple strategy discussed in their lecture and used by David, Kathy, Tammy, and Brian. Michael finally resorted to building models. He
held them next to each other as if they were reflected in a mirror and said, "... They're definitely different."

GL: "Okay, what would happen if you laid them right on top of one another?"

Michael: "They'd always be one off."

Marianne initially said that the structures were enantiomers, and when asked why, replied, "Because two things are different. I just know. Am I wrong?" Because she was not really sure, she was asked to build models. Once the structures were built, she was asked what the relationship was between the two, and she replied, "Mmm, they're different." She concluded this because she could not place one structure on top of the other and cause all of the substituents to coincide. But when asked if they were mirror images, she said, "No they're not."

GL: "Why don't you see if they're mirror images?"

Marianne: "... Like, you put them up and they're not."

GL: You're sure?"

Marianne: "I think so ... uh huh."

GL: "How many chiral atoms do they have in there?"

Marianne: "Four."

GL: "How many chiral atoms? Do they? They just have four carbons."

Marianne: "One, one, one! One chiral atom!"

Only after being shown that the molecules either had to be the same or mirror images did Marianne conclude, "Okay, they're mirror images."

GL: "Okay, then, show me."

Marianne: (Attempting to line them up as if they were being reflected in a mirror, without success) "... Like that?"

GL: "Oh, okay, what's reflecting what?"

Marianne: "I have no idea. It's a lot harder!"

But after manipulating it for awhile, she found it.
Marianne: "Oh, they're mirror images now!"

GL: "How can you tell?"

Marianne: "Um, it is just, kind of a plane, and you flip it (laugh), and then like... it gets turned the other way."

Everyone else initially built models to solve these problems. James built only the model of the first structure, and was able to demonstrate that he could not line his model up with the second structure, correctly concluding that the two structures must be enantiomers. However, this took some effort. He initially built the structure labeled 'A' and then attempted to align this with structure 'B' (Table 3.4, Question 6). He successfully aligned the methyl and hydroxyl groups on the chiral center, but found that hydrogen and ethyl were not aligned. He said, "And these two go up and these two go back and I can just flip it over like that and these two car now going back and these two are now coming forward." Now the hydrogen and ethyl were aligned at the expense of the methyl and hydroxyl groups.

GL: "But take a look, did that work?"

James: "No, it didn't."

GL: "Okay, when you turned the whole thing over, yeah, now, what happened?"

James: "Now it works. So they're the same. No, no, no, ooh... no, because of the oxygen...So they're enantiomers."

Anna tried to draw pictures "in her mind." She said, "Okay, in my mind right now I'm kind of doing some switching. Just kind of glancing at it. Um, and I'm not seeing it, so I'm going to build models." Once she had them built, she concluded, "Okay, and they've got to be mirror images because they're not superimposable." Jason built models of both structures (Table 3.4, Question 6) and concluded that the structures were stereoisomers but, "It's not a mirror image." Jason was asked to build the mirror image of the first structure, and he successfully did this. When he was able to line this model
up with his original model of the second structure, he correctly concluded that the two structures were enantiomers.

**Representations of (R)-2-chlorobutane.** Questions 8 and 9 (Table 3.4) gave two different representations of the same enantiomer of 2-chlorobutane and asked students to determine the relationship between them. Question 10 (Table 3.4) then asked students to name the same molecule. The first structure depicts the chiral carbon atom as having two substituents (chlorine and methyl) in the plane of the paper, one substituent (ethyl) above the plane, and one substituent (hydrogen) below the plane. The second structure depicts the chiral carbon atom as having two substituents (chlorine and hydrogen) above the plane of the paper and two substituents (methyl and ethyl) below the plane. In their lecture, students were told that this second type of structure could be called the 'bow tie' configuration.

Several strategies emerged in solving this set of questions. Some students initially built models of one structure and compared their first model to the other structure, concluding that they were the same. Others built one model for each structure and subsequently compared one model to the other. Some took structure 'A' and attempted to redraw it the "bow-tie" configuration used for structure 'B'. Finally, some took structure 'B' and attempted to redraw it in a form similar to that used for structure 'A' (Table 3.4, Question 8).

All of the students were eventually asked to build models of these structures. Most built a model of structure 'A' and subsequently aligned it with structure 'B', proving that they were the same.

Several difficulties became apparent from this exercise. Drawing both structures in the same format was difficult, and most students attempted to take structure 'A' and convert it into the "bow tie" configuration of structure 'B'. Any manipulation requiring rotation of either structures or models was difficult.
Michael initially confused the meanings of the dashes and wedges, thinking that dashes indicated substituents pointing above the plane of the paper. When he corrected this, he confused the two methyl groups in the molecule, thinking that the methyl group attached to the achiral methylene was actually attached to a chiral center. Thus, he could not properly rotate the molecule he had built representing structure 'A' and align it with structure 'B'. Andrea was not willing to rotate her model of 'A' at all, instead wanting to move substituents at the chiral center by breaking and reforming bonds.

Most students attempted to redraw structure 'A' into the "bow tie" configuration used for structure 'B'. Two different strategies were used. Some students rotated the methyl and ethyl groups to the wedge positions on the sides (left and right, respectively), leaving the chlorine and hydrogen in the dash positions (top and bottom, respectively). This strategy is illustrated in Figure 6.5. Others did a rotation that seemed to them to be clearer (although moving through a larger angle), and put the ethyl and hydrogen in the wedge positions (left and right, respectively), leaving the chlorine and methyl in the dash positions (top and bottom, respectively). This strategy is illustrated in Figure 6.10.

![Figure 6.10. Second commonly-employed rotational strategy.](image)

Students who used the second method insisted that it was easier for them to view in this manner; however, they had more difficulties than students using the first method. An example is given by James, who inadvertently exchanged the positions of the methyl and chlorine on doing this. Kathy was able to use this second method correctly, saying that she didn't use the first method (Figure 6.5) "cause that's too hard for me to construct in my mind." Kathy initially insisted on using the symbol 'C' for the chiral carbon atom, indicating this was because "I keep on forgetting about that stupid little thing." However,
as she worked, she adopted the convention that intersecting bonds indicate the presence of a carbon atom, and ceased drawing this symbol.

GL: "Now, something real interesting happened here. And this is neat. You told me you didn't like not having the carbon here in the middle, but as you went, you left it out. Why? I mean, what happened?"

Kathy: "Because, I think, when I do a cross like this, it kind of clicks that there's a 'C' there. And, plus, it's a lot easier to do a cross" (Figure 6.11).

![Figure 6.11. Kathy's method for examining enantiomers. Her first structure depicts the symbol of the chiral carbon atom, whereas her latter two do not.]

Anna attempted to redraw structure 'B' in a tetrahedral configuration similar to structure 'A' (Table 3.4, Question 8), but her original drawing had both dash and wedge placed to the viewer's left rather than to the viewer's right as given for structure 'A'. Anna didn’t see a problem with this, and concluded that the structures were identical, but when asked if she were positive, she laughed and said, "It doesn't, because it's rotating..." However, she wasn't sure that rotation was the right term, and when she tried to alter her diagram to place the dash and wedge on the right, she drew a series of structures that she produced by successively exchanging the positions of various substituents (Figure 6.12). Anna discovered that this method alone could never produce a drawing oriented in the same manner as structure 'A' (Table 3.4, Question 8). When asked to describe her difficulty, she said, "It looks like there's going to have to be some kind of ... well, I want to say 'rotation,' but I'm not sure that's going to work." She finally concluded that she had to rotate it "just a little bit."
Every student who initially attempted to solve this problem through the use of drawings eventually resorted to the previously-described "switching" strategy that they learned in class, which says that if the positions of any two substituents are switched, the enantiomer (mirror image) is formed. They were invariably successful upon reaching this point. Brian had little difficulty in either redrawing the structures on paper or employing this switching strategy; however, when asked to build models of the structures he had more trouble. Having already proven to himself that the two structures were identical, he knew that the model he built representing structure 'A' should align with structure 'B', but he attempted to place the chlorine, hydrogen, and methyl group in the plane of the paper, leaving the ethyl group perpendicular to this plane. He held the model in what could be termed a 'three-points-down' orientation. He said, "So, somewhere ... this three-dimensional stuff ... it's..." Almost accidentally, he aligned his model with the structure, finally agreeing that "It looks good." Several other students also attempted to use the "three-points-down" orientation, but it troubled Brian more than any of the others (Figure 6.13).

Naming the molecule was relatively more straightforward. A typical example is David's response. "Okay, um, I have a four-carbon chain. I started with the methyl group at the top. Down through the center carbon. And then down to the ethyl on the
bottom. On the second carbon, there’s a hydrogen and a chlorine. And then the third carbon, which is part of the ethyl group as it’s drawn here... um, has two hydrogens and the second carbon of the ethyl has three carbons.” (NB: He meant to use the word "hydrogens" here.) "You have a four-carbon chain. And so this would be butane. And the chlorine is on the second carbon, so it's 2-chlorobutane.”

Comparing a Newman Projection to a Dash-and-Wedge Diagram. Questions 11 - 12 (Table 3.4) asked students to compare a Newman projection (structure 'A') and a dash-and-wedge diagram (structure 'B') of the chiral molecule (S)-2,2-dibromo-3-chlorobutane in order to determine whether the given structures were enantiomers or two different representations of the same molecule. Several strategies were employed by students in order to answer this question. Some students built two models, one each of the Newman projection and dash-and-wedge diagram, and subsequently aligned these models with one another. When the models ultimately were shown to be identical, it could then be concluded that the diagrams were two different representations of the same structure. Other students built one model from the Newman projection and aligned this model with the dash-and-wedge formula, while still others built a model from the dash-and-wedge formula and then aligned it with the Newman projection. Finally, some students drew Fischer projections of each diagram and used these to determine that the diagrams represented identical structures.

Several difficulties emerged from this exercise. The structure contains only one chiral atom (the carbon atom labeled '3'; question 11, Table 3.4); however, several students were troubled by the configuration at the achiral atom labeled '2'. Related to this
was the idea that an atom whose configuration is drawn in three dimensions must be chiral. Other students were unwilling to rotate around the sigma bond connecting the middle carbon atoms when attempting to align one model with either another model or a diagram. One further difficulty was the conception that by physically rotating a model through 180 degrees forms the enantiomer.

The achiral atom labeled '2' gave several students difficulty. Jason, pointing to structure 'B' (Table 3.4, Question 11), asked, "Does this have to be level?" He wanted to know if it was actually planar. James asked the same question. He was asked if this mattered.

James: "Yeah. Well, I know this one (NB: carbon '3'), this is like, this is chiral right here. This (NB: carbon '2') is not, because you've got two Br's attached to it."

GL: "Okay, it's not chiral. Does it matter?"

James: "No. So, I would say they look the same."

Both David and Michael initially pointed out that carbon '3' was not chiral, but it troubled them anyway. After beginning to make a model of structure 'B', David switched the positions of a bromine on carbon 2 with the methyl substituent (carbon 1), an operation that makes no difference in the structure at this achiral center. When asked why he did that, he responded, "Uh, I don't know. I was just trying to go in order, I guess."

GL: "So does it matter how you connect the things on there?"

David: "No."

GL: "But that wasn't real obvious, was it?"

David: "Well, I guess it should have been."

Michael also struggled over the relative positions of the two bromine atoms at carbon '2'. When asked if it mattered, he said, "Um ... yeah". When asked why it mattered, he then responded, "Well, I guess it doesn't matter, since there's two bromines." Marianne assumed that any atom drawn in three dimensions was chiral until she was asked how
many chiral atoms were contained in the structure. She said, "Two ... no, one," and went on to successfully complete the exercise.

Neither Kathy nor Anna were initially willing to rotate their models around the sigma bond connecting the central carbon atoms. Anna built models of both structures, which ended up in different conformations. When asked if the two models represented the same structure or enantiomers, she hesitated before rotating one structure around the sigma bond connecting carbons '2' and '3' and asked, "Can I do that?"

Anna initially wanted to use a different color for each carbon atom, using a blue ball for carbon '1' (a methyl group).

GL: "What's that blue thing?"

Anna: "Um, well, I changed methyl to blue, since I have carbons ... I'm going to be denoting my carbons."

GL: "Oh, that's okay, but I don't think you need to. Put a black one on there. It'll be okay."

After she finished building her model, Anna was asked if she really needed a different color to designate the methyl carbon and responded that, no, it was part of "the carbon chain."

Andrea built a model using the dash-and-wedge formula and attempted to align it with the Newman projection, but inverted her entire model 180 degrees. She concluded that the two structures represented enantiomers.

Anna: "The hydrogen is up on the paper, and on the model, it's going down."

GL: "But can't you turn the model over? What would happen if I turned it over and set it right on top of structure 'A'?"

Anna: "The bromines would be different."

GL: "Couldn't you rotate it?"

Anna: "I didn't know I could rotate that side. So it would be like that?"
She then oriented the structures properly and concluded that the two structures were identical.

Most of the students were pleased to have the opportunity to use models on this question. The single exception was Brian, who had previously stated several times that he had difficulty working in three dimensions. Brian preferred to use a pencil-and-paper method. He said that the Newman projection was "very tough," and began looking for a chiral atom, but initially didn't find one. His attention was directed to carbon '2', and he then agreed that it had four substituents: carbon chain, methyl, chlorine, and hydrogen.

GL: "Now that one in the back, that's represented by the circle, is that one chiral?"

Brian: "I don't see why not."

GL: "Well, what's attached to it?"

Brian: "You have ... actually, no, because you have two bromines..."

GL: "Okay, good, two bromines on that one."

Brian: "It doesn't have four."

By this last statement, Brian implied that this carbon atom did not have four different substituents and was therefore not chiral. He then concluded that there was only one chiral atom in the structure.

Brian began by attempting to convert the Newman projection into a Fischer projection. He described this as drawing the molecule "flat."

Brian: "One, okay. ... Let's see how you would draw this. That's tough to draw."

GL: "Isn't that tough to draw?"

Brian: "Yeah... Um, I'm trying to draw it flat, but I'm stuck."

Because he was unsure how to reorient the diagram, Brian required some assistance to get started with his drawing.

GL: "Okay, well, let's try this. What about if you put the chlorine and the methyl as wedges out to left and right?"

Brian: "Okay, then that wouldn't be a problem."
GL: "Okay, what happens to the hydrogen on top? Where does that go?"

Brian (sighing): "That's on top."

After this clue, Brian proceeded to draw an excellent Fischer projection of the molecule. He then began drawing a Fischer projection of structure 'B', saying, "I'm going to start with my chiral carbon ... which would be this one right here. So I'm going to do the same thing. I'm going to pull chlorine and the rest of this ... to the sides. Okay. All right, hydrogen's in the back, so it's going to be at the bottom, and the methyl's at the top." Although he did not describe it in this manner, Brian was able to rotate the structure in order to draw the Fischer projection of structure 'B'..

GL: "Okay. So, are they the same, or are they different, or can you tell yet?"

Brian: "You definintely can't tell yet."

GL: "Okay! (laugh) What are you going to do to tell?"

Brian: "I don't know. Let me think here, let me see. First of all, I can take this...I'm just going to try my other tactic here. I'm going to switch the methyl and the hydrogen from top to bottom, and keep all this the same. Okay, we don't have a match yet, so I'm going to switch the 'big thing' with the methyl. And it looks like we have a match."

GL: "Oh, good!"

Brian: "So this is the mirror image, and this is the same, so I'd say they were the same."

Although Brian required some assistance beginning this exercise, his reasoning was excellent.

Representations of Diastereomers. Question 13 (Table 3.4) asked students to describe the relationships between and build two models of two representations of 1,2-dibromo-1,2-dichloroethane. Structure 'A' is the meso compound and structure 'B' is the optically active diastereomer, (1R,2R)-1,2-dibromo-1,2-dichloroethane. Structure 'A' (Table 3.4, Question 13) is intentionally drawn in a conformation such that the top
half of the molecule can be seen to be the mirror image of the bottom half. Upon observing this, an astute observer can then conclude that this is a meso compound. James was the only student who noticed this immediately, saying, "Well, because if you put like, an imaginary line, say it's a mirror image, to reflect. They're both identical, well, mirror images. Two chiral carbons." He thus reasoned that structure 'A' is a meso compound.

Some students chose to forego the use of models in this exercise whereas others requested them. Brian, Matthew, Kathy, and David used their molecular drawing skills without building models. In each case, they drew Fischer projections; nobody chose to draw either Newman projections or sawhorse diagrams. Kathy, James, and Tammy immediately set to work building models before attempting to answer the question; Marianne, Andrea, and Anna attempted to answer the question without using models, realized that they could not, and then built models.

In determining the actual relationships between the structures, James, Jason, Marianne, Andrea, Tammy, and Anna all chose to build two distinct models, one of structure 'A' and one of structure 'B'. Nobody chose to build a single model of one of the structures and then compare it to the other. The four students who drew Fischer projections (Brian, Matthew, Kathy, and David) all chose to use a "switching" strategy, in which they progressively switched positions of substituents at each chiral carbon, alternating its configuration each time. This strategy, when used correctly, correctly attributed the structures as diastereomers.

Several interesting difficulties emerged from the answers to this question. Three students (Anna, Brian, and Michael) attempted to draw structures that were described as "flat." Anna specifically stated that she wanted to draw each structure "without the stereochemistry", but actually drew Fischer projections.
Anna: "Alright, now I'm drawing out structure B without the stereochemistry.... Why is this bothering me?... Okay, Br, H, and... okay, I have mirror images in the two chiral compounds."

GL: "Okay, let me ask you a question. First of all, you said you're drawing without the stereochemistry, but that convention that you have drawn there, doesn't it really indicate the stereochemistry?"

AL: "Yeah, I guess it does, because the ones that are going up and down would be, you would automatically assume they're going back. And the ones to the side would automatically be coming forward. And I see your point now!"

Anna then said that in her drawings "bromine should be going back in both. I had the chlorines going back." She redrew her Fischer projections again in order to correctly represent the given structures. Brian and Michael also described the Fischer projections as flat, but in contrast to Anna, both drew them using the correct stereochemical conventions. Brian, who had several times mentioned his difficulties working in three dimensions, took a very mechanical approach to this problem, having attempted to memorize a method. He began working at the chiral carbon atom at the top, drawing chlorine and bromine in the top and bottom positions. He was then unsure how to proceed.

To determine if Brian might consider drawing the second chiral atom pointing down from the first, Brian was asked, "Are there two atoms that might be easier to work with?" He responded, "The two chiral carbons?" When asked what would happen to the position of bromine and chiral carbon if he placed the hydrogen in a horizontal position to the right and chlorine in a horizontal position to the left, he correctly placed the bromine up, the second chiral carbon down, and completed drawing his structures. He had no difficulty finishing the second structure.

In contrast to Brian and Anna, Michael correctly and confidently described the possible relationships between the two structures, but initially drew the Fischer
projections incorrectly, inverting the stereochemistry at the top carbon in both structure
'A' and structure 'B' (Table 3.4, Question 13).

Several interviewees initially were reluctant to use the term “diastereomer.” They
instead attempted to restrict their method of classifying the structures to the terms
"enantiomers", "the same compound", or "structural isomers", although everyone noticed
that the structures contained two chiral atoms. Most students described the top halves of
the structures as being the same, with the bottom halves being enantiomers. Jason then
described both structures as "structural isomers, yeah, 'cause they're just in a different
order." When asked to confirm this, he examined his models closely and said, "Nope!"
He confirmed that they were "not enantiomers, not mirror images" and went on to state
that they were not geometric isomers.

GL: "So they're not geometric. So they gotta be some kind of stereoisomers. What
kind are they? They're not enantiomers, you told me that, right? Because they're not
mirror images?"

Jason: "Yeah, they're not mirror images. So if they're not mirror images, they're
diastereomers?"

Kathy was also uncomfortable with the idea that these were isomers and yet were
neither structural isomers nor enantiomers, although she noticed that they were "not the
same, and they don't reflect each other."

Several students were reluctant to rotate either their written structures or their models
around the carbon-carbon sigma bond. James was particularly hesitant to do this and
queried, "Something I want to ask you, do they still rotate?" After being assured that
they did, he drew Fischer projections, and then asked again, "Can I rotate them?" Kathy
did not want to describe her operations as rotation. When asked how she produced the
top half of her diagram (Figure 6.14) from the diagram given in Table 3.4, Question 13,
she said that this amounted to "pulling the chlorine forward and pushing the bromine
back." She then said that she "pulled my chlorine and bromine apart." When asked if
what she had done was rotate them, she said, "basically." Jason was reluctant to rotate
his two models, even though it was necessary to do this in order to prove that they were
different. His initial statement was, "They're the same, obviously."

![Diagram]

Figure 6.14. Kathy's representation of the meso compound (1R,2S)-1,2-dibromo-1,2-
dichloroethane. Kathy drew this diagram by "pulling the chlorine forward and pushing
the bromine back."

Two final important difficulties were observed. Andrea had learned the "switching"
strategy that indicates that exchanging any two substituents at a chiral center inverts the
configuration. Doing this twice at the same chiral center therefore reproduces the original
structure. However, the structures in Question 13 (Table 3.4) contain two chiral centers.
Andrea attempted to switch one pair of substituents on each chiral center, and was unclear
as to why this did not produce the original structure. David initially attempted to do this
as well, but corrected himself. "One inversion, two inversions, they're the same. But
then I remembered, they would have to be two inversions around the same carbon. So I
knew that was not right." Finally, Marianne immediately identified the structures as
enantiomers, "because they're mirror images." She thought this was true because dash,
wedge, and line are drawn as mirror images in the two structures (Table 3.4, Question
13), without regard for the substituents attached to them.

Summary of Results from Third Interview. Some common strategies developed and
used by students in this study to compare two representations of chiral molecules are
given in Table 6.1. Seven broad categories of difficulties and strategies in learning
related to enantiomers, diastereomers, geometric isomers, and structural isomers among
the participants also emerged from this interview and are summarized in Table 6.2. These
categories are "difficulties related to rotation around bonds and molecules", "difficulties
related to mirror images and chirality," "difficulties related to nomenclature", "living in a
flat world", "difficulties involving the relationships between models and representations
on paper", "difficulties with rote rules", and "Preference for static structures - reluctance
to reorient/rotate."

Table 6.1. Strategies Used by Students in This Study to Compare Representations of
Chiral Molecules.

1) Building one model to compare with two drawn structures.

2) Building models of each of two drawn structures and comparing them with each
other.

3) Rotating drawn structures "in their mind's eye" without the use of models.

4) Drawing successive pairs of enantiomers
Table 6.2. Difficulties in Learning Derived From the Third Interview.

I) Difficulties related to rotation around bonds and molecules
   A) Restricted rotation around a bond
      1) Even after building a model and rotating around each bond, it is possible for a student to conclude that rotation is impossible, especially if it has "unusual" substituents (e.g. halogens) attached. These structures will sometimes be described as exhibiting geometric isomerism.
      2) Two representations of the same trans-geometric isomer rotated 180 degrees may be perceived by students to be different geometric isomers.
      3) Stereoisomers are frequently equated with geometric isomers. Simply being able to define these terms does not mean that students recognize which isomers are which.
   B) Rotation of an entire molecule
      1) Students may equate conformers with geometric isomers, failing to recognize that rotation is not restricted around a sigma bond in acyclic structures.
      2) Some students mistakenly perceive that physically rotating a chiral structure 180 degrees makes the enantiomer.
      3) Students frequently fail to recognize the difference between rotating around a bond and rotating an entire molecule.
      4) When aligning a structure with its mirror image, students will attempt continuous 60-degree rotations around the vertical bond (instead of the necessary 30-degree rotation).

II) Difficulties related to mirror images and chirality
   A) Mirror images
      1) Two identical structures will frequently not be perceived as identical unless they are drawn in the same orientation. If one structure is rotated or translated, it may be perceived as a different structure.
      2) If a student perceives that the frameworks of two structures are drawn or oriented as mirror images, the structures will also be perceived as mirror images, without regard for the attached substituents (Figure 6.15).
      3) Students find it difficult to recognize drawings of meso compounds even if they are drawn so that the plane of symmetry in the molecule is emphasized in the drawing (Figure 6.16).
      4) Two structures that contain the same number and type of atoms are generally assumed to be isomers if they are oriented differently.
   B) Chirality
      1) Students will worry about the configuration of an achiral atom if it is drawn in three dimensions.
      2) Stating that an atom is achiral does not insure that a student won't worry about its configuration.
   C) Students who detect the presence of two chiral atoms in a structure and perceive that the structures are neither identical nor enantiomers will frequently classify these structures as structural isomers rather than diastereomers.

III) Difficulties related to nomenclature
   A) Numbering
      1) Students frequently do not assign individual numbers to substituents on the same carbon atom, and fail to associate the need for doing this in order to distinguish between different structural isomers.
      2) Students tend to assign different numbers to substituents that are attached to the same carbon atom.
Table 6.2 (cont.),

B) Other

1) Students frequently fail to distinguish which atoms were part of the parent chain and which atoms would be considered as substituents.

2) Students tend to name each substituent on a chiral atom.
   a) Use of "hydro" to name hydrogen atoms.
   b) Naming each substituent on a chiral atom instead of viewing the chiral atom as part of a longer chain.

IV) "Living in a flat world"

A) A portion of a complex molecule drawn as a dash formula is planar.

B) Students frequently ask if a molecule drawn using a dash formula is planar.

C) When presented with difficult structures, students tend to draw them "without the stereochemistry," even when stereochemistry is important to the exercise.

V) Difficulties involving the relationships between models and representations on paper

A) In order to determine whether a model is identical to a drawing, a student will align two substituents from a structure with two on the paper, reorient the structure, and then align the other two, rather than aligning all four at once.

B) It is difficult for students to orient a three-dimensional model with its two-dimensional representation.

C) When students align a model with a structure, the model is placed on the paper "three points down" (Figure 6.13).

VI) Difficulties with rote rules

A) Switching substituents on chiral atoms

1) Students frequently attempt to compare two structures drawn using different representations by simply switching substituents.

2) Students frequently equate exchange of two substituents around a bond with restricted rotation with rotation of the entire molecule.

3) Students will invert the positions of two substituents at each of two different chiral atoms in an attempt to redraw the original structure in a different orientation.

4) When using models, students are reluctant to exchange any two substituents on a chiral carbon atom when making the mirror image. A student will insist on exchanging the same two that were used "on paper."

B) Other

1) In order to determine whether a model is identical to a drawing, a student will align two substituents from a structure with two on the paper, reorient the structure, and then align the other two, rather than aligning all four at once.

2) Students frequently confuse the meanings of dash and wedge notations.

VII) Preference for static structures - reluctance to reorient/rotate

A) Students are frequently reluctant to rotate around a sigma bond.

B) Reluctance to rotate entire structures.

1) Students are more reluctant to rotate complex molecules in order to compare them.

2) Students are often reluctant to reorient two identical models in order to conclude that they are the same.

3) When students rotate complex structures, they are reluctant to describe the operation as rotation.
Figure 6.15. Structures that may be perceived as mirror images because the frameworks are presented as mirror images.

Figure 6.16. Two representations of a meso compound (1,2-dibromo-1,2-dichloroethane) in which the plane of symmetry in the molecule is emphasized.
INTERVIEW 4 RESULTS

The fourth interview was conducted twelve to fourteen weeks after the beginning of the course, and was designed to probe student learning, understanding, and conceptions regarding the relationships between stereochemistry and chemical reactions and mechanisms. By this point in the semester, the students had studied the mechanisms of first and second order nucleophilic substitution reactions (Sn1 and Sn2 respectively) and first and second order elimination reactions (E1 and E2 respectively) in addition to the concepts of inversion and retention of configuration and racemization (Bailey & Bailey, 1995). Jason was ill during this portion of the semester and was unable to participate; thus, only nine students were interviewed.

Demonstrations of Second Order Nucleophilic Substitution. Questions 1 and 2 (Table 3.5) asked students to use two different types of models to demonstrate what occurs in a second order nucleophilic substitution (Sn2) reaction. In the mechanism of this reaction, the nucleophile enters at the same time that the leaving group departs, forming a transition state. If the reactant is chiral and substitution occurs at the chiral center, the product will consist of only one enantiomer with configuration inverted from that of the reactant. This process is illustrated in Figure 7.1.

\[
\text{Nu} + \begin{array}{c}
\text{A} \\
\text{B} \\
\text{C}
\end{array}
\begin{array}{c}
\text{LG}
\end{array}
\rightarrow
\begin{array}{c}
\text{Nu} \\
\text{A} \\
\text{B} \\
\text{C}
\end{array}
\begin{array}{c}
\text{LG}
\end{array}
\rightarrow
\begin{array}{c}
\text{Nu} \\
\text{A} \\
\text{B} \\
\text{C}
\end{array}
+ \begin{array}{c}
\text{LG}
\end{array}
\]

Figure 7.1. Inversion of configuration in second-order nucleophilic substitution (Sn2). Nu represents the nucleophile, LG the leaving group, and A, B, and C are other substituents on the central chiral carbon atom.

The first question requested the students to demonstrate the Sn2 mechanism using the wooden model illustrated in Figures 3.3 - 3.6, and the second question had them
repeat this process using the commercially available set of models (Prentice Hall Molecular Model Set for Organic Chemistry™) that are referred to in this study as static models. Both types of models are described under Materials and Methods.

Most of the students readily demonstrated the process of nucleophilic substitution using the wooden model, bringing the nucleophile in from the back side, attaching the rubber band representing its unshared electron pair to the central wooden ball to form the transition state, and then removing the rubber band holding the leaving group to the central wooden ball. Most students emphasized that approach of the nucleophile occurred simultaneously with departure of the leaving group, and Kathy made a point to say, "At the exact same time. But I don't have enough hands to do it at the exact same time."

Brian said that he thought this exercise would be "hard," but when asked to describe the mechanism, he said, "Okay, that means, um, that the leaving group is going to come off at the same time as the nucleophile." He attached the nucleophile using the rubber band and emphasized, "At the same time, the leaving group comes off." When asked why he thought this would be hard, he said, "I was trying to distinguish whether $S_N2$ was the intermediate or the transition state."

Only one student, Marianne, had real difficulty demonstrating this mechanism. When asked about the meaning of $S_N2$, she replied, "Isn't that a substitution one?"

GL: "Yeah. It's a substitution reaction. Is there something on there that could be a leaving group?"

Marianne: "I guess this could come off."

GL: "That makes sense to me."

Marianne: "This looks like a leaving group."

She identified the wooden ball attached to the post (Figure 3.3) as a potential leaving group, but had difficulty explaining her choice.

GL: "Well, why do you think that that would be the most likely leaving group, rather than one of the other things attached to the central atom? You're right, by the way."
Marianne: "Okay. Um, just 'cause, you know how when you have "something plus something," and then ... "

GL: "Okay"

Marianne: "... I don't know how to describe it, but, the last thing is most likely the leaving group. Easier to come off."

GL: "Okay, well, what side does it have to leave from?"

Marianne: "Like, do you mean like 'back-side attack', or...?"

Despite choosing a reasonable leaving group, she initially identified the nucleophile as one of the substituents attached to the chiral center, saying, "It's probably right here. The nucleophile." She then pointed to the wooden post containing the other wooden ball (the actual nucleophile), and asked, "Is that part of the thing, too?" Being assured that it was, she said, "I don't know; I don't think there is a nucleophile. Wouldn't it be like added onto it, like 'plus something'?" By this, she was asking if the nucleophile were a separate species.

GL: "Okay, fine, well, what's the other thing that could be 'plus something'?"

Marianne (pointing to the actual nucleophile): "I guess this!"

Marianne then proceeded to demonstrate the SN2 mechanism correctly, although she thought that it could be either SN1 or SN2.

Nature of the SN2 Transition State. Most of the participants described the leaving group, chiral center, and nucleophile as being linear, using the phrase "180 degrees apart." Only one participant, Anna, described the entire transition state as a trigonal bipyramid. Anna was the same student who, in the first interview, described how she had reviewed that portion of her freshman chemistry notes dealing with valence shell electron pair repulsion theory and the shapes of molecules.

Anna began by describing how she would draw a diagram of the transition state (Figure 3.4) on paper.
Anna: "The transition state's going to have both the, uh, the nucleophile and the leaving group still connected."

GL: "Okay"

Anna: "Um, if I was drawing this out on paper, instead of rubber bands, I would have three dots in between each to kind of indicate that a bond was forming between the nucleophile and the compound, and a bond was breaking between the leaving group and the compound."

Anna then drew a picture of the transition state and produced the drawing in Figure 7.2.

![Diagram of an SN2 transition state]

Figure 7.2. Anna's representation of an SN2 transition state. Anna has not indicated what atoms are attached to the central chiral carbon atom, but has attempted to show the planar nature of the chiral center and substituents 'A', 'B', and 'D'.

Anna: "Okay, what I've drawn is a 'C' (NB: a carbon atom) in the middle, with an 'A' pointing upwards, and um, a 'B' and a 'D' stereochemically pointing downwards, with the 'B' pointing out at us and the 'D' pointing towards the back. 'F' is the nucleophile, and it is entering from the left. And I have three dots showing its connection to the middle carbon.

GL: "Okay"

Anna: "Um, 'E' is the leaving group. It's to the ri ... leaving ... going right, and I also have three dots showing its connection to the middle carbon. They're both still connected, but 'F' is forming a bond and 'E' is breaking its bond."

Anna described her atoms 'A', 'B', and 'D', along with the central carbon atom as being trigonal planar, and when asked for an even simpler description, she said, "Oh,
they're flat!" She said that she used dash and wedge in her drawing (Figure 7.2) to "show that one is coming out and one is going back." However, she didn't initially describe the wooden model (Figures 3.3 - 3.5) in this manner. She was told that there were no dashes and wedges in the model, and was asked if one substituent "is coming out and one going back?"

Anna: "Mmm, no, because I see it as flat."

GL: "But I'm talking about... hold it so that it's oriented just like this, so that the "F" is on your left and the "E" is on your right."

Anna: "Oh, okay."

GL: "Now, don't you see one coming toward you and one going back?"

Anna: "Oh, I see what you mean. Yes."

Chirality and the $S_N^2$ Mechanism. Although the ability of students to demonstrate the $S_N^2$ mechanism using the wooden model (Figures 3.3 - 3.5) was generally satisfactory, some students had trouble correlating this mechanism with inversion of configuration (Figure 7.1). Tammy said that the nucleophile entered "from the back" and followed this up saying "the chiral atom is going to change position." She questioned, "the absolute configuration is going to change?" This type of uncertainty was common. Brian frankly stated, "I'm not sure" when asked what happened if the middle atom were chiral.

GL: "Okay, what would happen to the configuration? I mean, if it ... would it stay the same, would it undergo inversion...?"

Brian: "It would undergo inversion?"

GL: "Okay, why is that?"

Brian: "Uh, ... it's because you're breaking a bond?"

Although he knew that the nucleophile approached "just from the back", he never correlated this idea with inversion of configuration. Andrea was apologetic when asked...
about the consequences of the chirality of the central atom, and could not answer this question.

Michael and Anna were more successful with this question. Michael said, "You get ... the enantiomer?", and waved his hand back and forth across the central atom in order to show how it moved when the configuration inverted. He later said that he realized that, if the nucleophile and leaving group were different, a true enantiomer was not produced, but he had no other way to describe inversion. Anna immediately began, "If the middle atom is chiral, in SN2, um, well, I already said it causes inversion."

GL: "Right"

Anna: "But you're looking for something else..."

GL: "No, I'm not! What does that mean, that it causes inversion?"

Anna: "Well, the compound is pointing in a different way. It's..."

GL: "What do you mean by 'pointing in a different way'?"

Anna: "Well, it's pointing, um, when the nucleophile has connected and the leaving group has left, you have a, you have like the middle carbon is ... you have your tetrahedron, but the point of your tetrahedron, like "A" in my drawing, is pointing ... I'm sorry, let me back up. Um, ..."

GL: "Maybe this will help. What does that mean in terms of enantiomers?"

AL: "Oh, it's the mirror image!"

Static Models and Demonstration of Chirality. David, Kathy, Michael, and Brian quickly realized that the static model could not be used to represent inversion of configuration in the SN2 mechanism. David said, "Oh, well, I can show you right now, you can't ... you can't have the, uh, leaving group and the nucleophile attached at the same time," and he demonstrated that if the nucleophile attempted to come in from the back side, there was no place for it to attach. Kathy said, "It wouldn't be as effective," later noting, "There's no place to plug it in." Michael and Brian had similar comments.
Other students were not willing to give up the idea that the static models could be used to demonstrate inversion of configuration. James removed the leaving group and said, "Okay, it comes off flat, but now you've got a problem figuring out which one is going to be used." He pointed at the wooden model and said, "Like, would it shift this way?" He realized that something was different, picked up his nucleophile, attached it to the spot vacated by the leaving group, and without inverting the configuration he said, "Can you just do it like that? I don't know."

James then decided to build models of the two enantiomers of the product. When he finished, he said, "Okay, let's see if it will be mirror images. I don't think it will be." Only after comparing these structures did he conclude, "Hmm, so that wouldn't be, it wouldn't be a reversal." He then concluded that the problem with the static model was that "there's no peg in it."

Although she had correctly identified the nucleophile as a separate species when working with the wooden model, Tammy attempted to build the nucleophile into the structure of the initial reactant when using the commercial model set. She was questioned about this.

GL: "Doesn't the nucleophile have to be something separate?"

Tammy: "Oh, you're right."

She attempted to bring the nucleophile in from the back side, but when she found there was no place to put it, she simply removed the leaving group and replaced it with the nucleophile and asked, "Can I just put it on there like that?"

GL: "Can you?"

Tammy: "Okay, sure."

GL: "But is that legal?"

Tammy: "No, sir, because it's coming in from the opposite direction. This is the same ... I don't really know how to explain it. The nucleophile took the position of the leaving group." At this point, Tammy was really unsure what was correct.
GL: "What would happen to the configuration if you could do it that way?" (What would happen to the configuration if Tammy could simply remove the leaving group and replace it with the nucleophile?) Like James, she built models of the two possible enantiomers of the product, and then concluded "I don't know if I can do that."

When Anna was asked what would happen if she demonstrated the $S_N2$ reaction using the commercial models, she replied, "Well, for one thing, I wouldn't get the flatness." She then proceeded to remove the (yellow) leaving group and replace it with the (blue) nucleophile.

GL: "Where would the blue come in? You're putting the yellow and blue on the same side."

Anna: "Uh huh. The blue would have to come in from the opposite side. But I can't do that with this model. I would have to remove the yellow, which would mean I have an $S_N1$ reaction. Because then the leaving group would have to leave before the nucleophile can enter, and then the nucleophile has to enter the same spot. And there's a word for that, but I can't think of it right now."

Anna was prompted with the word "retention" and she responded, "Yes!" Anna's confusion was finally resolved when she investigated the $S_N1$ mechanism in the next portion of the interview.

**Comparison of Findings Regarding the $S_N2$ Mechanism**. Many of the students had difficulty with definitions in this section, confusing $S_N1$ with $S_N2$ and substitution with elimination. In addition, at various points, two different students attempted to build a tetrahedral reactant with the nucleophile already attached. However, the most common difficulty was a lack of correlation between the necessity of backside attack, formation of a trigonal bipyramidal transition state, and inversion of configuration. When given the model especially built for this purpose (Figures 3.3 - 3.6), students could describe and demonstrate the $S_N2$ mechanism showing inversion of configuration. However, when given a commercial model set that could not readily form a representation of the transition
state, the majority of the students were willing to form a product that did not invert configuration. When asked to describe the difficulties involved in using such a set, many were unable to state a reason why the model was inadequate and why the product they produced was incorrect.

**Demonstrations of First Order Nucleophilic Substitution Reactions.** The third question (Table 3.5) asked students to use the wooden model (Figures 3.3 and 3.6) to demonstrate what occurs in a first order nucleophilic substitution (SN1) reaction. In the first step of the mechanism of this reaction, the leaving group departs, forming a trigonal planar carbocation as an intermediate. In the second step, the nucleophile approaches to form a new bond from either side. If the reaction occurs at a chiral center, the product will consist of an equimolar mixture of enantiomers, one of which represents retention of configuration and the other inversion. This process is illustrated in Figure 7.3.

David had no difficulty with this question. He initially removed the wooden ball representing the leaving group, described the resulting intermediate as being planar and a carbocation, demonstrated that the nucleophile was equally likely to enter from either side, and said that if the initial reactant were chiral, the resulting product would be a racemic mixture, being equally likely to either invert or retain configuration.

Like David, Tammy performed this exercise perfectly. Unlike David, she was unsure of herself at almost every step. Although she did not receive any clues, she needed frequent encouragement to answer. At the end of the exercise she was asked to predict the configuration of the product.

GL: "Will you get one enantiomer when you do SN1?"

Tammy: "Oh, I'll end up with a racemic product ... I'm scared!"

Every other participant had some type of difficulty regarding this exercise. Two students explicitly described the SN1 mechanism as being more difficult than the SN2. Despite doing a very credible job with this exercise, James initially said, "See, this is
Figure 7.3. Mechanism of the first-order nucleophilic substitution (SN1) reaction. (a) Formation of the planar transition state. (b) Approach of the nucleophile showing retention of configuration. (c) Approach of the nucleophile from the opposite side, showing equal probability of inversion of configuration. Nu' represents the nucleophile, LG' the leaving group, and A, B, and C are other substituents on the central chiral carbon atom.

where I get confused, with that SN1 stuff." And Kathy began by saying, "The SN1 gets confusing for me."

**Nature of the SN1 Intermediate.** Two students, James and Marianne, were troubled by the charge on the carbocation intermediate. After Marianne formed the intermediate, she was asked, "It's only got three bonds to carbon, right? And we need to have four. So what do you call that thing?" She hesitated, looking puzzled.

GL: "Okay, let me ask you a question. When the leaving group left, it took its pair of electrons with it, right?"

Marianne: "Right"

GL: "So what's the charge on that thing?"

Marianne: "Positive. Negative, no positive."
GL: "Okay, it's positive. So what do you call something, a species with a carbon, three bonds, and a positive charge?"

Marianne: "... A carbocation!"

Like Marianne, James also had difficulty with the charge on the intermediate. He explained, "The leaving group has to leave first. Okay, so it leaves and you have this intermediate right here. Which is going to be... negative or positive... negative, right? I'm trying to think."

GL: "Isn't it a carbocation?" (NB: emphasis on the 'cat' syllable)

James (laughing): "Yeah, yeah, okay. I'm thinking I'm always getting that stuff backwards. It's going to be positive."

Many students had difficulties explaining the planar nature of the intermediate carbocation. Michael had only very minor difficulties with most this exercise, but had trouble explaining the nature of the intermediate carbocation. When asked, "Now, what happened stereochemically if it's $S_N1$?", Michael replied, "If it's $S_N1$, it's planar."

GL: "What's planar?"

Michael: "The molecule that's being substituted."

This being incorrect, he was then asked, "Let me ask you this question first. Does it go through an intermediate or a transition state."

Michael: "Okay, it goes through an intermediate. It's a carbocation."

GL: "Perfect. What's planar now? You said it's planar."

Michael: "It's flat."

GL: "But what is..."

Michael: "It's all in one..."

GL: "I agree. But, I mean, what is it that's flat? It's not the initial molecule. The initial molecule isn't flat."

Michael: "It's like, the intermediate is flat."
When asked what difference that made, Michael replied, "It means that it can come in on either side. It's not hindered." Michael proceeded to complete this exercise without any more difficulties.

When constructing the intermediate carbocation, Tammy, Kathy, and Andrea initially built a model that actually represented the Sn2 transition state (bringing in the nucleophile before removing the leaving group). Tammy did this despite explicitly explaining that in the Sn1 mechanism, the leaving group departed prior to approach of the nucleophile. In contrast, Andrea was confused regarding terminology. She said, "Okay. The nucleophile has to force the leaving group off."

GL: "In Sn1?"
Andrea: "Which one are we doing? Sn1?"
GL: "We're doing Sn1 now; we did Sn2 before."
Andrea: "Okay, Sn1 is two steps."

Kathy described the intermediate as a carbocation, but brought her nucleophile in before releasing the leaving group (forming the Sn2 transition state instead of the Sn1 intermediate carbocation). Kathy was then asked, "What else could you do instead of having the nucleophile come off?", and she answered, "Take off your leaving group."

Kathy then reconstructed the model of the initial starting material and removed the leaving group (forming the planar carbocation intermediate). She picked up her nucleophile and said, "Your nucleophile comes in where your leaving group left at. And it attaches."

Kathy then built a model of the product with its configuration retained but did not build a model with the configuration inverted.

**Importance of the Carbocation Intermediate to the Stereochemistry of the Product.**

Most of the interviewees did not initially associate the shape of the Sn1 intermediate with the stereochemistry of the product. As an example, after forming the planar carbocation intermediate, James proceeded to attach the nucleophile on the side opposite from that
formerly occupied by the leaving group, and said, "I mean, ooh, it looks like the same thing as the SN2."

GL: "Does the nucleophile have to come in on that side?"

James: "Uh, from this side?"

GL: "Yeah"

James hesitated and then explained, "No, it can come in on this side and still be the same thing. And that's why you get both products! Because, because, it leaves right away." As he did this portion of the exercise, it appeared that James was explaining this to himself as well as to the interviewer. Describing the difference between the SN2 and the SN1 mechanisms, James said, "Um, you can have, you can have both forms of this molecule... occur in the reaction... with an SN2 you can only have one form. And, which is like the inversion of it."

Kathy had similar problems. She recognized that she formed "a carbocation intermediate," but stated that the nucleophile approached from only one side "because that's where your charge is at."

GL: "But it's flat. It looks flat to me. Isn't it flat?"

Kathy: (laughing) "I guess so."

GL: "So where's the charge? Which atom is the charge on?"

Kathy: "The carbon." She (correctly) pointed to the central carbon atom.

Kathy was then asked about the charge. "But does it point to your left, to your right, or is it just on a carbon atom?" She replied, "It's around the carbon atom."

GL: "But is it more to the left, more to the right, or neither."

Kathy: "Either on this side or on this side. Wherever it can fit." She finally decided that the nucleophile could enter from either direction, saying, "Right. Either side."

GL: "So, which percent do you get? Do you get more from the left or more from the right? Or is there any preference?"

Kathy: "I don't think there is any preference, because of where it comes in."
GL: "Which one do you get? Do you get that one, or do you get the one with the nucleophile coming in from the other side?"

Kathy: "You get this one."

GL: "Why?"

Kathy: "Because your nucleophile takes the place of where the leaving group was."

After deciding that the nucleophile could enter from either side of the planar carbocation, Kathy was still unsure as to how this affected the stereochemistry of the product. She was asked, "Okay. So what about the product? What are your choices, as far as the configuration of the product? What could happen?"

Kathy: "It could either, your nucleophile coming in on the right side or the left side."

GL: "Okay, so what happens if the nucleophile comes in on the same side as the leaving group left?"

Kathy: "It'll stay the same."

GL: "Okay. What happens if the nucleophile comes in from the other side?"

Kathy: "It switches."

GL: "And so what happens to the configuration at that carbon?"

Kathy: "... It's different. It's 'anti' configuration (laughs)."

Kathy demonstrated this mechanism again, with the leaving group coming in opposite the site of the leaving group. She was asked how she could describe what was happening to the configuration of the molecule. She laughed and said, "... good question." Only after reviewing the SN2 mechanism she had worked with previously, was Kathy confident enough to describe the stereochemical consequences of the SN1 mechanism. At this point, Kathy was asked how many of the SN1 reactant molecules are inverted, and she replied, "Half of it gets inverted and the other half doesn't."

After constructing the carbocation intermediate for the SN1 mechanism, Andrea was asked about the chirality of the product.

GL: "Now, if that middle atom was chiral, what happens to it at the end?"
Andrea: "Well, it's not chiral right now, because it only has three groups."

She was told that this was a good observation and was further pressed as to whether this meant that the stereochemistry would be inverted. She said, "Yeah, 'cause this one will come in on the other side. Well, no, because since this one is already gone, the nucleophile can come to where the other one was?" She successfully demonstrated approach of the nucleophile from both sides, but was unsure what product or products actually formed.

GL: "Which one do you get? Do you get the one where it came in from the left or from the right?"

Andrea: "I don't know..."

GL: "Or do you get both? What do you think? What does your common sense tell you?"

Andrea: "Both, maybe?"

After deciding that she would get both products, she then stated more confidently that the mixture of products would not rotate plane-polarized light.

Comparison of Findings Regarding the SN1 Mechanism. Although the intermediate was generally described as planar, most of the students did not readily associate the necessity of having a planar intermediate to the formation of equal amounts of enantiomeric products. This was in part because many students did not visualize approach of the nucleophile as being equally likely from either side. There were several variations on this theme. Simply being able to explain that the leaving group departed before the nucleophile approached did not mean that a subject would actually illustrate this with a model. Two subjects stated that the leaving group departed first while demonstrating that the nucleophile forced the leaving group to leave. A planar intermediate never formed, and formation of only one product could be demonstrated. Several students formed the planar intermediate, but visualized approach of the nucleophile from only the side opposite the leaving group. One student, after forming the
planar intermediate, had the nucleophile approach from the same side that had been occupied by the leaving group (explaining that this had something to do with the charge). The idea that approach of the nucleophile from either side was equally likely once the leaving group departed was not readily apparent.

Students also had difficulty explaining the relationship between the shape of the intermediate and the stereochemistry of the product. Inversion of configuration in the $\text{Sn}_2$ mechanism was much more readily apparent than was racemization, or formation of a mixture of mirror images, in the $\text{Sn}_1$ mechanism.

**Study of the $\text{Sn}_2$ Mechanism of a Specific Reaction.** The next four questions of the fourth interview (Table 3.5, Questions 4-7) asked students about the mechanism of the $\text{Sn}_2$ reaction of bisulfide ion (the nucleophile) with the chiral reagent (S)-2-chlorobutane. The chiral molecule is drawn on the paper in a manner such that the leaving group is not oriented at a 180 degree angle from the approaching nucleophile, and thus the observer must either rotate the chiral molecule or reorient the nucleophile. Possible strategies for each are given in Figures 7.4 and 7.5.

![Diagram of Sn2 mechanism](image)

**Figure 7.4.** Possible strategy to correctly orient nucleophile and chiral molecule. These structures are given in questions 4 - 7, interview 4 (Table 3.5). (a) Rotation of chiral molecule. (b) Approach of nucleophile and formation of product.

Most of the students laughed when asked what kind of reaction was being discussed, because the diagram of the reaction (Table 3.5, Question 4) is clearly labeled "$\text{Sn}_2$."
Nevertheless, this question was not as trivial as might be assumed. Only four of nine interviewees unhesitatingly identified the reaction as a type of substitution. Of the remaining five, James laughed and identified the reaction as "$S_{N2}$," but when further pressed, he asked, "Okay, you mean, is it like addition, or....."

GL: "Yeah, what kind of reaction is that?"

James: "Um,..., golly, I don't really know. Is it going to be a substitution?"

This type of hesitation was common. Tammy said, "You mean $S_{N2}$?"

GL: "Okay, it's $S_{N2}$. Tell me something. Is it elimination, substitution...?"

Tammy: "Okay, um... oh, it's substitution!", followed by a laugh.

When told that "There's a big hint on there," Anna replied, "Yeah, that '$S_{N2}$' is the hint!", and she laughed. But when asked to give a word to describe the reaction, she said, "Um, I... it's going to be either elimination or substitution. We were just tested over this, so I should know it. Let's see, you had it paired off the hydrochloric acid on the test. Um, I think that... oh..."

GL: "What does the 'S' stand for?"

Anna: ""Oh, wait a minute! Wait a minute! You know what? I'm thinking, I'm looking at this like it's 'tin'." (NB: 'Sn' is the chemical symbol for tin.) "It's $S_{N2}$, it's nucleophilic substitution."

Kathy also noted that the notation '$S_{N2}$' was important, but had difficulty identifying the reaction type. When asked to "Tell me something else besides $S_{N2}$," she
noted that the bisulfide ion was a common nucleophile and that the leaving group was attached to a tertiary carbon atom, finally correcting this to a secondary carbon. When asked if the reaction was elimination, addition, or substitution, she identified it as substitution, admitting that "I guessed."

GL: "What does the 'SN2 stand for?"  
Kathy: "The mechanism, bimolecular."
GL: "Okay, what does the 'S' stand for?"
Kathy: (laugh) "Oh, that I don't know! I don't know what the 'S' stands for. That I don't know... Substitution!"

Finally, Andrea did not know how to determine what kind of reaction she had, saying, "...Um, what do you mean, reaction, like..."

GL: "Is it substitution? Elimination? Addition?"
Andrea: "Addition ... Oh, I don't know, I can't tell. There's no products."
However, when asked, "What does the little symbol above the arrow tell you?", she answered, "... Substitution?"

Everyone correctly identified the bisulfide ion as the nucleophile (Table 3.5, Question 5). Because the nomenclature of this ion had not been discussed in class, it was usually called "H-S-minus" or some variant, or simply identified by pointing. Seven participants immediately identified chloride as the leaving group. However, the identity of the leaving group was not as obvious as that of the nucleophile. Marianne initially identified the leaving group as "the ethyl group. No, wait. Oh, chlorine, chlorine!" Brian said, "The leaving group would probably be ... the hydrogen." When asked further what a good candidate for the leaving group would be, he then answered, "... Mmm, oh, chlorine!" Anna initially identified the leaving group as "um... ethyl," and when questioned about this, replied, "Well, no, wait. No, I'm sorry. It would have, well, no ... wait ... it's going to be the chlorine." When asked why this was so hard to see, she said, "Well, at first I was looking at it to just do a simple inversion. You know,
the ethyl was on the opposite side of the carbon than the nucleophile coming in. But if I rotate that …"

All of the subjects confidently described the mechanism as proceeding through a transition state, and in addition, everyone stated that inversion of stereochemistry will occur (Table 3.5, Question 6). Drawing the mechanism in three dimensions (Table 3.5, Question 7) was much more difficult, and several of the students discussed the reasons why. Brian said, "The problem that I'm having is to figure out now what comes in front." Tammy described the problem as being "because this (NB: the leaving group) looks like it's coming out." James knew there was a problem and when told by the interviewer that "I did a mean thing on this," he replied, "Yeah, I haven't figured it out."

But in spite of realizing that the molecule was not oriented on the paper so that one could easily illustrate back-side attack by the nucleophile, only four students attempted to redraw the structure without prompting (Table 3.5, Question 4). Anna used a strategy similar to that shown in Figure 7.4.

Anna: "I'm going to make one little change here. I'm going to rotate this so that it's clear that I have the chlorine opposite where the ... and now I have the ethyl going back. And the hydrogen coming forward. I believe I've drawn that correctly (Figure 7.6). Okay, this is S_N2. All right... the transition state, which I'm going to put in brackets ... we're going to have the H-S-minus, dot, dot, dot, then the carbon, then dot, dot, dot, then the chlorine. I'll still have the methyl sticking straight up, and going down, more towards a downwards angle will be the hydrogen coming out, and actually I meant to draw this a little farther over. I'll go ahead and do that. Okay, pretty much going almost straight downwards, the hydrogen, wedged out, and the ethyl group on the dotted lines going back."

GL: "Man, I should have you teach this in class."

Anna (laughing): "Oh, I like public speaking. I have fun with it. But you can't shut me up!"
Figure 7.6. Anna's representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. Anna had to reorient the reactant to draw this transition state that correctly depicts its geometry.

She continued, drawing the structure of the product with inverted configuration (Figure 7.6), and said, "And the, um ... I may not be drawing this correctly ... um, okay, the methyl, I'm sorry, the ethyl and the hydrogen ... the hydrogen's still wedged out and the methyl (NB: the ethyl) I still have with dotted lines going back. And they're more angled to the right." All this was drawn well, and in describing the product, she said, "And you have a 'quote, unquote' mirror image."

Like Anna, Michael knew that he needed to reorient the molecule, but was initially unsure what to do. He pointed to the right side of the molecule and said, "I'm going to flip the chlorine over here." His reason was, "I'm trying to get it over here, just because that's how I looked at it in the book and the examples." But he was unsure what to do until he was asked, "Without drawing anything, what options have you got? To try to move that chlorine over there."

Michael: "You mean, just rotate the molecule?"

GL: "That's one excellent way. Which axis are you going to use to rotate it around?"

Michael was unsure what this meant. After building a model, he oriented it with the drawing and was again asked, "If the chlorine is like that, which axis are you going to rotate it around to get the chlorine over on the other side." Michael rotated around the
bond connecting methyl group to central hydrogen (Table 3.5, Question 4) and said "Like that."

GL: "On your paper, which axis is that? Between which two atoms?"
Michael: "Oh, between the hydrogen and the ethyl."

GL: "Which bond are you holding between your two fingers, that you're rotating around?"
Michael: "Oh, the methyl! Are you saying that the methyl's going to stay in the same place, but these are going to change?"

GL: "That's what I was asking you. Does that seem like a reasonable thing to do?"
Michael: "So the ethyl would come where the hydrogen is and the hydrogen's where the chlorine is. And the chlorine would go over there." Michael produced the diagram shown in Figure 7.7 and was told that he was close, but the nucleophile and leaving group were not quite 180 degrees apart. (NB: Michael's original drawing, as shown in Figure 7.7, had the nucleophile on the left. It can be seen as the "HS-" that has been partially crossed out.)

![Figure 7.7](image-url)

**Figure 7.7.** Michael's initial representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. In this diagram, the 180° angle between the nucleophile (HS⁻), central atom, and leaving group (Cl⁻) is unclear.

GL: "But they're close! What else could you do to get them 180 degrees apart? Do you see what I'm saying?"
Michael: "Yeah. So that ... no, I don't understand what you're saying."
GL: "What I'm saying is, if you look at the model up there, the nucleophile has to come in 180 degrees opposite from the leaving group. But the way you have it drawn here, this isn't quite a 180 degree angle between the sulfur, the carbon, and the chlorine. Do you see what I mean?"

Michael: "Mm hmm." He decided that he could either rotate the molecule again or move the nucleophile, and chose the latter. He then drew the transition state as shown (Figure 7.8), and was asked whether "the methyl, the ethyl, the hydrogen, and the carbon. Shouldn't they form a plane?" He agreed that they did not.

![Figure 7.8](image)

Figure 7.8. Michael's modified representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. The methyl, ethyl, hydrogen, and central carbon should form a plane.

James chose a different strategy to reorient the molecule. He said, "Okay, um, like, if you switch two groups, that makes the enantiomer. And if you switch two more, that makes it the same thing. So that's that over there." James produced the diagram shown in Figure 7.9, switching the positions of the methyl and hydrogen, and the ethyl and chlorine. Like Michael, James' drawing of nucleophile, central carbon, and leaving group was not quite linear. James wanted reassurance, and asked, "Now, doesn't it have to be, like, do you have to switch the catty-corner ones, opposite, or can you switch just any one out?"

GL: "Can you? Don't switch them, just tell me. Looking at this thing (NB: a three-dimensional model of a tetrahedron), does it matter?"

James: "Mm hmm"

GL: "Is there such a thing as catty-corner, or opposite, or aren't they all the same?"
Figure 7.9. James' representation of the approach of bisulfide ion to (S)-2-chlorobutane. In this drawing, James has switched the positions of the methyl and hydrogen, and the ethyl and chlorine.

James: "They're all the same!" He began drawing the transition state, and asked, "Do I have to kind of draw it flat, or just draw it three-dimensional, still?"

GL: "Oh, you want to draw it three-dimensional, if you can."

James produced the transition state given in Figure 7.10 and began drawing the product (Figure 7.11), saying "I don't know if I should crowd it so much." While showing him a model of a tetrahedron, James was asked, "Does this look like a tetrahedron?", and he responded, "What I've got to do is move this over and ...", and he drew the products shown in Figure 7.12. James chose to draw a mixture of enantiomers instead of an inverted product.

Unlike the other students who reoriented the reactant molecule, David initially attempted to draw a transition state based on the original position of the reactant. Figure 7.13 is a computer-generated reproduction of his drawing. He was asked about his representation of the molecule.

Figure 7.10. James' representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. The 180° angle between nucleophile, central carbon atom, and leaving group is not accurately drawn.
Figure 7.11. James' initial representation of the product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion. The structure as drawn is not tetrahedral around the central carbon atom.

Figure 7.12. James' final representations of the product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion (2-butanethiol). Although missing a hydrogen (H) atom that should be attached to the sulfur (S), the structures appear to be tetrahedral around the central carbon atom.

Figure 7.13. Reproduction of David's transition state for the reaction of bisulfide ion with (S)-2-chlorobutane. Nucleophile, central carbon atom, and leaving group are not oriented at a 180° angle.

GL: "You drew a wedge and a wedge. Is that the right angle? I mean you have a wedge on the chlorine and a wedge for the SH."

David: "Tell you what. Let's do this. I'm going to show ... I'm going to actually draw out the transition state." He drew the transition state given in Figure 7.14, and when asked what he had done, he responded as follows:

David: "Okay, when it goes through this transition state, it becomes planar."

GL: "Okay, what atoms become planar?"
Figure 7.14. David's initial representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. Although he has redrawn the structure, nucleophile, central carbon atom, and leaving group still are not drawn at a 180° angle.

David: "Okay. The ... well, if you look at it from this way, the whole thing ... the whole thing is flat. If you look at it head-on, the hydrogen would go back here ... the ethyl group out here, the carbon in the center with the methyl at the top."

David illustrated perfectly the shape of the transition state. He finished by drawing the product (Figure 7.15). When asked how he did this, he replied, "Well, you take off the leaving group for one thing, and then I drew the rest of it basically from there. This is the mirror image of the starting material."

GL: "So you used the starting material to tell you the shape of the product?"

David: "Yes."

One other student, Brian, also chose to redraw the starting material. However, his experience was much different. Because he was unsure how to begin, Brian was prompted as follows. "Okay, let me make a suggestion. Would it help you, I mean ... What's the problem that is different from the way we usually do these?"

Brian: "The problem is that I'm having to figure out now what comes in front."

GL: "Okay. But it's not drawn the way we usually draw them, is it?"

Brian: "Right, no."
Figure 7.15. David's final representation of the product that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. The configuration of the product has been properly inverted.

GL: "Would it help to redraw the reactant?"

Brian: "You could."

Brian described the mechanism using these words. "Well, let's see. The chlorine has to come off. The leaving group. And, uh, bisulfide would have to, again, come onto it. So I would say that, if I had to, just by looking at it, just by straight substitution, that it would do this." The dash formulas of the overall reaction that he then produced (Figure 7.16) eliminated any three-dimensional representation of the stereochemistry, a major difference between Brian and anyone else who chose to redraw the starting material. However, he was aware that the stereochemistry was important, because he then stated, "But I know that it's inverted, so..."

When asked to draw the transition state, Brian hesitated. In demonstrating this mechanism using the wooden model (Figures 3.3 - 3.5), he detached the leaving group before bringing in the nucleophile (as in the $\text{SN}_1$ mechanism, Figure 7.3). He was asked, "Okay now, doesn't the transition state ... doesn't the nucleophile come in at the same time?"

Brian: "Right"

GL: "So aren't all five of those things attached?"
Figure 7.16. Brian's representation of the SN2 reaction of bisulfide ion with 2-chlorobutane. Brian has eliminated any three-dimensional drawing conventions in his diagrams.

Brian: "Yeah, you're right. I'll put this back on there." He then returned to his drawing, admitting, "I wouldn't know where to put..." He drew a linear diagram consisting of nucleophile, central atom, and leaving group only (Cl - C - HS).

GL: "I mean, you can draw it the way you did. But that's not what the model looks like."

Brian: "Right"

GL: "Okay, what goes on there?"

Brian: "What goes on?"

GL: "Yeah. On those three substituents that you have coming off the carbon? So far, all you've shown is the chlorine and the nucleophile. But there's three other substituents on that carbon."

Brian: "Okay, do you want me to draw these?"

GL: "Yeah, what the heck."

Brian reluctantly added hydrogen, methyl, and ethyl to his drawing, and when asked how he knew where to put them, he responded, "I guessed." His transition state is shown in Figure 7.17.
Only Anna, Michael and James attempted to reorient the structure before illustrating approach of the nucleophile. David adopted the intermediate strategy of reorienting the transition state. Except for Brian, the others attempted to show the nucleophile entering from the back of the molecule, behind the plane of the paper, in a manner somewhat similar to the strategy shown in Figure 7.5. Nobody was completely successful when using this strategy.

Kathy initially drew a diagram showing the position of approach of the bisulfide nucleophile (Figure 7.18) and then drew the transition state (Figure 7.19), saying, "What's going to happen is, your HS-negative is going to come in on the opposite side of your chlorine. And I'm going to put my little hydrogen on to the back." At this point, in order to show that the remaining substituents form a plane in the transition state, Kathy could have drawn the bond to her hydrogen (H) with a solid line instead of dashes, but she did not.

Initially Kathy drew the transition state with the hydrogen atom from the nucleophile (HS-) approaching the central carbon atom. She was asked about this.

GL: "What atom is attacking the carbon, from the HS?"

Kathy: "S!"
She then redrew the nucleophile (Figure 7.19). She was less successful drawing the structure of the product because her drawing does not represent a regular tetrahedron (Figure 7.20).

![Figure 7.18. Kathy's representation of the approach of bisulfide ion to (S)-2-chlorobutane. Approach of the nucleophile (HS\textsuperscript{-}) should be 180° from the departing leaving group (Cl\textsuperscript{-}).](image)

![Figure 7.19. Kathy's representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane. This drawing apparently shows nucleophile, central atom, and leaving group in the proper orientation, but the planar orientation of the remaining substituents (ethyl, hydrogen, methyl on the central carbon) is inaccurate.](image)

GL: "What I want to know is, what happens to the configuration at that carbon?"

Kathy: "It changed."

GL: "Does it look like it changed on your drawing?"

Kathy: "No, no, it sure doesn't."
Figure 7.20. Kathy's final representation of the product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion. Kathy has attempted to depict the inversion of configuration of the product, but the structure is not tetrahedral around the central atom.

Andrea's experience was similar to Kathy's. She drew approach of the nucleophile from the back fairly successfully, although, like Kathy, she used the hydrogen from the bisulfide ion as the nucleophilic atom (Figure 7.21). Describing her transition state, she said, "The chlorine's still on there," and pointed to the bisulfide she had drawn, saying, "So this one has to come from this side." Because she had not used sulfur as the nucleophilic atom, she was told, "By the way, it's the sulfur that's attached." She crossed out the nucleophile and drew it again.

Figure 7.21. Andrea's representation of the transition state that forms on the reaction of bisulfide ion with (S)-2-chlorobutane.

When asked about the shape of the methyl, hydrogen, ethyl, and central carbon in her transition state (Figure 7.21), she said they were flat, but admitted that she couldn't draw them flat. She admitted, "I'm not sure which one ... I guess the hydrogen would be coming out." She then drew the final product depicted in Figure 7.23, again attaching...
hydrogen instead of sulfur to the central carbon atom. Although she described the product as having inverted configuration, this cannot be determined from her drawing.

![Diagram](image1.png)

**Figure 7.22.** Andrea's final representation of the product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion (2-butanethiol). Andrea correctly described inversion of configuration in the product, but the relative configuration of the product cannot be determined from this diagram.

Tammy drew the transition state correctly, but drew a product with retained configuration (Figure 7.23). When asked where she would put the nucleophile, she answered, "Where the chlorine is. This is what I think, but I don't know. I took the chlorine, and I replaced it, because since there's substitution, I thought that, like I should take half like this ..." Although she was able to state that the configuration should be inverted and had earlier demonstrated this using the wooden model, she was unable to draw the product in an inverted configuration.

![Diagram](image2.png)

**Figure 7.23.** Tammy's representation of the transition state that forms on the reaction of (S)-2-chlorobutane with bisulfide ion.

In contrast, Marianne drew the inverted product perfectly (Figure 7.24), but when asked to draw the transition state, she admitted, "I don't know. I forgot how to do that."
I know it's somewhere in between, because both of these have to be connected, for one thing."

\[
\begin{align*}
\text{CH}_3 \\
\text{C} & \text{H}^+ \\
\text{SH} \\
\text{CH}_2\text{CH}_3
\end{align*}
\]

Figure 7.24. Marianne's representation of the product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion. Inversion of configuration in the product is correctly depicted in this diagram.

GL: "You're right. So how many bonds am I going to have to carbon?"

Marianne: "Five, right?"

GL: "That's right."

Marianne (drawing the transition state): "Oh, you can just do that?"

GL: "Yeah, do you have a choice?"

Marianne: "No. So it'd be like that?" Marianne's transition state attempted to illustrate back-side attack by the nucleophile but is not a trigonal bipyramid (Figure 7.25).

\[
\begin{align*}
\text{CH}_3 \text{SH} \\
\text{C} & \text{H} \\
\text{H} \\
\text{Cl} \\
\text{CH}_2\text{CH}_3
\end{align*}
\]

Figure 7.25. Marianne's representation of the transition state that forms on the reaction of (S)-2-chlorobutane with bisulfide ion.

Comparison of Findings Regarding \text{SN}2 Substitution in (S)-2-Chlorobutane. Two distinct strategies emerged when students were confronted with this problem. Some
students chose to reorient the reactant molecule in their drawings in order to place the leaving group in the plane of the paper. Others chose to draw approach of the nucleophile from behind the leaving group. Students who adopted the former strategy were more successful in drawing a satisfactory mechanism.

All of the participants described this mechanism as proceeding through a transition state, all of them knew that the nucleophile approached from the back side of the leaving group, and all of them described the resulting product in terms of inversion of configuration. This knowledge did not necessarily translate into the ability to satisfactorily draw the intermediate or the inverted product.

**Study of SN1 Substitution in (S)-2-Chlorobutane.** The next four questions of the fourth interview (Table 3.5, Questions 8 - 11) asked students about the mechanism of the SN2 reaction of bisulfide ion (the nucleophile) with the chiral reagent (S)-2-chlorobutane. The leaving group (chloride) is oriented in the same manner as in questions 4 - 7 (Table 3.5). This reaction proceeds through a planar carbocation intermediate (the sec-butyl carbocation), which could be depicted either flat on the page or perpendicular to it (Figure 7.26).

![Figure 7.26. Representations of a planar carbocation intermediate. (a) The carbocation written in the plane of the paper. (b) The carbocation written perpendicular to the plane of the paper.](image)

Because only one hour was allotted for this interview, only six students completed this set of questions. Each of the six students identified the reaction (Table 3.5, Question 8) using the term substitution and identified the nucleophile (bisulfide ion, HS⁻) and leaving group (chloride ion, Cl⁻). Five of the six participants easily recognized that the
mechanism of this reaction would be different from the mechanism of the reaction previously studied (Table 3.5, Question 4). James, however, did not immediately recognize the mechanism even though the reaction was clearly labeled "SN1."

JT: "Can I look at that one again?" (NB: the SN2 reaction, Table 3.5, question 4)

GL: "Yeah! The only difference is..."

JT: "What is the difference? I mean, they're the same things."

GL: "Just different mechanism."

James then reassembled the wooden models, said, "Okay, so I have this. And what it does first is, the leaving group leaves." Pointing to the intermediate, he continued, "So that would be flat." He then drew a diagram showing formation of the intermediate (Figure 7.27).

![Figure 7.27](image)

**Figure 7.27.** James' initial T-shaped representation of the sec-butyl carbocation intermediate. The bond angles in this diagram appear to be 90°; a more accurate representation would depict the intermediate as being trigonal planar.

GL: "What are the bond angles in that thing?"

James: "They're all going to be ninety degrees? Oh, it'll be ... oh, what is it called? I can do it here.... It's flat, but it's not ninety degrees. It's , 180 divided by 3 is ...

GL: "It's really 120 degrees, but is that what you have drawn there?"

James then redrew the intermediate (Figure 7.28) in a manner similar to Figure 7.26(a).

Michael described this mechanism very well. He initially said, "Okay, it goes through two steps. It goes through an intermediate, carbocation intermediate," pointed out the leaving group, and drew the intermediate (Figure 7.29).
Figure 7.28. James' final representation of the sec-butyl carbocation intermediate. The trigonal planar shape is accurately drawn with appropriate bond angles.

Figure 7.29. Michael's representation of the sec-butyl carbocation intermediate. This drawing illustrates the equal probability of approach of the nucleophile from either side.

When using the models, everyone else also removed the leaving group first (producing a planar carbocation intermediate) and then brought the nucleophile in.

Tammy described the mechanism as follows. "Okay, SN1 has two steps. So, okay, this is the nucleophile. And the one on the right's going to be the leaving group. Okay, so first I'm going to have the leaving group leave. And then the nucleophile can either enter from the left or it can enter from the right."

Andrea said that the mechanism "happens in two steps."

GL: "And, um, ..., what does that mean stereochemically? What kind of products are you going to get?"

Andrea: ...

GL: "I mean, is it going to ..."
AP: "Both inverted and, like not. Regular. Not inverted."

Brian and Anna described formation of the intermediate in similar terms. Both Tammy and Anna volunteered that the product would be racemic, and Brian and Anna both described the intermediate carbocation as having a positive charge. Tammy was somewhat unsure of the charge on the intermediate, describing it as "a carbocation??", and Andrea paused when asked if the intermediate had a charge. She was asked what she had removed, and said, "'Cause the leaving group left, so it'd be ... positive."

When using the models, most of the students also were able to describe why two enantiomers would be obtained from a chiral reactant. Looking at the planar intermediate, Brian said, "The nucleophile could come from this side, or it could come from the totally opposite side, with a fifty percent chance." Tammy said, "And the nucleophile can either enter from the left or it can enter from the right," and Andrea said, "You could either draw it with ... the nucleophile in the front, or it could be in the back. Right, yeah."

Anna removed the leaving group, saying, "Well, it's going to kind of go off into limbo, right now," looked at the planar intermediate, and said, "Now, I could go with the 'regular' product, with the nucleophile entering from the left." This was the side opposite from where the leaving group departed. She continued, "I get what looks like an inverted compound, or my nucleophile can go around and enter from the right, and enter the same spot where the leaving group was. And then I have retention."

Students were generally less successful when drawing the mechanism, and their verbal descriptions suffered as well. The most successful student was Michael, who drew a carbocation intermediate leading to a racemic mixture (Figure 7.29). Michael's intermediate was drawn in a plane perpendicular to the paper. Other students expressed reservations regarding their abilities to draw the mechanism on paper. Anna said, "All right. I'm not quite sure I'm going to be able ... that I'm going to know how to do it without a model." Anna attempted to draw a mechanism similar to Michael's, but her carbocation intermediate was T-shaped (Figure 7.30). When asked, "Is that the shape of
the carbocation?", she responded, "Um, no. I need to draw that sterically." She began to draw (Figure 7.31), looked at her diagram, and said, "Okay ... um ... that still doesn't look right." She heeded the suggestion that she "make the carbocation on the wooden model and see what it looks like," and drew the intermediate once again (Figure 7.32). Her final drawing appears to be a hybrid of the two extremes depicted in Figure 26.

![Figure 7.30. Anna's initial representation of the sec-butyl carbocation intermediate. Although the bonding is correct, the shape is not depicted as trigonal planar.](image)

![Figure 7.31. Anna's second representation of the sec-butyl carbocation intermediate. Because Anna had begun to portray the bond angles and then abandoned this diagram, most of the atoms are missing from this structure.](image)

![Figure 7.32. Anna's final representation of the sec-butyl carbocation intermediate. Anna has attempted to show both that the intermediate is trigonal planar and that it is to be depicted perpendicular to the plane of the paper.](image)

Both James and Brian also drew a T-shaped planar intermediate (Figures 7.27 and 7.33). James described his intermediate, saying, "It's flat, but it's not ninety degrees. It's, 180 divided by three is ..." Although the bond angle in the carbocation is actually 120 degrees (360 degrees divided by three), it was clear that James knew the actual shape.
but had not drawn it properly. Because his intermediate as drawn did not actually have 120° bond angles, he was asked what he had actually drawn.

Figure 7.33. Brian’s T-shaped representation of the sec-butyl carbocation intermediate.

GL: "But is that what you have drawn here?"
James: "It’s sixty? You want me to draw it like that?"

James then drew a planar intermediate with the appropriate 120° bond angles (Figure 7.28). Brian was also asked about his T-shaped intermediate. "Now, are the bond angles really ninety degrees like that?", and he replied, "No. I’d rather draw them like that than three dimensional. I can see it better."

Andrea’s intermediate was drawn well, and, like James’ intermediate, was drawn in the plane of her paper (Figure 7.34). Tammy drew an intermediate that might be described as “almost” in the plane of the paper, with solid lines connecting methyl and ethyl to the central carbon atom and a dashed line connecting the remaining hydrogen atom. Upon being asked about the shape of her intermediate, she corrected her drawing (Figure 7.35).

Figure 7.34. Andrea’s representation of the sec-butyl carbocation intermediate. This intermediate is correctly drawn as trigonal planar and depicted in the plane of the paper.
Figure 7.35. Tammy's corrected representation of the sec-butyl carbocation intermediate. This intermediate is trigonal planar and depicted in the plane of the paper.

GL: "Okay, that's very nice. Now I have one question to ask you. What's the shape of that intermediate?"

Tammy: "Trigonal planar."

GL: "Okay, what you have drawn there, is it trigonal planar?"

TB (correcting her drawing): "Um, oh, I should probably just have a straight line."

After drawing the intermediate, each student was asked to draw the racemic mixture of products. Two strategies emerged for drawing this set of enantiomers. These may be described as reflecting one structure in a mirror plane to form the second (Figure 7.36a) and exchanging the position of two substituents on the chiral center to form an enantiomer (Figure 7.36b). Although four of the six students drew this mixture correctly, only Michael and Anna drew the two products using the first strategy, thus clearly demonstrating that they were actually mirror images (Figures 7.37 and 7.38). The other two used the second strategy of exchanging the positions of substituents. Tammy simply exchanged the positions of the thiol and methyl substituents (Figure 7.39), and Andrea exchanged the positions of the thiol and hydrogen substituents (Figure 7.40).

James drew one of the products, (R)-2-butanethiol (Figure 7.41), and when attempting to draw the enantiomer, he said to himself, "Okay .... same thing ... think about this now...this one ... and now ... scratch that out, that's nothing." He began to draw the (R)-enantiomer again, crossed out the bond to his methyl group to the viewer's..."
right, and placed this methyl group to the viewer's left. This supposed enantiomer is not a true tetrahedron (Figure 7.42).

Figure 7.36. Two strategies for drawing mirror images. a) Reflecting one structure in a mirror plane. b) Exchanging the positions of two substituents.

Figure 7.37. Michael's representation of the racemic mixture of thiols that forms on the SN1 reaction of bisulfide ion with (S)-2-chlorobutane. These correctly-drawn structures are depicted as though they were actually reflected in a mirror.
Figure 7.38. Anna's representation of the racemic mixture of thiols that forms on the SnI reaction of bisulfide ion with (S)-2-chlorobutane. Like Michael's (Figure 7.37), these structures are depicted as though they were actually reflected in a mirror.

Figure 7.39. Tammy's representation of the racemic mixture of thiols that forms on the SnI reaction of bisulfide ion with (S)-2-chlorobutane. The second enantiomer was drawn from the first by exchanging the positions of the thiol (HS) and methyl (CH₃) groups.
Figure 7.40. Andrea's representation of the racemic mixture of thiols that forms on the SN1 reaction of bisulfide ion with (S)-2-chlorobutane. The second enantiomer was drawn from the first by exchanging the positions of the thiol (HS) and hydrogen (H).

Figure 7.41. James' first representation of (R)-2-butanethiol. This structure as drawn is tetrahedral around the central carbon atom.

Figure 7.42. James' final representation of (R)-2-butanethiol. This structure as drawn is not tetrahedral around the central carbon atom.
Finally, Brian did not use any three-dimensional conventions in drawing his products. It is clear that he wished to show that he had formed two different products, but as they are both drawn in a plane, it is not possible to draw any conclusions about their three-dimensional shapes (Figure 7.43).

\[
\begin{align*}
\text{CH}_3 & \quad \text{CH}_3 \\
HS & \quad C \quad C\text{H}_2\text{CH}_3 \\
\text{H} & \quad \text{H} \\
\end{align*}
\]

Figure 7.43. Brian's representation of the racemic product that forms on the reaction of (S)-2-chlorobutane with bisulfide ion under $S_N1$ conditions. Brian has not attempted to illustrate the configuration around the central carbon atom in his drawings.

Comparison of Findings Regarding $S_N1$ Substitution in (S)-2-Chlorobutane.

Having previously worked with the $S_N2$ substitution reaction of bisulfide ion with (S)-2-chlorobutane, all of the students easily identified this reaction (Table 3.5, Question 4) as another substitution reaction. When using the models, the students readily removed the leaving group, described the shape of the intermediate, and subsequently brought the nucleophile in from either side to form a racemic product. Translating these ideas to paper was more difficult. Because the intermediate is planar, its trigonal planar shape can accurately be depicted on a piece of paper without the use of dash or wedge. However, several students had difficulties drawing this intermediate. Some drew it using a T-shape. Despite describing the intermediate using the terms "planar" or "trigonal planar," others attempted to draw it with at least one substituent pointing out of the plane of the molecule.

Students who initially drew the intermediate perpendicular to the plane of the paper were generally more successful in subsequently drawing the proper stereochemistry of the products than were students who drew the intermediate in the plane of the paper. Two strategies could be seen when drawing the racemic product. Two students drew the
two enantiomers as though they were actually reflecting each other in a mirror plane. Others drew one enantiomer and then interchange two substituents to form its mirror image. These two strategies are illustrated in Figure 7.36.

Modeling an E2 Elimination. The last set of questions (Table 3.5, Questions 12 - 15) asked about the E2 elimination of hydrogen chloride from (S)-2-chlorobutane (Table 3.5, Question 12). Students were taught that elimination reactions such as this proceed according to Saytzeff's rule, giving the most highly substituted product (Bailey & Bailey, 1995). According to what the students had been taught, the product of this reaction should consist of a mixture of cis- and trans-2-butene isomers, with little 1-butene present.

For cis- and trans-2-butene to form, the molecule must adopt a conformation such that either the hydrogen atom labeled Hₐ or the hydrogen labeled Hₖ is antiperiplanar to the chlorine atom (Table 3.5, Question 12). Elimination of the chlorine atom and Hₖ yields cis-2-butene, whereas elimination of the chlorine atom and Hₐ yields trans-2-butene. These conformations (shown as Newman projections) and their respective elimination products are illustrated in Figure 7.44. Although the mechanism of this reaction was taught to these students, the idea that one conformation led to the cis isomer and the other led to the trans isomer was not presented as part of the coursework.

Identifying the E2 reaction type. Without much hesitation, most of the participants said that this was an elimination reaction (Table 3.5, Question 12). Marianne said, "...I don't know. You mean, like, elimination?", and Brian initially hesitated before committing himself, but everyone else confidently stated that the reaction was an elimination. Andrea said that it was elimination "because it's E2" and James said, "It's easy because you've got an 'E' right here."

Identifying the E2 Reaction Product. Recognizing that the reaction was elimination did not imply that everyone would identify either what atoms would eliminate or what class of compound would form (Table 3.5, Questions 13, 14). Only Michael and David
initially identified the chlorine and a vicinal hydrogen as the atoms that would eliminate and clearly stated that the product would be an alkene. Everyone else experienced some type of difficulty. Tammy and Brian both recognized that hydrogen and halogen both were eliminated, but when asked what class of compound would form, Tammy hesitated.

\[
\text{a) } \begin{array}{c}
\text{CH}_3 \\
\text{H} \\
\text{H}_b \\
\text{H}_a \\
\text{Cl} \\
\text{CH}_3
\end{array}
\quad \begin{array}{c}
\text{OCH}_2\text{CH}_3 \\
\text{E2}
\end{array}
\quad \begin{array}{c}
\text{H}_3\text{C} \\
\text{C} \\
\text{CH}_3 \\
\text{H} \\
\text{H}
\end{array}
\]

\[
\text{b) } \begin{array}{c}
\text{CH}_3 \\
\text{H} \\
\text{H}_b \\
\text{H}_a \\
\text{Cl} \\
\text{CH}_3
\end{array}
\quad \begin{array}{c}
\text{OCH}_2\text{CH}_3 \\
\text{E2}
\end{array}
\quad \begin{array}{c}
\text{H}_3\text{C} \\
\text{C} \\
\text{CH}_3 \\
\text{H} \\
\text{H}
\end{array}
\]

Figure 7.44. Formation of cis- and trans-2-butene by elimination of chlorine and hydrogen. Elimination of $H_a$ yields the cis product, and elimination of $H_b$ yields the trans product.

GL: "Okay, what kind of product am I going to get?"

Tammy: (quizzical look)

GL: "Just what class of compound is going to form?"

Tammy: "Um, like it'll go through a transition state..."

GL: "I mean, will it be an alkane, an alkene, an alcohol, what class? An ether..."

Tammy: "Okay, um, it's going to be an alkene."
Brian identified the product as "Um ... an alcohol."

GL: "It's elimination, remember?"

Brian: "Oh, yeah. Alkene. Yeah, it's going to form a double bond."

He then pointed to the location where the new double bond would form.

Four students (James, Marianne, Andrea, and Anna) attempted to remove only the chlorine. When asked, "What kind of compound am I going to get?", Anna sighed and said, "I don't like eliminations." When further asked what was eliminated, she responded, "...Um, I think it's the halogen."

GL: "The halogen, okay. Do you eliminate an atom or a molecule?"

Anna: "... We're just eliminating an atom."

GL: "Okay, can I just eliminate one atom? I'm not going to do a substitution."

Anna: "Am I going to get rid of water here?"

GL: "Well, is there any way to get rid of water off an alkyl halide?"

Anna: "No, not off an alkyl halide."

GL: "I'm going to eliminate a small molecule that has chlorine in it. What's got to be attached to that chlorine? I can't just eliminate chlorine, right?"

Anna pointed to a vicinal hydrogen and said, "Right. That hydrogen, I believe, is going to go with it." At this point, Anna still had difficulty identifying the class of compound that would form, and she questioned herself. "Um, when I eliminate HCl, the kind of species that's going to form?"

GL: "We're thinking about Saytzeff's rule here."

Anna: "Oh, okay. Um, that has to do with, we want the more highly substituted species to form." When then asked to clarify this, she apologized and then said, "Um, carbocation. No, no..." She was finally asked if the product was an alkane, alkene, or alkyne, and she agreed that it would be an alkene.

Marianne, Andrea, and James had similar problems. They all stated that chlorine would be eliminated, but were unwilling to choose to eliminate a hydrogen atom along
with it. All of them needed encouragement to eliminate a hydrogen atom. When Marianne finally said, "Probably an 'H'" and pointed to the correct hydrogen atoms. But she then identified the product as "an alkane."

**GL:** "Is it an alkane? Are there enough atoms to make an alkane?"

**Marianne:** "Alkene!"

Like Marianne, Andrea hesitated, finally identified the atoms eliminated as hydrogen and chlorine, pointed to the correct hydrogen atoms, and then identified the product as "an alkane?" She then corrected herself, saying, "An alkene?" James' experience was similar.

Like Anna, Kathy attempted to eliminate a water molecule from the alkyl halide.

**GL:** "What's going to leave; what's going to eliminate?"

**Kathy:** "Your Cl and an H." She attempted to remove chlorine and hydrogen from the same carbon atom, producing the partially-completed structure shown in Figure 7.45.

**GL:** "What are you going to form?"

![Figure 7.45](image)

**Kathy:** "It's going to form water."

**GL:** "To form water?"

Pointing to the ethoxide ion, Kathy said, "Yeah, with the '-OH'."

**GL:** "What's the 'Cl' going to do?"

**Kathy** (laughing): "It'll go off in bye-bye land!"
Pointing to the structure she had drawn (Figure 7.45), Kathy was then asked, "How many bonds to carbon do you have right now?"

Kathy: "Way too many!"

GL: "How many do you have?"

Kathy: "I have five." She agreed that she needed only four. When asked how she could "get around that problem," she responded, "Eliminating this hydrogen." She then eliminated the hydrogen designated "Ha" and produced a correct structure for the product (Figure 7.46).

![Image](image_url)

Figure 7.46. Kathy's final representation of the elimination product that forms on the reaction of (S)-2-chlorobutane with ethoxide ion.

Like Kathy, several other students had some difficulty drawing the structure of the product. Some students were unsure of the role of the ethoxide ion. Tammy and Michael both identified the ethoxide as a nucleophile. Attempting to draw the product, Tammy stated, "First I need to find like the nucleophile," and identified it as the ethoxide ion. She hesitated and called the ethoxide ion "a catalyst?", and when asked with what atom the ethoxide would react, she replied, "chloride?".

Tammy was told that the reaction was elimination, not substitution, and she replied that she knew a double bond should form. When told that ethoxide was a base, she was remained reluctant to use this base to remove a hydrogen ion from the reactant. Like Kathy, she ultimately attempted to remove the hydrogen atom geminal to the halide, but agreed that this would not help her in attempting to form a double bond.
Michael correctly positioned the double bond according to Saytzeff's rule to form the more highly substituted alkene and correctly described why he had done so, but in addition, he removed a second hydrogen atom and replaced it with an ethoxy group. He finally crossed out his extraneous ethoxy group to produce the structure shown in Figure 7.47. Everyone else drew either the cis- or trans-isomer of 2-butene as the product, although Marianne drew a product that was not planar around the double bond (Figure 7.48). She was asked to build a model of her product, and successfully built a model of trans-2-butene. When asked, "Is it three-dimensional?", she said, "No ... It's flat!" She drew a flat molecule with bond angles of ninety degrees (Figure 7.49), and when questioned about this, she agreed that the ninety degree angles she had drawn did not match the bond angles in the model and finally drew a structure with appropriate bond angles (Figure 7.50).

Figure 7.47. Michael's initial representation of the elimination product that forms on the reaction of ethoxide ion with (S)-2-chlorobutane. The extraneous ethoxy group is in the upper right corner of the diagram.

Figure 7.48. Marianne's initial representation of trans-2-butene. The structure illustrated is not planar.

Products of the E2 Elimination. James initially said that the major product, 2-butene, did not exhibit cis-trans isomerism. Brian initially stated that only the cis isomer would
Figure 7.49. Marianne's second representation of \textit{trans}-2-butene. Although planar, this structure does not correspond to the shape of the actual molecule.

Figure 7.50. Marianne's final representation of \textit{trans}-2-butene. This planar structure corresponds to the actual shape of the molecule.

form. James reasoned that the product did not exhibit cis-trans isomerism because "You can't rotate around the double bond." He had drawn a condensed formula (Figure 7.51); when encouraged to draw a dash formula (Figure 7.52), he then agreed that two isomers were feasible. Brian was not able to elucidate a reason that only the cis isomer formed. Everyone else stated that formation of both \textit{cis}- and \textit{trans}-2-butene would occur. When subsequently asked what difference it made whether the hydrogen atoms marked 'a' or 'b' eliminated (H\textsubscript{a} or H\textsubscript{b}, Table 3.5, Question 12) the most common reactions were either to state that it didn't matter or to pick up a set of models and begin to investigate. Anna investigated this question through the use of models.

Figure 7.51. James' condensed formula of 2-butene. On viewing this structure, James stated that cis-trans isomerism was not possible in 2-butene.
GL: "If you wanted to eliminate hydrogen "a," what has to happen?"
Anna: "Wait a minute. No, wait. No, if I'm eliminating the chlorine, it would need to be hydrogen 'b'."
GL: "The way you have it held right there, right?"
Anna: "Right"
GL: "Now, is there any way you could eliminate hydrogen 'a'?"
Anna: "Mm hmm. If, if I eliminated the hydrogen on the other carbon."

Although some students clearly stated that elimination could only occur when a hydrogen atom was anti-periplanar to the chlorine atom (the commonly used phrase was "elimination occurs anti"), they had difficulty orienting their models in this manner. Others simply forgot that this conformation was necessary for elimination. Anna had built a model in which the substituents around the C-C bond were in an eclipsed conformation.

GL: "If I have it just like you have it here, where this is eclipsed, can elimination occur now?"
Anna: "Um, no, I think that ... I want to say that they need to be staggered."
GL: "You are right. And what else has to happen?"
Anna: Um, ew!

GL: "Besides being staggered, what else has to happen?"

Anna: ...

GL: "Could elimination occur from either of those hydrogens right now, or just from one of them?"

Anna: "Well, it could occur from either."

GL: "Okay, does the term "antiperiplanar" mean anything to you?"

Anna: "Oh, yeah, yes it does! Antiperiplanar. Okay, it needs to be pointing opposite from the other hydrogen. So, okay, hydrogen 'a' would have to be the one."

Michael, who otherwise did this elimination flawlessly, oriented his model in such a manner that $H_a$ was antiperiplanar to the chlorine atom while he was attempting to eliminate $H_b$. When then asked, "What has to be anti?", he was puzzled, and responded, "Oh, it has to be this one?" Like Anna, he originally thought that either hydrogen atom could eliminate when one of them was antiperiplanar to the chlorine.

Once halogen and either $H_a$ or $H_b$ were oriented in an antiperiplanar conformation, the subject then had to determine which geometric isomer would form as a product. Several participants stated that the product would always be trans-2-butene no matter which hydrogen atom, $H_a$ or $H_b$, was eliminated. Brian's reasoning was that the atoms being eliminated were oriented "one up and one down," and when asked what he was pointing at "that's up and down," he confirmed that he was looking at the atoms being eliminated rather than the substituents that would remain. When encouraged to instead look at what remained in the product, he decided to focus on the terminal methyl groups, and then concluded that elimination of $H_a$ and the chlorine atom would give the cis product whereas elimination of $H_b$ and chlorine yields the trans product.

Having correlated elimination of one hydrogen atom with formation of one geometric isomer did not mean that a subject automatically associated elimination of the other hydrogen atom with formation of the other isomer. Only after investigation of both
antiperiplanar conformers leading to elimination were most of the subjects confident that
elimination of H\textsubscript{A} led to the cis product and corresponding elimination of H\textsubscript{B} gave the trans.

Most students felt that they could not have done this without the use of models. When asked what he would do without models, David candidly said, "Quite honestly, I'd have to guess." When asked to draw this reaction on paper, only Andrea initially chose to use Newman projections (Figure 7.53), saying "I couldn't think of any other way to draw it." More common was the use of dash-and-wedge structures such as that initially drawn by Michael (Figure 7.54). Michael's reaction was typical; when it was suggested that he instead draw a Newman projection, he responded that it was indeed much easier to visualize this elimination using this type of drawing.

Figure 7.53. Andrea's Newman projections of (S)-2-chlorobutane, showing the chlorine and hydrogen atoms in an antiperiplanar conformation.

Figure 7.54. Michael's dash-and-wedge representation of (S)-2-chlorobutane, showing hydrogen and chlorine in an antiperiplanar conformation.
After the exercise was complete, several students attempted to identify the product as a mixture of enantiomers, although when asked if the product contained a chiral atom, each participant immediately recognized that it did not. A common question was whether each geometric isomer formed in equal amounts, in a manner analogous to the formation of an equimolar mixture of enantiomers by $S_N1$ substitution. Brian asked, "Okay, is that a 50-50 chance for that, too?" When asked if the products were enantiomers, he agreed that they were not, and concluded that he could not tell whether or not an equimolar mixture of products would form.

**Summary of Results from Fourth Interview.** Four broad categories of difficulties and learning strategies regarding the relationships between stereochemistry and chemical reactions and mechanisms among beginning organic chemistry students emerged from this interview. These were termed "association of stereochemistry and mechanism," "rote rules and reorientation," "what students say vs. what they do," and "bond making and bond breaking." The first category includes those difficulties experienced by students when they attempt to visualize and describe the stereochemistry of the product when using a given mechanism. The second category describes the difficulties encountered by students when they attempt to apply rote rules regarding the depiction and reorientation of three dimensional structures on a two-dimensional surface. The third category includes any statements about rotation and shapes of molecules or chemical processes that vary from what students draw or depict with models. The last category involves those difficulties encountered by students when they are required to demonstrate bond making and bond breaking in chemical reactions. These four categories are described and summarized in Table 7.1.
Table 7.1. Difficulties in Learning Derived from the Fourth Interview.

I) Association of stereochemistry and mechanism
   A) SN1 substitution
      1) Forming the planar intermediate
         a) Some students indicate that the leaving group cannot depart
            unless forced away by the nucleophile.
         b) Students frequently do not associate departure of leaving group
            with formation of a planar intermediate.
      2) Reaction of the planar intermediate
         a) After forming a planar carbocation intermediate, students
            indicate that there must be a preference for one side or the other in
            nucleophilic attack. Students can make up several reasons for this,
            mostly involving the supposed preference of one side or the other
            for bearing the positive charge.
         b) Students do not readily associate the necessity of having a
            planar intermediate to the formation of equal amounts of
            enantiomeric products.
         c) Students who do not draw the planar intermediate perpendicular
            to the plane of the paper have more difficulty visualizing the
            stereochemistry of the resulting product.
   B) SN2 substitution
      1) Some students are not able to correlate approach of the nucleophile
         from the back side with inversion of configuration.
      2) Some students do not correlate inversion of configuration with
         formation of a mirror image.
   C) E2 elimination
      1) Students tend to focus on the atoms that are eliminated rather than those
         remaining when determining which geometric isomer forms. Students
         who do this always state that the resulting geometric isomer is trans.
         Some students indicate that as long as any hydrogen atom on a vicinal
         carbon atom is antiperiplanar to the leaving group (e.g. halogen), a
         hydrogen atom that is gauche to the halogen can be removed.
      2) Some students indicate that elimination of any vicinal hydrogen can
         yield either the cis or trans product.

II) Rote rules and reorientation
   A) Unwillingness to rotate when using rote rules
      1) Students will reorient structures to facilitate viewing the process of
         substitution but will still fail to place the leaving group 180 degrees from
         the approaching nucleophile.
      2) A nucleophile such as bisulfide ion will be drawn the same way (HS- instead of SH- or SH). Students will then draw a structure with a C-H-S
         bond.
      3) In describing the SN2 mechanism, students often use whatever
         substituent that is drawn ISO degrees from the nucleophile as the leaving
         group.
      4) When describing E2 elimination, students will say that only one
         geometric isomer forms "because you can't rotate around a double bond."
      5) Students are reluctant to rotate molecules to facilitate drawing a
         mechanism.
      6) Students tend to reorient tetrahedral structures by switching two pairs
         of substituents instead of by rotating the structure.

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Table 7.1 (cont.).

B) Rote rules and difficulties with complex structures

1) Students sometimes assume that cis and trans geometric isomers form in equimolar amounts in E2 elimination.
2) When students use a switching rule to form enantiomers, they will be troubled about which two substituents to choose. Substituents on a tetrahedron may be described as "catty-corner" to each other.
3) When attempting to draw enantiomers, some students will abandon use of stereochemical conventions.
4) When chiral molecules are oriented in unusual positions, some students will redraw them in a way to eliminate any stereochemical designations.

III) What students say vs. what they do

A) What they say about rotation

1) A student may say that "elimination occurs anti," but fail to rotate the molecule to form a conformer in which the leaving groups are antiperiplanar.
2) When describing the S_N2 mechanism, students will identify a good leaving group on a structure, but will not rotate the structure in order to use it. Instead, whatever substituent that is drawn 180 degrees from the approaching nucleophile will be forced to leave.

B) What they say about shapes

1) Carbocation intermediates may be drawn T-shaped even if their shape is described as trigonal planar.
2) Some students will describe the S_N2 product as having inverted configuration, but draw it with retained configuration.

C) What they say about processes

1) Given a static model, some students will attempt to demonstrate the S_N2 mechanism without inverting the configuration of the product. Instead, they just substitute nucleophile for leaving group.
2) When describing the S_N1 mechanism, a student may say that a racemic mixture forms from a chiral reactant but will only draw one chiral product.

IV) Bond making and bond breaking

A) Elimination

1) When describing E2 elimination in alkyl halides, students will frequently attempt to eliminate only one atom (e.g. halogen without hydrogen).
2) When describing E2 elimination in alkyl halides, students are sometimes unable to describe the product as containing a new double bond and instead describe the product as an alkane.

B) Substitution

1) After describing both S_N1 and S_N2 mechanisms, some students will say that they are "really the same."
2) In describing substitution reactions, some students will attempt to build the nucleophile into the reactant.
3) Students will identify the nucleophile as a moiety already attached to the chiral center before reaction occurs, and are unsure that the nucleophile is a separate species.

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RESULTS FROM CONCEPT MAPS

Analysis of Concept Maps. Each of the concept maps from both the Fall, 1997 and Spring, 1998 semesters was analyzed through the use of various nonparametric statistical tests. The superordinate concepts for each map were tabulated and the percent occurrence of each superordinate concept was calculated. An ordinal rank was then assigned to each seed concept on each student map based on the level in the map at which the concept was found. If two or more concepts occurred at the same level, a tie was assigned. For example, if the seed concept "hydrocarbon" were found at the highest level in a given map, and the terms "alkane" and "alkene" both were found at the next level, then "hydrocarbon" would be assigned a value of 1.0, whereas "alkane" and "alkene", being tied, would both be assigned a value of 2.5. Both the Kendall coefficient of concordance (W) and the level of significance were calculated for each set of concept maps. Finally, each pair of concepts in a given set of maps was analyzed by a similar procedure, yielding a relative rank for each concept in the pair, a value for W, and a significance level. These data were tabulated for each set of concept maps. Calculations were performed using the Statistical Package for the Social Sciences™ (SPSS), and appear in Tables 8.1, 8.2, 8.3, 8.6, 8.7, 8.8, 8.11, 8.12, 8.15, 8.16, 8.19, 8.20, 8.21, 8.24, 8.25, 8.26, 8.27, 8.28, 8.31, 8.32, 8.33, 8.36, 8.37, 8.38, 8.41, 8.42, 8.43, 8.46, 8.47, 8.48, 8.51, 8.52, and 8.53. The relative rankings were used as an indication of which seed concepts were perceived as most general or most specific by the classes as a whole, and Kendall's W was used as a measure of the concordance of individual classes with regards to the hierarchical placement of the seed concepts.

Each concept map was also qualitatively analyzed for difficulties as follows. Each proposition within a concept map was evaluated for its scientific accuracy. In addition, propositions within a map were compared to each other, because at times two or more propositions within a given concept map were contradictory. Propositions leading to difficulties were tabulated and categorized by type. Duplicate difficulties (occurring in
more than one student map) were discarded. The resulting categories of difficulties are given in Tables 8.4, 8.9, 8.13, 8.17, 8.22, 8.29, 8.34, 8.39, 8.44, 8.49, and 8.54. Examples of difficulties deemed as being most interesting or significant were tabulated and are listed in Tables 8.5, 8.10, 8.14, 8.18, 8.23, 8.30, 8.35, 8.40, 8.45, 8.50, and 8.55. Each example is referenced by type to its corresponding table of categories. Any and all difficulties identified were listed and tabulated, whether or not they dealt directly with the learning of stereochemistry.

Results of Concept Map 1. Concept map 1, which had the seed concepts "alkane", "alkene", "alkyne", "hydrocarbon", and "multiple bond", was assigned as the first concept map in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of superordinate concept for this map was "hydrocarbon" (88.2% and 95.1% of respondents, respectively). Analysis of concordance of ordinal rank of these concepts for each semester gave values of Kendall's W of .6030 and .6368, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.1, 8.2, and 8.3.

Qualitative analysis of the concept maps yielded four major types of propositions. First were conceptions that were interesting or unusual but not necessarily incorrect. Next were difficulties regarding chemical bonds. The third type of difficulty identified dealt with the differences between saturated and unsaturated compounds, and the last type of alternative conception dealt with isomers. These types are listed in Table 8.4, with specific examples given in Table 8.5.

Results of Concept Map 2. Concept map 2, which had the seed concepts "conformer", "equilibrium", "staggered", "eclipsed", and "rotation", was assigned as the second concept map in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of superordinate concept for this map was "conformer" or "conformational isomer" (74.6% and 91.3% of respondents, respectively). Analysis of concordance of ordinal rank of these concepts for each semester gave values of Kendall's W of .6030 and .6368, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.1, 8.2, and 8.3.

Qualitative analysis of the concept maps yielded four major types of propositions. First were conceptions that were interesting or unusual but not necessarily incorrect. Next were difficulties regarding chemical bonds. The third type of difficulty identified dealt with the differences between saturated and unsaturated compounds, and the last type of alternative conception dealt with isomers. These types are listed in Table 8.4, with specific examples given in Table 8.5.
### Table 8.1. Statistical Analysis of Concept Map 1.

Seed concepts: alkane, alkene, alkyne, hydrocarbon, multiple bond

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Percent of students choosing concept</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrocarbon</td>
<td></td>
<td>88.2%</td>
<td>95.1%</td>
</tr>
<tr>
<td>alkane</td>
<td></td>
<td>4.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>alkene</td>
<td></td>
<td>1.6%</td>
<td>0.0%</td>
</tr>
<tr>
<td>organic compound(s)</td>
<td></td>
<td>1.6%</td>
<td>0.0%</td>
</tr>
<tr>
<td>others(^b)</td>
<td></td>
<td>3.9%</td>
<td>0.0%</td>
</tr>
<tr>
<td>unclear choice(^c)</td>
<td></td>
<td>0.0%</td>
<td>4.9%</td>
</tr>
</tbody>
</table>

#### Mean rank of seed concept

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrocarbon</td>
<td>1.09</td>
<td>1.00</td>
</tr>
<tr>
<td>alkane</td>
<td>3.06</td>
<td>3.02</td>
</tr>
<tr>
<td>multiple bond</td>
<td>3.22</td>
<td>3.36</td>
</tr>
<tr>
<td>alkene</td>
<td>3.80</td>
<td>3.81</td>
</tr>
<tr>
<td>alkyne</td>
<td>3.82</td>
<td>3.81</td>
</tr>
</tbody>
</table>

#### Statistic Value

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(W^d)</td>
<td>.6030</td>
<td>.6368</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

\(^a\) Represents 127 concept maps from Fall, 1997 and 81 concept maps from Spring, 1998.

\(^b\) Represents concepts chosen by only one participant.

\(^c\) Represents maps without a clear superordinate concept.

\(^d\) Represents the Kendall coefficient of concordance.
Table 8.2. Individual Statistical Comparisons of Seed Concepts from Map 1 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrocarbon</td>
<td>1.04</td>
<td>alkane</td>
<td>1.96</td>
<td>.8336</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.02</td>
<td>multiple bond</td>
<td>1.98</td>
<td>.9230</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.01</td>
<td>alkene</td>
<td>1.99</td>
<td>.9568</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.01</td>
<td>alkyne</td>
<td>1.99</td>
<td>.9568</td>
<td>.0000</td>
</tr>
<tr>
<td>alkane</td>
<td>1.53</td>
<td>multiple bond</td>
<td>1.47</td>
<td>.0037</td>
<td>.5128</td>
</tr>
<tr>
<td>alkane</td>
<td>1.29</td>
<td>alkene</td>
<td>1.71</td>
<td>.3578</td>
<td>.0000</td>
</tr>
<tr>
<td>alkane</td>
<td>1.29</td>
<td>alkyne</td>
<td>1.71</td>
<td>.3663</td>
<td>.0000</td>
</tr>
<tr>
<td>multiple bond</td>
<td>1.39</td>
<td>alkene</td>
<td>1.61</td>
<td>.0576</td>
<td>.0100</td>
</tr>
<tr>
<td>multiple bond</td>
<td>1.38</td>
<td>alkyne</td>
<td>1.62</td>
<td>.0628</td>
<td>.0072</td>
</tr>
<tr>
<td>alkene</td>
<td>1.50</td>
<td>alkyne</td>
<td>1.50</td>
<td>.0085</td>
<td>.3218</td>
</tr>
</tbody>
</table>

Table 8.3. Individual Statistical Comparisons of Seed Concepts from Map 1 for the Spring, 1998 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrocarbon</td>
<td>1.00</td>
<td>alkane</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.00</td>
<td>multiple bond</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.00</td>
<td>alkene</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>hydrocarbon</td>
<td>1.00</td>
<td>alkyne</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>alkane</td>
<td>1.47</td>
<td>multiple bond</td>
<td>1.53</td>
<td>.0045</td>
<td>.5586</td>
</tr>
<tr>
<td>alkane</td>
<td>1.27</td>
<td>alkene</td>
<td>1.73</td>
<td>.4545</td>
<td>.0000</td>
</tr>
<tr>
<td>alkane</td>
<td>1.27</td>
<td>alkyne</td>
<td>1.73</td>
<td>.4545</td>
<td>.0000</td>
</tr>
<tr>
<td>multiple bond</td>
<td>1.42</td>
<td>alkene</td>
<td>1.58</td>
<td>.0282</td>
<td>.1725</td>
</tr>
<tr>
<td>multiple bond</td>
<td>1.42</td>
<td>alkyne</td>
<td>1.58</td>
<td>.0292</td>
<td>.1725</td>
</tr>
<tr>
<td>alkene</td>
<td>1.50</td>
<td>alkyne</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

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Table 8.4. Types of Propositions and Difficulties Identified from Concept Map 1.

I) Interesting/unusual but not incorrect.
II) Problems with bonding.
   A) Factual problems
   B) Grammatical problems.
III) Problems with saturated and unsaturated.
   A) Factual problems
   B) Grammatical problems.
IV) Problems with isomers
   A) Factual problems.
   B) Grammatical problems.

Table 8.5. Selected Difficulties Identified From Concept Map 1.

<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Hydrocarbon formed from decayed plants and animals.</td>
</tr>
<tr>
<td>I</td>
<td>(Superordinate concept is &quot;Shared electron pairs.&quot;)</td>
</tr>
<tr>
<td>IIA</td>
<td>A hydrocarbon as a chain with one open end is an alkyl group.</td>
</tr>
<tr>
<td>IIB</td>
<td>An alkyne has no single bonds.</td>
</tr>
<tr>
<td>IIB</td>
<td>Hydrocarbons ... must have one double bond include alkynes.</td>
</tr>
<tr>
<td>IIB</td>
<td>Hydrocarbons with carbon-carbon single bonds are alkanes that can be alkenes.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Alkane is a saturated hydrocarbon, base for alkene, base for alkyne.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Saturated hydrocarbons also can be alkene forms double bonds.</td>
</tr>
<tr>
<td>IVA</td>
<td>Hydrocarbons create isomers.</td>
</tr>
<tr>
<td>IVB</td>
<td>Structural formulas can contain hydrocarbons.</td>
</tr>
</tbody>
</table>

*a Item in parentheses is summarized from individual concept maps.

*b Refers to difficulty type identified in Table 8.4.
W of .6368 and .7155, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.6, 8.7, and 8.8.

Qualitative analysis of the concept maps yielded four major types of conceptions. These major types of difficulties were problems involving rotation, problems involving equilibrium, problems involving conformer extremes, and problems involving the definition of conformer. These types are listed in Table 8.9, with specific examples given in Table 8.10.

**Results of Concept Map 3.** Concept map 3, which had the seed concepts "isomer", "structural isomer", "stereoisomer", "geometric isomer", and "conformer", was only assigned in the Spring, 1998, semester. The first choice of superordinate concept for this map was one of the related terms "isomer", "isomers" or "isomerism" (88.9% of respondents). Analysis of concordance of ordinal rank of these concepts for each semester gave a values of Kendall's W of .7380, which is significant at the .0000 level. Results of these calculations are given in Tables 8.11 and 8.12.

Qualitative analysis of this concept maps yielded five major types of conceptions. First were conceptions that were interesting or unusual but not necessarily incorrect. Next were difficulties involving molecular and structural formulas, difficulties involving conformers, difficulties involving the nature of geometric isomers, and finally some other difficulties involving isomers. These types are listed in Table 8.13, with specific examples given in Table 8.14.

**Results of Concept Map 4.** Concept map 4, which had the seed concepts "reaction", "substitution", "elimination", and "addition", was only assigned in the Spring, 1998, semester. The first choice of superordinate concept for this map was one of the related terms "reaction" or "organic reaction" (79.3% of respondents). Analysis of concordance of ordinal rank of these concepts for each semester gave a values of Kendall's W of .9703, which is significant at the .0000 level. Results of these calculations are given in Tables 8.15 and 8.16.
Table 8.6. Statistical Analysis of Concept Map 2.

Seed concepts: conformer, equilibrium, staggered, eclipsed, rotation

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Percent of students choosing concept</th>
<th>Fall 1997a</th>
<th>Spring 1998a</th>
</tr>
</thead>
<tbody>
<tr>
<td>conformer(s)/conformational isomers</td>
<td>74.6 %</td>
<td>91.3%</td>
<td></td>
</tr>
<tr>
<td>isomer(s)/isomerism</td>
<td>13.8%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>stereoisomers</td>
<td>3.8%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>othersb</td>
<td>6.9%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>unclearc</td>
<td>0.9%</td>
<td>1.2%</td>
<td></td>
</tr>
</tbody>
</table>

Mean rank of seed concept

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Fall 1997a</th>
<th>Spring 1998a</th>
</tr>
</thead>
<tbody>
<tr>
<td>conformer</td>
<td>1.10</td>
<td>1.01</td>
</tr>
<tr>
<td>rotation</td>
<td>2.68</td>
<td>2.58</td>
</tr>
<tr>
<td>staggered</td>
<td>3.48</td>
<td>3.48</td>
</tr>
<tr>
<td>eclipsed</td>
<td>3.54</td>
<td>3.49</td>
</tr>
<tr>
<td>equilibrium</td>
<td>4.20</td>
<td>4.44</td>
</tr>
</tbody>
</table>

Statistic  

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997a</th>
<th>Spring 1998a</th>
</tr>
</thead>
<tbody>
<tr>
<td>WD</td>
<td>.6368</td>
<td>.7155</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

aRepresents 130 concept maps from Fall, 1997 and 80 concept maps from Spring, 1998.
bRepresents concepts chosen by only one participant.
cRepresents maps without a clear superordinate concept.
dRepresents the Kendall coefficient of concordance.
Table 8.7. Individual Statistical Comparisons of Seed Concepts from Map 2 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>conformer</td>
<td>1.04</td>
<td>rotation</td>
<td>1.96</td>
<td>.8403</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.02</td>
<td>staggered</td>
<td>1.98</td>
<td>.9484</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.02</td>
<td>eclipsed</td>
<td>1.98</td>
<td>.9484</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.03</td>
<td>equilibrium</td>
<td>1.97</td>
<td>.9080</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.25</td>
<td>staggered</td>
<td>1.75</td>
<td>.3077</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.24</td>
<td>eclipsed</td>
<td>1.76</td>
<td>.3255</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.23</td>
<td>equilibrium</td>
<td>1.77</td>
<td>.3275</td>
<td>.0000</td>
</tr>
<tr>
<td>staggered</td>
<td>1.48</td>
<td>eclipsed</td>
<td>1.52</td>
<td>.0312</td>
<td>.0833</td>
</tr>
<tr>
<td>staggered</td>
<td>1.27</td>
<td>equilibrium</td>
<td>1.73</td>
<td>.2604</td>
<td>.0000</td>
</tr>
<tr>
<td>eclipsed</td>
<td>1.28</td>
<td>equilibrium</td>
<td>1.72</td>
<td>.2297</td>
<td>.0000</td>
</tr>
</tbody>
</table>

Table 8.8. Individual Statistical Comparisons of Seed Concepts from Map 2 for the Spring, 1998 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>conformer</td>
<td>1.01</td>
<td>rotation</td>
<td>1.00</td>
<td>.9429</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.00</td>
<td>staggered</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.00</td>
<td>eclipsed</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.00</td>
<td>equilibrium</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.22</td>
<td>staggered</td>
<td>1.78</td>
<td>.3270</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.22</td>
<td>eclipsed</td>
<td>1.78</td>
<td>.3391</td>
<td>.0000</td>
</tr>
<tr>
<td>rotation</td>
<td>1.85</td>
<td>equilibrium</td>
<td>1.15</td>
<td>.5386</td>
<td>.0000</td>
</tr>
<tr>
<td>staggered</td>
<td>1.50</td>
<td>eclipsed</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>staggered</td>
<td>1.20</td>
<td>equilibrium</td>
<td>1.80</td>
<td>.3636</td>
<td>.0000</td>
</tr>
<tr>
<td>eclipsed</td>
<td>1.20</td>
<td>equilibrium</td>
<td>1.80</td>
<td>.3748</td>
<td>.0000</td>
</tr>
</tbody>
</table>

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Table 8.9. Types of Difficulties Identified from Concept Map 2.

I) Problems with rotation
   A) What rotates?
   B) Rotation and isomers

II) Problems with equilibrium
   A) What is in equilibrium?
      1) Species that "have equilibrium"
      2) Impossible items in equilibrium
      3) Other
   B) Problems with staggered and eclipsed/chair and boat/axial and equatorial
      1) axial/equatorial
      2) chair/boat
      3) staggered/eclipsed
         a) staggered is at equilibrium, eclipsed is not (or similar)
         b) other

III) Problems with conformer extremes
   A) Equating staggered/eclipsed with boat/chair
   B) Problems with the nature of conformers

IV) Problems with the definition of conformer
   A) Conformers and bonds
      1) Equating conformers with bonds
      2) Problems with the nature of the bonds in conformers
   B) Problems involving structural isomers
Table 8.10. Selected Difficulties Identified from Concept Map 2.

<table>
<thead>
<tr>
<th>Type(^a)</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA</td>
<td>Atoms have unrestricted and continual rotation in space around C-C bonds allowing electrons to be as far apart or close together as possible.</td>
</tr>
<tr>
<td>IA</td>
<td>Conformer is the rotation of a carbon-carbon single bond.</td>
</tr>
<tr>
<td>IB</td>
<td>Molecules with no free rotation are alkenes or alkynes (NB: cyclic compounds?) that may have isomers or pretend to be isomers as conformers.</td>
</tr>
<tr>
<td>IIA1</td>
<td>A Newman projection can have equilibrium. A sawhorse diagram can have equilibrium.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Conformers: isomers which have equilibrium of their molecular formula.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Conformers can be staggered, considered stable, possesses equilibrium between atoms. Conformers can be eclipsed considered unstable presents steric effect (without mention of equilibrium).</td>
</tr>
<tr>
<td>IIA2</td>
<td>Double bonds, when spaced equally, are in equilibrium.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Single bonds are usually in equilibrium.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Constitutional isomers must keep equilibrium to be stable.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Equilibrium is either &quot;axially or equatorially&quot;</td>
</tr>
<tr>
<td>IIB2</td>
<td>A carbon-carbon single bond where the atoms are far apart is staggered as found in chair conformation which is most stable and closer to equilibrium.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Conformers isomers can be staggered and are more stable and therefore have equilibrium.</td>
</tr>
<tr>
<td>IIB3a</td>
<td>Conformers can be eclipsed and are at equilibrium. Conformers can be staggered.</td>
</tr>
<tr>
<td>IIB3a</td>
<td>Rotation of carbons forms staggered which creates more equilibrium.</td>
</tr>
<tr>
<td>IIB3a</td>
<td>Single bonds may be eclipsed with an equilibrium that is least stable, and staggered with an equilibrium that is more stable.</td>
</tr>
<tr>
<td>IIB3a</td>
<td>The staggered conformer is more stable and closer to equilibrium, and the eclipsed is less stable and is also in equilibrium.</td>
</tr>
<tr>
<td>IIB3b</td>
<td>Molecules that are staggered have stable atoms with &quot;good equilibrium.&quot;</td>
</tr>
<tr>
<td>IIIA</td>
<td>A conformer is an isomer that can be eclipsed which is called the boat conformation.</td>
</tr>
<tr>
<td>IIIA</td>
<td>A conformer is an isomer that can be staggered which is called the chair conformation.</td>
</tr>
<tr>
<td>IIIA</td>
<td>The eclipsed conformer forms the boat conformation and the staggered forms the chair.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Eclipsed conformation occurs where electrons are close together.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Eclipsed conformers are smaller and staggered conformers are larger.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Staggered conformation occurs where electrons are far apart.</td>
</tr>
<tr>
<td>IVA1</td>
<td>A conformational isomer cannot be a pi bond but can be a sigma bond.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Carbon bonds help make up a molecular formula.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Carbon bonds which are single bonds are alkanes.</td>
</tr>
<tr>
<td>IVA1</td>
<td>One type of isomer is the Newman projection.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Conformers are made of sigma bonds.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Conformers do not have multiple bonds.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Conformers occur in carbon-carbon single bonds.</td>
</tr>
<tr>
<td>IVB</td>
<td>Cycloalkanes are conformers, example is ethane.</td>
</tr>
</tbody>
</table>

\(^a\)Refers to difficulty type identified in Table 8.9.
Table 8.11. Statistical Analysis of Concept Map 3\textsuperscript{a}.

Seed Concepts: isomer, structural isomer, stereoisomer, geometric isomer, conformer

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Percent of students choosing concept\textsuperscript{b}</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer(s)/isomerism</td>
<td>88.9%</td>
</tr>
<tr>
<td>conformer(s)/conformational isomers</td>
<td>8.3%</td>
</tr>
<tr>
<td>others\textsuperscript{c}</td>
<td>2.8%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Mean rank of seed concept</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer</td>
<td>1.11</td>
</tr>
<tr>
<td>structural isomer</td>
<td>2.89</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>2.95</td>
</tr>
<tr>
<td>conformer</td>
<td>3.56</td>
</tr>
<tr>
<td>geometric isomer</td>
<td>4.49</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(W)\textsuperscript{e}</td>
<td>.7380</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Assigned only in Spring, 1998.
\textsuperscript{b} Represents 72 concept maps from Spring 1998.
\textsuperscript{c} Represents concepts chosen by only one participant.
\textsuperscript{d} Represents maps without a clear superordinate concept.
\textsuperscript{e} Represents the Kendall coefficient of concordance.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer</td>
<td>1.01</td>
<td>structural isomer</td>
<td>1.99</td>
<td>.9467</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.01</td>
<td>stereoisomer</td>
<td>1.99</td>
<td>.9467</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.07</td>
<td>conformer</td>
<td>1.93</td>
<td>.7480</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.01</td>
<td>geometric isomer</td>
<td>1.99</td>
<td>.9467</td>
<td>.0000</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.48</td>
<td>stereoisomer</td>
<td>1.52</td>
<td>.0174</td>
<td>.2569</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.33</td>
<td>conformer</td>
<td>1.67</td>
<td>.2166</td>
<td>.0001</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.09</td>
<td>geometric isomer</td>
<td>1.91</td>
<td>.8108</td>
<td>.0000</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.34</td>
<td>conformer</td>
<td>1.66</td>
<td>.1853</td>
<td>.0002</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.10</td>
<td>geometric isomer</td>
<td>1.90</td>
<td>.7237</td>
<td>.0000</td>
</tr>
<tr>
<td>conformer</td>
<td>1.30</td>
<td>geometric isomer</td>
<td>1.70</td>
<td>.3201</td>
<td>.0000</td>
</tr>
</tbody>
</table>

Table 8.13. Types of Difficulties Identified from Concept Map 3.

I) Interesting or unusual
   A) Recognizing a relationship between geometric and stereoisomers
   B) Interesting descriptions of conformers and isomers

II) Problems with molecular and structural formulas.
   A) Confusing the formula with the molecule.
   B) Other problems with formulas.

III) Problems with conformers
   A) Problems with the relationship between conformers and other types of isomers.
   B) Problems with the nature of different types of conformers.

IV) Problems with the nature of geometric isomers.
   A) Problems recognizing the structural features of geometric isomers.
   B) Problems with the relationship between stereoisomers and geometric isomers.

V) Other problems with isomers

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Table 8.14. Selected Difficulties Identified from Concept Map 3a.

<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulties</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA</td>
<td>Geometric isomer is a type of stereoisomer.</td>
</tr>
<tr>
<td>IB</td>
<td>Geometric isomers differ by bond arrangement.</td>
</tr>
<tr>
<td>IB</td>
<td>Conformational isomers differ in distance between attached atoms. Skeletal isomers differ in carbon-carbon arrangement and positional isomers differ in non-carbon group arrangement.</td>
</tr>
<tr>
<td>IIA</td>
<td>An isomer is a molecular formula.</td>
</tr>
<tr>
<td>IIA</td>
<td>Sawhorse diagrams, Newman diagrams are examples of alkanes.</td>
</tr>
<tr>
<td>IIB</td>
<td>$C_5H_{16}$ is molecular formula of pentane &amp; 2-methylbutane.</td>
</tr>
<tr>
<td>IIB</td>
<td>Isomers are different compounds with the same molecular formula but different structural formulas.</td>
</tr>
<tr>
<td>IIIA:</td>
<td>Conformers are seen as isomers but are not seen as types of stereoisomers, even though they both have the same &quot;bonding attachments.&quot;</td>
</tr>
<tr>
<td>IIIB</td>
<td>Isomers are conformers in the &quot;chair&quot; or &quot;boat.&quot;</td>
</tr>
<tr>
<td>IVA</td>
<td>Geometric isomers differ in orientation around double bonds.</td>
</tr>
<tr>
<td>IVA</td>
<td>Geometric isomers occur in rings.</td>
</tr>
<tr>
<td>IVA</td>
<td>Rotation around single carbon bonds causes conformers, whereas rotation around double carbon bonds causes geometric isomers.</td>
</tr>
<tr>
<td>IVB</td>
<td>(Geometric isomers are not seen as types of stereoisomers.)</td>
</tr>
<tr>
<td>IVB</td>
<td>(Stereoisomers are a different category from geometric isomers)</td>
</tr>
<tr>
<td>V</td>
<td>(Different bonding attachments result in stereoisomers.)</td>
</tr>
<tr>
<td>V</td>
<td>(Skeletal and constitutional isomers are not seen as types of structural isomers)</td>
</tr>
</tbody>
</table>

---

aItems in parentheses are summarized from individual concept maps.

bRefers to difficulty type identified in Table 8.13.
Qualitative analysis of this concept map yielded five major types of difficulties. First were difficulties involving a narrow focus on the catalyst. Next were difficulties involving addition, difficulties involving substitution, difficulties involving elimination, and finally some other miscellaneous difficulties involving reactions. These types are listed in Table 8.17, with specific examples given in Table 8.18.

Results of Concept Map 5. Concept map 5, which had the seed concepts "carbocation", "carbanion", "free radical", "nucleophile", and "electrophile", was assigned in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of superordinate concept for this map was "intermediates" (68.9% and 65.4% of respondents, respectively). Analysis of concordance of ordinal rank of these concepts for each semester gave values of Kendall's W of .5203 and .2508, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.19, 8.20, and 8.21.

Qualitative analysis of the concept maps yielded four major types of difficulties. The first type of difficulty involved bond cleavage and the odd electron, and the next involved charges, electrophiles, nucleophiles, and free radicals. The third type involved improper generalization, and the last involved the process or progress of the mechanism. These types are listed in Table 8.22, with specific examples given in Table 8.23.

Results of Concept Map 6. Concept map 6, which had the seed concepts "carbocation", "carbanion", "free radical", "homolytic cleavage", "heterolytic cleavage," and "reaction intermediate", was only assigned in the Fall, 1997, semester. The first choice of superordinate concept for this map was "reaction intermediates" (69.6% of respondents). Analysis of concordance of ordinal rank of these concepts for each semester gave a values of Kendall's W of .8308, which is significant at the .0000 level. Results of these calculations are given in Tables 8.24 and 8.25.

Far fewer difficulties were found during analysis of concept map 6 than were found in analysis of any other set of concept maps. Only two difficulties were discovered, and...
Table 8.15. Statistical Analysis of Concept Map 4.

Seed concepts: reaction, substitution, elimination, addition

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Mean rank of seed concept:</th>
</tr>
</thead>
<tbody>
<tr>
<td>reaction(s)</td>
<td>1.00</td>
</tr>
<tr>
<td>equation(s)</td>
<td>2.96</td>
</tr>
<tr>
<td>elimination</td>
<td>2.98</td>
</tr>
<tr>
<td>others(^c)</td>
<td>3.06</td>
</tr>
<tr>
<td>unclear(^d)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>W(^e)</td>
<td>.9703</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>3</td>
</tr>
</tbody>
</table>

\(^a\) Assigned only in Spring, 1998.
\(^b\) Represents 87 concept maps from Spring, 1998.
\(^c\) Represents concepts chosen by only one participant.
\(^d\) Represents maps without a clear superordinate concept.
\(^e\) Represents the Kendall coefficient of concordance.

---

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Table 8.16. Individual Statistical Comparisons of Seed Concepts from Map 4 for the Spring, 1998 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>reaction</td>
<td>1.00</td>
<td>substitution</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction</td>
<td>1.00</td>
<td>addition</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction</td>
<td>1.00</td>
<td>elimination</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.49</td>
<td>addition</td>
<td>1.51</td>
<td>0.0129</td>
<td>0.3183</td>
</tr>
<tr>
<td>substitution</td>
<td>1.47</td>
<td>elimination</td>
<td>1.53</td>
<td>0.0649</td>
<td>0.0254</td>
</tr>
<tr>
<td>addition</td>
<td>1.47</td>
<td>elimination</td>
<td>1.53</td>
<td>0.0519</td>
<td>0.0455</td>
</tr>
</tbody>
</table>

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Table 8.17. Types of Difficulties Identified from Concept Map 4.

I) Narrow focus involving the catalyst.
   A) Elimination requires a catalyst.
      1) dehydrohalogenation occurs in acid
      2) elimination requires a catalyst
         a) must be acid catalyst
         b) base can be a catalyst in elimination reactions.

II) Difficulties involving addition.
    A) Focus too narrow
       1) Confusion of atoms with substituents
       2) Narrow focus on the products
    B) What happens?
       1) Improper mechanism
       2) Where does addition occur?

III) Difficulties involving substitution
    A) Focus too narrow
       1) Nature of leaving group
          a) Leaving group is an atom.
          b) Leaving group is a molecule.
       2) What forms?
    B) Alternative conceptions regarding the process of substitution

IV) Difficulties involving elimination.
    A) Focus too narrow
       1) Atoms are eliminated.
       2) Narrow focus on process
    B) Other alternative conceptions about elimination

V) Other difficulties.
Table 8.18. Selected Difficulties Identified from Concept Map 4.

<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA1</td>
<td>Elimination needs an acidic catalyst. Elimination can be dehydrohalogenation.</td>
</tr>
<tr>
<td>IA2</td>
<td>Elimination reaction contains a catalyst.</td>
</tr>
<tr>
<td>IA2a</td>
<td>Elimination has H⁺ catalyst.</td>
</tr>
<tr>
<td>IA2a</td>
<td>Reactions can be elimination reactions that have an acid catalyst.</td>
</tr>
<tr>
<td>IB</td>
<td>Dehydrohalogenation elimination of H &amp; halogen by use of catalyst must be a base.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Addition atoms are added (sic) to multiple bonds.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Addition occurs when an atom is added to adjacent atoms.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Addition of atoms to adjacent atoms creates hydration reactions.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Reactions may gain atoms which is addition reaction.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Addition of atoms to adjacent atoms creates hydration reactions.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Addition reactions are also called dehydration reactions.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Addition reduces an alkene to an alkane.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Addition reaction that is an electrophile that accepts an electron pair.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Addition reaction adds atoms to adjacent carbon atoms.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Addition reactions occur when atoms are added.</td>
</tr>
<tr>
<td>IIIA1a</td>
<td>Substitution atoms are replaced.</td>
</tr>
<tr>
<td>IIIA1a</td>
<td>Substitution in which atoms replace other atoms.</td>
</tr>
<tr>
<td>IIIA1a</td>
<td>Substitution reactions are easiest to identify because atoms are replaced.</td>
</tr>
<tr>
<td>IIIA1a</td>
<td>Substitution replaces atoms with another species.</td>
</tr>
<tr>
<td>IIIA1a</td>
<td>Substitution where atoms are replaced but remains an alkane.</td>
</tr>
<tr>
<td>IIIA2</td>
<td>Substitution has H⁺ catalyst and forms H₂O molecule.</td>
</tr>
<tr>
<td>IIIA2</td>
<td>Substitution occurs where the hydrogen atom of a hydrocarbon is replaced by a substituent.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Substitution occurs when an atom or substituent is replaced by a different atom or substituent which is more electronegative.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Substitution reaction that is a nucleophile that donates an electron pair that is a free radical.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Elimination atoms are removed to form multiple bonds.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Elimination occurs when atoms on adjacent carbon atoms are removed to form a small molecule and a double or triple bond.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Elimination occurs when atoms on adjacent carbon atoms are removed.</td>
</tr>
<tr>
<td>IVA1</td>
<td>Elimination occurs with removal of atoms.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Elimination eliminates atoms or groups of atoms by adding an acid catalyst to form a small molecule, also forms double or triple bonds.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Elimination reactions are also known as dehydration reactions.</td>
</tr>
<tr>
<td>IVA2</td>
<td>Reactions can be elimination reactions that eliminate a water molecule.</td>
</tr>
<tr>
<td>IVB</td>
<td>Elimination does not have group of atoms.</td>
</tr>
<tr>
<td>IVB</td>
<td>Elimination occurs when adjacent carbons are removed to form a new molecule.</td>
</tr>
<tr>
<td>V</td>
<td>Equations are reactions.</td>
</tr>
<tr>
<td>V</td>
<td>Reaction is a step-by-step mechanism.</td>
</tr>
<tr>
<td>V</td>
<td>Reaction occurs between two atoms in which bonds are broken and created.</td>
</tr>
</tbody>
</table>

^Refers to difficulty type identified in Table 8.17.
Table 8.19. Statistical Analysis of Concept Map 5.

Seed concepts: carbocation, carbanion, free radical, nucleophile, electrophile

<table>
<thead>
<tr>
<th>Superordinate Concept</th>
<th>Percent of Students Choosing Concept</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>intermediates</td>
<td>68.9%</td>
<td>65.4%</td>
<td></td>
</tr>
<tr>
<td>organic reactions</td>
<td>9.8%</td>
<td>11.1%</td>
<td></td>
</tr>
<tr>
<td>reaction mechanisms</td>
<td>10.7%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>chemical reactions</td>
<td>0.0%</td>
<td>3.7%</td>
<td></td>
</tr>
<tr>
<td>species</td>
<td>0.8%</td>
<td>4.9%</td>
<td></td>
</tr>
<tr>
<td>electrophile</td>
<td>0.0%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>others(^b)</td>
<td>7.3%</td>
<td>7.4%</td>
<td></td>
</tr>
<tr>
<td>unclear choice(^c)</td>
<td>2.4%</td>
<td>2.5%</td>
<td></td>
</tr>
</tbody>
</table>

Mean rank of seed concepts:

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbocation</td>
<td>2.27</td>
<td>2.50</td>
</tr>
<tr>
<td>carbanion</td>
<td>2.30</td>
<td>2.51</td>
</tr>
<tr>
<td>free radical</td>
<td>2.30</td>
<td>2.56</td>
</tr>
<tr>
<td>nucleophile</td>
<td>4.06</td>
<td>3.72</td>
</tr>
<tr>
<td>electrophile</td>
<td>4.06</td>
<td>3.70</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997(^a)</th>
<th>Spring 1998(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(W^d)</td>
<td>.5203</td>
<td>.2508</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

\(^a\) Represents 122 concept maps from Fall, 1997 and 81 concept maps from Spring, 1998.

\(^b\) Represents concepts chosen by only one participant.

\(^c\) Represents maps without a clear superordinate concept.

\(^d\) Represents the Kendall coefficient of concordance.
<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbocation</td>
<td>1.50</td>
<td>carbanion</td>
<td>1.50</td>
<td>.0083</td>
<td>.3192</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.50</td>
<td>free radical</td>
<td>1.50</td>
<td>.0028</td>
<td>.5652</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.15</td>
<td>electrophile</td>
<td>1.85</td>
<td>.5235</td>
<td>.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.14</td>
<td>nucleophile</td>
<td>1.86</td>
<td>.5485</td>
<td>.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.50</td>
<td>free radical</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.15</td>
<td>electrophile</td>
<td>1.85</td>
<td>.5235</td>
<td>.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.15</td>
<td>nucleophile</td>
<td>1.85</td>
<td>.5235</td>
<td>.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.15</td>
<td>electrophile</td>
<td>1.85</td>
<td>.5158</td>
<td>.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.15</td>
<td>nucleophile</td>
<td>1.85</td>
<td>.5158</td>
<td>.0000</td>
</tr>
<tr>
<td>electrophile</td>
<td>1.50</td>
<td>nucleophile</td>
<td>1.50</td>
<td>.0017</td>
<td>.6560</td>
</tr>
</tbody>
</table>

Table 8.20. Individual Statistical Comparisons of Seed Concepts from Map 5 for the Fall, 1997 Semester.
<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbocation</td>
<td>1.50</td>
<td>carbanion</td>
<td>1.50</td>
<td>0.000</td>
<td>1.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.49</td>
<td>free radical</td>
<td>1.51</td>
<td>0.0139</td>
<td>0.3175</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.26</td>
<td>electrophile</td>
<td>1.74</td>
<td>0.2590</td>
<td>0.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.25</td>
<td>nucleophile</td>
<td>1.75</td>
<td>0.2903</td>
<td>0.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.49</td>
<td>free radical</td>
<td>1.51</td>
<td>0.0278</td>
<td>0.1574</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.26</td>
<td>electrophile</td>
<td>1.74</td>
<td>0.2590</td>
<td>0.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.26</td>
<td>nucleophile</td>
<td>1.74</td>
<td>0.2509</td>
<td>0.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.27</td>
<td>electrophile</td>
<td>1.73</td>
<td>0.2401</td>
<td>0.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.26</td>
<td>nucleophile</td>
<td>1.74</td>
<td>0.2509</td>
<td>0.0000</td>
</tr>
<tr>
<td>electrophile</td>
<td>1.50</td>
<td>nucleophile</td>
<td>1.50</td>
<td>0.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Table 8.22. Types of Difficulties Identified from Concept Map 5.

I) Difficulties regarding bond cleavage and the odd electron.
   A) Source of the odd electron in free radicals
   B) Formation of carbocations and carbanions

II) Difficulties regarding charges, electrophiles, nucleophiles, and free radicals.
   A) Nature of nucleophile and electrophile.
      1) Wrong charges
      2) Equating free radicals with other species
         a) Equating free radical with electrophile
         b) Equating free radical with nucleophile
         c) Equating free radical with both
      3) Intermediates are formed from electrophiles and nucleophiles
   B) Accepting and donating electron pairs; nature of Lewis acids and bases.
      1) Carbanion as Lewis acid or electrophile; carbocation as Lewis base or
         nucleophile
      2) How electrophiles and nucleophiles react
      3) Equating organic species with inorganic examples
   C) Where free radicals occur

III) Improper generalization.
   A) Key link missing.
      1) Carbanion not linked to nucleophile (or Lewis base)
      2) Carbocation not linked to electrophile (or Lewis acid)
   B) Improper route from general to specific
      1) Not sure if carbanions are always nucleophiles
      2) Not sure if carbocations are always electrophiles
      3) All nucleophiles are seen as carbanions
      4) All electrophiles are seen as carbocations
      5) Improper attribution of cause and effect

IV) Difficulties regarding the process or progress of the mechanism.
   A) Role of the catalyst
   B) Number of steps in a mechanism
   C) Intermediate as a product
Table 8.23. Selected Difficulties Identified from Concept Map 5\(^a\).

<table>
<thead>
<tr>
<th>Type(^b)</th>
<th>Difficulties</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA</td>
<td>Free radical formed by heterolytic cleavage.</td>
</tr>
<tr>
<td>IA</td>
<td>Free radical is neutral because of homolytic cleavage divides bonding electrons unevenly.</td>
</tr>
<tr>
<td>IA</td>
<td>Reaction intermediate with free electron is formed by heterolytic cleavage.</td>
</tr>
<tr>
<td>IB</td>
<td>Carbanion is formed by homolytic cleavage.</td>
</tr>
<tr>
<td>IB</td>
<td>Carbocation formed by homolytic cleavage or heterolytic cleavage.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Carbanion has a positive charge and can be an electrophile.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Carbocation has a negative charge and can be a nucleophile.</td>
</tr>
<tr>
<td>IIA2a</td>
<td>Electrophiles can be free radicals.</td>
</tr>
<tr>
<td>IIA2a</td>
<td>Free radical can act as electrophile.</td>
</tr>
<tr>
<td>IIA2a</td>
<td>Free radicals and carbocations can be electrophiles.</td>
</tr>
<tr>
<td>IIA2b</td>
<td>Free radical has one unshared unpaired electron, example of nucleophile.</td>
</tr>
<tr>
<td>IIA2c</td>
<td>Free radical has a neutral charge, can either be electrophile or nucleophile.</td>
</tr>
<tr>
<td>IIA3</td>
<td>Reaction intermediates are formed by electrophiles.</td>
</tr>
<tr>
<td>IIA3</td>
<td>Reaction intermediates are formed by nucleophiles.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Carbanion has a pair of unshared electrons, example of electrophile.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Carbanion is an electrophile electron pair is accepted this is a Lewis acid.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Carbanions are neutralized by nucleophiles.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Carbocation is a nucleophile electron pair is donated this is a Lewis base.</td>
</tr>
<tr>
<td>IIB3</td>
<td>Reaction intermediate formed by heterolytic cleavage can be electrophile AKA Lewis acid e.g. HNO(_3).</td>
</tr>
<tr>
<td>IIB3</td>
<td>reaction intermediate formed by heterolytic cleavage can be nucleophile AKA Lewis base e.g. NH(_3).</td>
</tr>
<tr>
<td>IIC</td>
<td>Free radicals occur in substitution reactions.</td>
</tr>
<tr>
<td>IIIA1</td>
<td>Carbanion likes to react with electrophile (but not seen as nucleophile).</td>
</tr>
<tr>
<td>IIIA1</td>
<td>(Carbanion not linked to nucleophile or Lewis base.)</td>
</tr>
<tr>
<td>IIIA2</td>
<td>Carbocation likes to react with nucleophile (but not seen as an electrophile).</td>
</tr>
<tr>
<td>IIIIB1</td>
<td>Carbanion can be a nucleophile.</td>
</tr>
<tr>
<td>IIIIB1</td>
<td>Carbanion is similar to nucleophile.</td>
</tr>
<tr>
<td>IIIIB2</td>
<td>Carbocation also called electrophile.</td>
</tr>
<tr>
<td>IIIIB2</td>
<td>Carbocation can be an electrophile.</td>
</tr>
<tr>
<td>IIIIB2</td>
<td>Carbocation is similar to electrophile.</td>
</tr>
<tr>
<td>IIIIB3</td>
<td>Nucleophiles are carbanions.</td>
</tr>
<tr>
<td>IIIIB4</td>
<td>Electrophiles are carbocations.</td>
</tr>
<tr>
<td>IIIIB5</td>
<td>Electrophiles cause carbocations.</td>
</tr>
<tr>
<td>IIIIB5</td>
<td>Nucleophiles cause carbanions.</td>
</tr>
<tr>
<td>IVA</td>
<td>Carbanions which carry a negative charge often found as nucleophiles in the presence of a catalyst.</td>
</tr>
<tr>
<td>IVA</td>
<td>Catalyst may be a base which removes a hydrogen atom and a halogen in a process called dehydrohalogenation.</td>
</tr>
<tr>
<td>IVB</td>
<td>Elimination is multi-step.</td>
</tr>
<tr>
<td>IVB</td>
<td>Substitution occurs in a single step.</td>
</tr>
<tr>
<td>IVC</td>
<td>Addition reactions may form carbocations or carbanions.</td>
</tr>
<tr>
<td>IVC</td>
<td>Elimination reactions may form carbocations or carbanions.</td>
</tr>
</tbody>
</table>

\(^a\)Items in parentheses are summarized from individual concept maps.

\(^b\)Refers to difficulty type identified in Table 8.22.

Seed concepts: carbocation, carbanion, free radical, homolytic cleavage, heterolytic cleavage, reaction intermediate

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Percent of students choosing concept</th>
</tr>
</thead>
<tbody>
<tr>
<td>reaction intermediate(s)</td>
<td>69.6%</td>
</tr>
<tr>
<td>organic reaction(s)</td>
<td>9.6%</td>
</tr>
<tr>
<td>reaction mechanisms</td>
<td>8.0%</td>
</tr>
<tr>
<td>chemical reaction(s)</td>
<td>3.2%</td>
</tr>
<tr>
<td>others^c</td>
<td>9.6%</td>
</tr>
</tbody>
</table>

Seed concept                                                                 | Mean rank of seed concept |
-----------------------------------------------------------------------------|---------------------------|
reaction intermediate                                                       | 1.00                      |
 carbocation                                                                  | 3.19                      |
 carbanion                                                                   | 3.19                      |
 free radical                                                                 | 3.19                      |
 homolytic cleavage                                                          | 5.20                      |
 heterolytic cleavage                                                        | 5.22                      |

Statistic                                                                 | Value |
---------------|--------|
W^d            | .8308  |
significance   | .0000  |
degrees of freedom | 5     |

^a Assigned only in Fall, 1997.
^b Represents 127 concept maps from Fall, 1997.
^c Represents concepts chosen by only one participant.
^d Represents the Kendall coefficient of concordance.
<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>reaction intermediate</td>
<td>1.00</td>
<td>carbocation</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction intermediate</td>
<td>1.00</td>
<td>carbanion</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction intermediate</td>
<td>1.00</td>
<td>free radical</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction intermediate</td>
<td>1.00</td>
<td>homolytic cleavage</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>reaction intermediate</td>
<td>1.00</td>
<td>heterolytic cleavage</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.50</td>
<td>carbanion</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.50</td>
<td>free radical</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.10</td>
<td>homolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>carbocation</td>
<td>1.10</td>
<td>heterolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.50</td>
<td>free radical</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.10</td>
<td>homolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>carbanion</td>
<td>1.10</td>
<td>heterolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.10</td>
<td>homolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>free radical</td>
<td>1.10</td>
<td>heterolytic cleavage</td>
<td>1.90</td>
<td>.6608</td>
<td>.0000</td>
</tr>
<tr>
<td>homolytic cleavage</td>
<td>1.49</td>
<td>heterolytic cleavage</td>
<td>1.51</td>
<td>.0256</td>
<td>.1575</td>
</tr>
</tbody>
</table>
very few student maps contained these difficulties. These two difficulties were the
statements that carbocations and carbanions are formed through homolytic cleavage and
the statement that free radicals are formed through heterolytic cleavage.

**Results of Concept Map 7.** Concept map 7, which had the seed concepts
"enantiomer", "physical properties", "chemical properties", "plane-polarized light", and
"racemic mixture", was assigned in both the Fall, 1997, and Spring, 1998, semesters.
For both semesters, the first choice of superordinate concept for this map was
"enantiomers" (43.4% and 65.8% of respondents, respectively). Analysis of
concordance of ordinal rank of these concepts for each semester gave values of Kendall’s
W of .5852 and .5125, respectively, both of which are significant at the .0000 level.
Results of these calculations are given in Tables 8.26, 8.27, and 8.28.

Qualitative analysis of the concept maps yielded five major types of propositions.
First were propositions that were interesting or unusual but not necessarily incorrect.
Next were difficulties regarding physical and chemical properties. The third type of
difficulty identified dealt with sources and causes of optical activity and chirality, the
fourth involved differences between types of optical isomers, and the last dealt with
distinguishing chiral atoms from molecules. These types are listed in Table 8.29, with
specific examples given in Table 8.30.

**Results of Concept Map 8.** Concept map 8, which had the seed concepts
"enantiomer", "racemate", "mirror image", "inversion", "absolute configuration," and
"resolution", was assigned in both the Fall, 1997, and Spring, 1998, semesters. For
both semesters, the first choice of superordinate concept for this map was "enantiomers"
(42.2% and 75.0% of respondents, respectively). Analysis of concordance of ordinal
rank of these concepts for each semester gave values of Kendall’s W of .4542 and .5637,
respectively, both of which are significant at the .0000 level. Results of these
calculations are given in Tables 8.31, 8.32, and 8.33.

Seed concepts: enantiomer, physical properties, chemical properties, plane-polarized light, racemic mixtures

<table>
<thead>
<tr>
<th>Superordinate Concept</th>
<th>Percent of students choosing concept</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>enantiomer(s)</td>
<td>43.4%</td>
<td>65.8%</td>
<td></td>
</tr>
<tr>
<td>optical isomer(ism)</td>
<td>30.2%</td>
<td>19.0%</td>
<td></td>
</tr>
<tr>
<td>chiral atoms</td>
<td>7.0%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>isomers</td>
<td>3.9%</td>
<td>3.8%</td>
<td></td>
</tr>
<tr>
<td>stereoisomers/ism</td>
<td>3.1%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>chiral compound(s)</td>
<td>3.1%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>chiral atom(s)</td>
<td>2.3%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>nonsuperimposable mirror images</td>
<td>0.0%</td>
<td>2.5%</td>
<td></td>
</tr>
<tr>
<td>racemic mixtures</td>
<td>1.6%</td>
<td>3.8%</td>
<td></td>
</tr>
<tr>
<td>others&lt;sup&gt;b&lt;/sup&gt;</td>
<td>5.4%</td>
<td>2.5%</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Seed concept</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>enantiomer(s)</td>
<td>1.14</td>
<td>1.04</td>
</tr>
<tr>
<td>physical properties</td>
<td>2.94</td>
<td>2.84</td>
</tr>
<tr>
<td>chemical properties</td>
<td>3.24</td>
<td>2.94</td>
</tr>
<tr>
<td>racemic mixture</td>
<td>3.55</td>
<td>3.82</td>
</tr>
<tr>
<td>plane polarized light</td>
<td>4.13</td>
<td>4.37</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;c&lt;/sup&gt;</td>
<td>.5852</td>
<td>.5125</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents 129 concept maps from Fall, 1997 and 79 concept maps from Spring, 1998.

<sup>b</sup>Represents concepts chosen by only one participant.

<sup>c</sup>Represents the Kendall coefficient of concordance.
Table 8.27. Individual Statistical Comparisons of Seed Concepts from Map 7 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer</td>
<td>1.03</td>
<td>physical properties</td>
<td>1.97</td>
<td>.9098</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.02</td>
<td>chemical properties</td>
<td>1.98</td>
<td>.9200</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.05</td>
<td>plane-polarized light</td>
<td>1.95</td>
<td>.8508</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.05</td>
<td>racemic mixture</td>
<td>1.95</td>
<td>.8406</td>
<td>.0000</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.43</td>
<td>chemical properties</td>
<td>1.57</td>
<td>.1111</td>
<td>.0010</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.16</td>
<td>plane-polarized light</td>
<td>1.84</td>
<td>.5421</td>
<td>.0000</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.38</td>
<td>racemic mixture</td>
<td>1.62</td>
<td>.0918</td>
<td>.0027</td>
</tr>
<tr>
<td>chemical properties</td>
<td>1.24</td>
<td>plane-polarized light</td>
<td>1.76</td>
<td>.3447</td>
<td>.0000</td>
</tr>
<tr>
<td>chemical properties</td>
<td>1.45</td>
<td>racemic mixture</td>
<td>1.55</td>
<td>.0155</td>
<td>.2184</td>
</tr>
<tr>
<td>racemic mixture</td>
<td>1.42</td>
<td>plane-polarized light</td>
<td>1.58</td>
<td>.0277</td>
<td>.0997</td>
</tr>
</tbody>
</table>

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Table 8.28. Individual Statistical Comparisons of Seed Concepts from Map 7 for the Spring, 1998 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer</td>
<td>1.00</td>
<td>physical properties</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.00</td>
<td>chemical properties</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.01</td>
<td>plane-polarized light</td>
<td>1.99</td>
<td>.9844</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.03</td>
<td>racemic mixture</td>
<td>1.97</td>
<td>.8789</td>
<td>.0000</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.48</td>
<td>chemical properties</td>
<td>1.52</td>
<td>.0156</td>
<td>.3173</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.09</td>
<td>plane-polarized light</td>
<td>1.91</td>
<td>.6815</td>
<td>.0000</td>
</tr>
<tr>
<td>physical properties</td>
<td>1.27</td>
<td>racemic mixture</td>
<td>1.73</td>
<td>.3057</td>
<td>.0000</td>
</tr>
<tr>
<td>chemical properties</td>
<td>1.13</td>
<td>plane-polarized light</td>
<td>1.87</td>
<td>.5850</td>
<td>.0000</td>
</tr>
<tr>
<td>chemical properties</td>
<td>1.28</td>
<td>racemic mixture</td>
<td>1.72</td>
<td>.2552</td>
<td>.0001</td>
</tr>
<tr>
<td>racemic mixture</td>
<td>1.40</td>
<td>plane-polarized light</td>
<td>1.60</td>
<td>.0498</td>
<td>.0742</td>
</tr>
</tbody>
</table>

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Table 8.29. Types of Difficulties Identified from Concept Map 7.

I) Interesting

A) Descriptions involving chemical or physical properties
   1) Unusual chemical or physical properties as examples.
   2) Unusual methods for distinguishing stereoisomers.

B) Relationships between structure and chirality
   1) Statements that could anticipate chiral molecules containing no chiral atoms.
   2) Statements that could anticipate meso compounds
   3) Statements that clarify chirality at an atom

II) Difficulties involving physical or chemical properties.

A) Naive statements regarding chemical and physical properties
   1) Simple statements that substances have properties
   2) Enantiomers have different chemical properties

B) Confusion of chemical and physical properties
   1) Chemical properties categorized incorrectly
   2) Physical properties categorized incorrectly

C) Confusion of structure with chemical or physical properties
   1) Structure confused with chemical properties
   2) Structure confused with physical properties

D) Rotation of plane polarized light not recognized as a physical property

III) Sources and causes of optical activity and chirality.

A) Structural source of optical activity
   1) Optical activity and plane polarized light
   2) Nature of enantiomers and diastereomers

B) Sources of enantiomers

C) Nature of racemic mixtures

IV) Differences between types of optical isomers.

A) Optical isomers are enantiomers

B) Other

V) Distinguishing chiral atoms from molecules.
<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA1</td>
<td>Chemical properties are different, <em>e.g.</em> drug effects.</td>
</tr>
<tr>
<td>IA1</td>
<td>Chemical properties: teratogen, Thalidomide.</td>
</tr>
<tr>
<td>IA1</td>
<td>Enantiomers have chemical properties (*structure, smell, <em>etc.</em>) that are different.</td>
</tr>
<tr>
<td>IA2</td>
<td>Enantiomers have identical stabilities therefore chemical properties are the same.</td>
</tr>
<tr>
<td>IA2</td>
<td>Interesting: Physical properties distinguish enantiomers.</td>
</tr>
<tr>
<td>IA2</td>
<td>Interesting: Racemic mixtures have the same stabilities; therefore, chemical properties are the same.</td>
</tr>
<tr>
<td>IB1</td>
<td>Enantiomers almost always need chiral atoms.</td>
</tr>
<tr>
<td>IB1</td>
<td>Enantiomers usually have a chiral carbon. Enantiomers have similar chemical and physical properties.</td>
</tr>
<tr>
<td>IB2</td>
<td>Steroisomer that can be superimposable &amp; Steroisomer that can be nonsuperimposable.</td>
</tr>
<tr>
<td>IB3</td>
<td>Chiral carbons are $sp^3$-hybridized.</td>
</tr>
<tr>
<td>IB3</td>
<td>Enantiomers are chiral compounds in which configuration around the carbon varies.</td>
</tr>
<tr>
<td>IB3</td>
<td>Enantiomers with single configuration.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Chiral carbons form enantiomers having many different chemical properties.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Enantiomer has chemical properties.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Enantiomers are chiral compounds and have different chemical properties.</td>
</tr>
<tr>
<td>IIA1</td>
<td>Enantiomers demonstrate physical properties such as melting point. <em>Do other compounds demonstrate physical properties?</em></td>
</tr>
<tr>
<td>IIA2</td>
<td>Enantiomers have chemical properties and physical properties.</td>
</tr>
<tr>
<td>IIA2</td>
<td>Enantiomers exhibit different chemical properties with different results in organic reactions. Enantiomers come in pairs (50/50) racemic mixture.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers have different chemical properties.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Chemical properties such as melting point.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Chemical properties, <em>e.g.</em> boiling point.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers all have same physical properties. Enantiomers have different chemical properties such as R and S which rotates the plane polarization of light.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers are nonsuperimposable mirror images that rotate plane-polarized light which is a chemical property. <em>(not okay!)</em></td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers have different chemical properties such as solubilities, melting point, boiling point.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers have the same chemical properties such as electronegativity.</td>
</tr>
<tr>
<td>IIB1</td>
<td>Enantiomers have the same chemical properties, <em>e.g.</em> molar mass, melting point, boiling point.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Physical properties such as nonsuperimposable mirror images.</td>
</tr>
<tr>
<td>IIC1</td>
<td>50/50 racemic mixtures in which chemical properties are in equal amounts.</td>
</tr>
<tr>
<td>IIC1</td>
<td>Chemical properties of enantiomers include R-(-) and S-(+).</td>
</tr>
<tr>
<td>IIC1</td>
<td>Chemical properties which are identical such as chemical formula</td>
</tr>
<tr>
<td>IIC1</td>
<td>Enantiomer has a chemical property of chiral carbon.</td>
</tr>
</tbody>
</table>
Table 8.30 (cont).

IIC2 Enantiomers have physical properties like nonsuperimposable mirror images can also rotate clockwise or counterclockwise because you do not change chemical composition.

IID Enantiomers have identical physical and chemical properties, but enantiomers differ in the rotation of plane polarized light.

IID Enantiomers have same physical properties. BUT R-(-) rotates p polarization counterclockwise and R-(+) rotates p polarization clockwise.

IIIA1 A right-handed image might have counterclockwise rotation of plane-polarized light, and a left-handed image might have clockwise rotation of plane-polarized light.

IIIA1 Enantiomers occur in equal amounts of R- and S-; this is called racemic; this type of mixture occurs in plane polarized light.

IIIA1 Enantiomers have different physical properties in their rotation coming out to be either positive or negative where 50% of the two makes a racemic mixture.

IIIA1 Enantiomers having different rotations which are equal but in opposite directions known as plane polarized light.

IIIA1 If plane polarized light is not rotated, this indicates a racemic mixture.

IIIA1 Physical and chemical properties differ only in plane polarized light which is negative when it rotates counterclockwise and positive when it rotates clockwise.

IIIA2 Isomers that are nonsuperimposable include enantiomers that do not rotate.

IIIA2 Optical isomers having no mirror images are diastereomers. Optical isomers having mirror images may be meso compounds and are superimposable.

IIB Enantiomers are formed from racemic mixtures.

IIB Enantiomers are nonsuperimposable mirror images are in racemic mixture and occur in equal proportions.

IIIC Achiral atoms result in a 50/50 mixture of enantiomers.

IIIC Enantiomers have racemic mixtures which are superimposable and are inactive.

IIIC Optical isomers can be optically inactive which are racemic mixtures.

IVA Chiral compounds are called enantiomers.

IVA Optical isomers are enantiomers.

IVA: Optical isomers have the same chemical properties but different physical properties.

IVA Optical isomers, also called enantiomers ...

IVB Enantiomers can be diastereomers which changes physical properties which causes change to chemical properties.

V A chiral atom has one pair of enantiomers. Enantiomers are also called optical isomers.

V Chiral carbons can be a racemic mixture. Chiral carbons can have optical isomerism.

V Optical isomerism depends on chiral carbons which have enantiomers.

---

^tems in parentheses are summarized from individual concept maps.

^Refers to difficulty type identified in Table 8.29.

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Qualitative analysis of the concept maps yielded eight major types of difficulties. First were propositions that were interesting or unusual but not necessarily incorrect and next were propositions that, while not incorrect, would be considered naive in the context of the assigned map. Third were difficulties regarding the meaning of inversion and fourth were difficulties involving absolute configuration. The next three types of difficulties dealt with resolution, racemates, and relationships between types of isomers. Finally, the eighth type of difficulty involved the meaning of chirality. These types are listed in Table 8.34, with specific examples given in Table 8.35.

Results of Concept Map 9. Concept map 9, which had the seed concepts "isomer", "structural isomer", "stereoisomer", "enantiomer", and "diastereomer", was assigned in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of superordinate concept for this map was "isomer" or "isomers" (79.8% and 93.4% of respondents, respectively). Analysis of concordance of ordinal rank of these concepts for each semester gave values of Kendall's W of .7930 and .8771, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.36, 8.37, and 8.38.

Qualitative analysis of the concept maps yielded six major types of propositions. First were propositions that were interesting or unusual but not necessarily incorrect and next were propositions that, while not incorrect, would be considered naive in the context of the assigned map. Third were difficulties regarding mirror images and chirality and fourth were difficulties involving what may be described as the geometric isomer-diastereomer problem. The fifth type of difficulty dealt with improper relationships between structural isomers and stereoisomers. Finally, the sixth type of difficulty involved definitions that were too narrow. These types are listed in Table 8.39, with specific examples given in Table 8.40.

Results of Concept Map 10. Concept map 10, which had the seed concepts "nucleophile", "leaving group", "racemization", "inversion", and "substitution", was
Table 8.31. Statistical Analysis of Concept Map 8.

Seed concepts: enantiomer, racemate, mirror image, inversion, absolute configuration, resolution

<table>
<thead>
<tr>
<th>Superordinate Concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer(s)</td>
<td>42.2%</td>
<td>75.0%</td>
</tr>
<tr>
<td>optical isomer(ism)</td>
<td>28.4%</td>
<td>10.5%</td>
</tr>
<tr>
<td>isomer(s)</td>
<td>6.9%</td>
<td>5.3%</td>
</tr>
<tr>
<td>stereochemistry</td>
<td>4.3%</td>
<td>0.0%</td>
</tr>
<tr>
<td>chiral carbon/atom(s)</td>
<td>4.3%</td>
<td>0.0%</td>
</tr>
<tr>
<td>racemate</td>
<td>3.4%</td>
<td>3.9%</td>
</tr>
<tr>
<td>nucleophilic substitution</td>
<td>0.0%</td>
<td>2.6%</td>
</tr>
<tr>
<td>absolute configuration</td>
<td>1.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>resolution</td>
<td>1.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>others&lt;sup&gt;b&lt;/sup&gt;</td>
<td>6.9%</td>
<td>2.6%</td>
</tr>
</tbody>
</table>

Percent of students choosing concept

Mean rank of seed concepts:

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer</td>
<td>1.40</td>
<td>1.17</td>
</tr>
<tr>
<td>mirror image</td>
<td>2.76</td>
<td>2.67</td>
</tr>
<tr>
<td>racemate</td>
<td>3.77</td>
<td>3.85</td>
</tr>
<tr>
<td>inversion</td>
<td>4.31</td>
<td>4.58</td>
</tr>
<tr>
<td>absolute configuration</td>
<td>4.36</td>
<td>4.36</td>
</tr>
<tr>
<td>resolution</td>
<td>4.40</td>
<td>4.36</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;c&lt;/sup&gt;</td>
<td>.4542</td>
<td>.5637</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents 116 concept maps from Fall, 1997 and 76 concept maps from Spring, 1998.

<sup>b</sup>Represents concepts chosen by only one participant.

<sup>c</sup>Represents the Kendall coefficient of concordance.
Table 8.32. Individual Statistical Comparisons of Seed Concepts from Map 8 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer</td>
<td>1.03</td>
<td>racemate</td>
<td>1.97</td>
<td>.9098</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.05</td>
<td>inversion</td>
<td>1.95</td>
<td>.8373</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.05</td>
<td>resolution</td>
<td>1.95</td>
<td>.8030</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.06</td>
<td>absolute</td>
<td>configuration</td>
<td>1.94</td>
<td>.7986</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.21</td>
<td>mirror image</td>
<td>1.79</td>
<td>.3603</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.31</td>
<td>racemate</td>
<td>1.69</td>
<td>.2164</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.24</td>
<td>inversion</td>
<td>1.76</td>
<td>.3148</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.22</td>
<td>resolution</td>
<td>1.78</td>
<td>.4070</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.20</td>
<td>absolute</td>
<td>configuration</td>
<td>1.80</td>
<td>.4294</td>
</tr>
<tr>
<td>racemate</td>
<td>1.38</td>
<td>inversion</td>
<td>1.62</td>
<td>.0852</td>
<td>.0104</td>
</tr>
<tr>
<td>racemate</td>
<td>1.32</td>
<td>resolution</td>
<td>1.68</td>
<td>.1697</td>
<td>.0003</td>
</tr>
<tr>
<td>racemate</td>
<td>1.41</td>
<td>absolute</td>
<td>configuration</td>
<td>1.59</td>
<td>.0439</td>
</tr>
<tr>
<td>inversion</td>
<td>1.47</td>
<td>resolution</td>
<td>1.53</td>
<td>.0059</td>
<td>.5002</td>
</tr>
<tr>
<td>inversion</td>
<td>1.51</td>
<td>absolute</td>
<td>configuration</td>
<td>1.49</td>
<td>.0002</td>
</tr>
<tr>
<td>resolution</td>
<td>1.46</td>
<td>absolute</td>
<td>configuration</td>
<td>1.54</td>
<td>.0081</td>
</tr>
</tbody>
</table>
Table 8.33. Individual Statistical Comparisons of Seed Concepts from Map 8 for the Spring, 1998, Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>enantiomer</td>
<td>1.06</td>
<td>racemate</td>
<td>1.94</td>
<td>.7996</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.02</td>
<td>inversion</td>
<td>1.98</td>
<td>.9091</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.00</td>
<td>resolution</td>
<td>2.00</td>
<td>1.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.02</td>
<td>absolute configuration</td>
<td>1.98</td>
<td>.9091</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.07</td>
<td>mirror image</td>
<td>1.93</td>
<td>.7404</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.27</td>
<td>racemate</td>
<td>1.73</td>
<td>.2907</td>
<td>.0004</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.13</td>
<td>inversion</td>
<td>1.87</td>
<td>.6615</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.20</td>
<td>resolution</td>
<td>1.80</td>
<td>.5240</td>
<td>.0000</td>
</tr>
<tr>
<td>mirror image</td>
<td>1.15</td>
<td>absolute configuration</td>
<td>1.85</td>
<td>.6156</td>
<td>.0000</td>
</tr>
<tr>
<td>racemate</td>
<td>1.34</td>
<td>inversion</td>
<td>1.66</td>
<td>.1628</td>
<td>.0082</td>
</tr>
<tr>
<td>racemate</td>
<td>1.43</td>
<td>resolution</td>
<td>1.57</td>
<td>.0262</td>
<td>.2888</td>
</tr>
<tr>
<td>racemate</td>
<td>1.41</td>
<td>absolute configuration</td>
<td>1.59</td>
<td>.0438</td>
<td>.1701</td>
</tr>
<tr>
<td>inversion</td>
<td>1.55</td>
<td>resolution</td>
<td>1.45</td>
<td>.0109</td>
<td>.4927</td>
</tr>
<tr>
<td>inversion</td>
<td>1.52</td>
<td>absolute configuration</td>
<td>1.48</td>
<td>.0027</td>
<td>.7316</td>
</tr>
<tr>
<td>resolution</td>
<td>1.53</td>
<td>absolute configuration</td>
<td>1.47</td>
<td>.0084</td>
<td>.5485</td>
</tr>
</tbody>
</table>
Table 8.34. Types of Difficulties Identified from Concept Map 8.

I) Interesting or unusual
   A) Comments about absolute configuration
   B) Comments about enantiomers
      1) Enantiomers and chirality
      2) Other comments about enantiomers
   C) Comments about resolution

II) Naive

III) Difficulties with meaning of inversion
   A) Inversion as exchange of substituents
   B) Inversion as only possible with certain classes of compounds
   C) Inversion as a property instead of a process
   D) Inversion and chirality

IV) Difficulties with absolute configuration

V) Difficulties involving resolution
   A) Resolution of diastereomers
   B) Resolution as a process that does not involve separation
   C) Processes used to effect resolution

VI) Difficulties involving racemates
   A) Racemates as single compounds
   B) Racemates as achiral.
   C) Inevitability of formation of racemates.
      1) From achiral reagents
      2) From chiral reagents

VII) Difficulties regarding relationships between types of isomers.
   A) Enantiomers and diastereomers
   B) Geometric isomers and enantiomers

VIII) Meaning of chirality
   A) Mirror images of diastereomers
   B) Chirality of enantiomers
   C) Chirality and structure
   D) Other
Table 8.35. Selected Difficulties Identified from Concept Map 8.

<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA</td>
<td>Absolute configuration is asking, &quot;What is the shape of the actual molecule?&quot;</td>
</tr>
<tr>
<td>IA</td>
<td>Absolute configuration is their position in space.</td>
</tr>
<tr>
<td>IB1</td>
<td>Enantiomers have at least one chiral atom, usually carbon.</td>
</tr>
<tr>
<td>IB1</td>
<td>One chiral atom implies one pair of enantiomers.</td>
</tr>
<tr>
<td>IB2</td>
<td>Enantiomers may be optically inactive especially racemic mixtures and meso compounds.</td>
</tr>
<tr>
<td>IB2</td>
<td>Enantiomers undergo inversion in $S_n2$ reactions.</td>
</tr>
<tr>
<td>IC</td>
<td>Resolution can be done by mechanical means, microorganisms, diastereomers. (The first two are &quot;impractical;&quot; the last is &quot;most practical.&quot;)</td>
</tr>
<tr>
<td>II</td>
<td>Chiral atoms form enantiomers. Chiral atoms form diastereomers.</td>
</tr>
<tr>
<td>II</td>
<td>Diastereomers involve inversion.</td>
</tr>
<tr>
<td>II</td>
<td>Optical isomerism involves mirror images.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Chiral carbon compounds may have inversion of their stereochemistry if exchange only two substituents.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Enantiomers always have a chiral atom when 2 of the atoms substituents are swapped inversion occurs.</td>
</tr>
<tr>
<td>IIIA</td>
<td>If the substituents are inverted, an inversion of configuration takes place.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Inversion of any two substituents on a chiral atom gives you an enantiomer.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Inversion occurs when the alkyl halide is optically active.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Optical isomers of alkyl halides can undergo inversion of configuration.</td>
</tr>
<tr>
<td>IIIC</td>
<td>Enantiomer can have inversion, e.g. socks, achiral.</td>
</tr>
<tr>
<td>IIIC</td>
<td>Enantiomer is a molecule with a mirror images which is inversion.</td>
</tr>
<tr>
<td>IIIC</td>
<td>Enantiomers can be thought of in pairs differing in a 90° inversion around a chiral carbon.</td>
</tr>
<tr>
<td>IIIC</td>
<td>R- and S- are inversions.</td>
</tr>
<tr>
<td>IIID</td>
<td>Enantiomers have the same physical properties except for the direction of inversion of plane polarized light.</td>
</tr>
<tr>
<td>IIID</td>
<td>Enantiomers undergo rotation and inversion to form nonsuperimposable mirror images.</td>
</tr>
<tr>
<td>IIID</td>
<td>Mirror images are not meso compounds which are superimposable and formed by inversion.</td>
</tr>
<tr>
<td>IV</td>
<td>Enantiomers are composed of racemates can be chemically separated includes physical separation than inversion resulting in absolute configuration.</td>
</tr>
<tr>
<td>IV</td>
<td>Enantiomers consist of chiral carbon defined as a carbon atom attached to four different substituents rotates to form absolute configuration.</td>
</tr>
<tr>
<td>IV</td>
<td>Enantiomers have 2 different absolute configurations; each is called a racemate.</td>
</tr>
<tr>
<td>IV</td>
<td>Inversion results in absolute configuration.</td>
</tr>
<tr>
<td>IV</td>
<td>Racemic mixture are inversions have absolute configuration have different resolutions.</td>
</tr>
<tr>
<td>VA</td>
<td>Diastereomers are separated by resolution.</td>
</tr>
<tr>
<td>VA</td>
<td>Enantiomers are diastereomers separated by resolution.</td>
</tr>
<tr>
<td>VA</td>
<td>Enantiomers or mirror images are not diastereomers which have to be separated by resolution.</td>
</tr>
</tbody>
</table>
Table 8.35 (cont.).

VB Enantiomers: in nature they cause resolution.
VB Optical isomers can be chiral diastereomers are not mirror images but can be converted to enantiomers by resolution.
VB Optical isomers can be enantiomers which are in resolution when in nature.
VC Enantiomers are nonsuperimposable mirror images in their absolute configuration and can only be separated by resolution because of inversion of structure.
VC Enantiomers are nonsuperimposable mirror images separated by resolution (which is) crystallization or distillation.
VC Nonsuperimposable mirror images are separated by mechanical resolution.
VIA Enantiomers are isomers that are nonsuperimposable mirror images or compounds which are resolved naturally into racemic mixtures.
VIA Enantiomers are mirror images that are inversions known as racemate.
VIA Enantiomers are mirror images that are racemates.
VIA Enantiomers are racemates that cause the rotation of plane polarized light.
VIA Enantiomers include racemate enantiomers which are "resolved enantiomers."
VIA Racemate is considered a salt of a racemic mixture.
VIB Enantiomers may be achiral reagents that are racemates.
VIB Isomers can be achiral, has two substituents the same, like RCHX₂, can have racemic mixture.
VIB Racemic mixture is optically inactive and an example is a meso compound.
VIC1 Achiral reagents lead to racemates.
VIC2 Optical isomers are not achiral atoms form racemic products.
VIIA Enantiomer is opposite of diastereomer.
VIIA Enantiomers are mirror images are not diastereomers.
VIIA Enantiomers which vary only in the arrangements of their atoms in space are called diastereomers and can be separated from one another by resolution.
VIIIB Geometric isomers can be cis-trans can be enantiomers.
VIIIB Geometric isomers can be enantiomers.
VIIIA Optical isomer can be diastereomers do not have mirror images.
VIIIA Optical isomerism consists of chiral carbon compounds which don't have mirror images such as diastereomers.
VIIAI Optical isomers without mirror images are diastereomers.
VIIIB Enantiomers are mirror images can be superimposable which is achiral.
VIIIB Enantiomers may be achiral reagents.
VIIIC Optical isomers are identical in structure but vary as mirror images.
VIIIC Optical isomers are identical in structure. (Examples are the two enantiomers of lactic acid.)
VIID A chiral carbon atom has isomers called enantiomers.
VIID Mirror images that are superimposable are meso compounds have at least 2 chiral atoms.

aRefers to difficulty type identified in Table 8.34.
Table 8.36. Statistical Analysis of Concept Map 9.

Seed concepts: isomer, structural isomer, stereoisomer, enantiomer, diastereomer

<table>
<thead>
<tr>
<th>Superordinate Concept</th>
<th>Percent of Students Choosing Concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer(s)</td>
<td>79.8%</td>
<td>93.4%</td>
<td></td>
</tr>
<tr>
<td>optical isomer(s)</td>
<td>5.0%</td>
<td>2.6%</td>
<td></td>
</tr>
<tr>
<td>compound(s)</td>
<td>4.2%</td>
<td>2.6%</td>
<td></td>
</tr>
<tr>
<td>enantiomers</td>
<td>2.5%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>stereoisomers</td>
<td>1.7%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>diastereomers</td>
<td>1.7%</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>others&lt;sup&gt;b&lt;/sup&gt;</td>
<td>5.0%</td>
<td>3.9%</td>
<td></td>
</tr>
</tbody>
</table>

Mean rank of seed concept

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer</td>
<td>1.05</td>
<td>1.00</td>
</tr>
<tr>
<td>structural isomer</td>
<td>2.72</td>
<td>2.54</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>2.84</td>
<td>2.83</td>
</tr>
<tr>
<td>enantiomer</td>
<td>4.24</td>
<td>4.29</td>
</tr>
<tr>
<td>diastereomer</td>
<td>4.15</td>
<td>4.35</td>
</tr>
</tbody>
</table>

Value

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;c&lt;/sup&gt;</td>
<td>.7930</td>
<td>.8771</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents 119 concept maps from Fall, 1997 and 76 concept maps from Spring, 1998.

<sup>b</sup>Represents concepts chosen by only one participant.

<sup>c</sup>Represents the Kendall coefficient of concordance.
Table 8.37. Individual Statistical Comparisons of Seed Concepts from Map 9 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer</td>
<td>1.00</td>
<td>structural isomer</td>
<td>2.00</td>
<td>.9909</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.01</td>
<td>stereoisomer</td>
<td>1.99</td>
<td>.9553</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.01</td>
<td>enantiomer</td>
<td>1.99</td>
<td>.9820</td>
<td>.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.02</td>
<td>diastereomer</td>
<td>1.98</td>
<td>.9202</td>
<td>.0000</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.45</td>
<td>stereoisomer</td>
<td>1.55</td>
<td>.0649</td>
<td>.0075</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.13</td>
<td>enantiomer</td>
<td>1.87</td>
<td>.6554</td>
<td>.0000</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.14</td>
<td>diastereomer</td>
<td>1.86</td>
<td>.6465</td>
<td>.0000</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.15</td>
<td>enantiomer</td>
<td>1.85</td>
<td>.6002</td>
<td>.0000</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.16</td>
<td>diastereomer</td>
<td>1.84</td>
<td>.5825</td>
<td>.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.53</td>
<td>diastereomer</td>
<td>1.47</td>
<td>.0126</td>
<td>.2368</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>isomer</td>
<td>1.00</td>
<td>structural isomer</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.00</td>
<td>stereoisomer</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.00</td>
<td>enantiomer</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>isomer</td>
<td>1.00</td>
<td>diastereomer</td>
<td>2.00</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.43</td>
<td>stereoisomer</td>
<td>1.57</td>
<td>0.1116</td>
<td>0.0067</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.05</td>
<td>enantiomer</td>
<td>1.95</td>
<td>0.8646</td>
<td>0.0000</td>
</tr>
<tr>
<td>structural isomer</td>
<td>1.05</td>
<td>diastereomer</td>
<td>1.95</td>
<td>0.8939</td>
<td>0.0000</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.14</td>
<td>enantiomer</td>
<td>1.86</td>
<td>0.6019</td>
<td>0.0000</td>
</tr>
<tr>
<td>stereoisomer</td>
<td>1.12</td>
<td>diastereomer</td>
<td>1.88</td>
<td>0.7015</td>
<td>0.0000</td>
</tr>
<tr>
<td>enantiomer</td>
<td>1.48</td>
<td>diastereomer</td>
<td>1.52</td>
<td>0.0091</td>
<td>0.4387</td>
</tr>
</tbody>
</table>

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Table 8.39. Types of Difficulties Identified from Concept Map 9.

I) Interesting or unusual
   A) Relationships between types of stereoisomers
      1) Classification of stereoisomers primarily through use of mirror images
      2) Classification of stereoisomers primarily through absolute configuration or chirality
      3) Relationship between enantiomers and diastereomers
      4) Relationship between geometric isomers, stereoisomers, and diastereomers
   B) Issues of superimposability
   C) Classification of given types of isomers
      1) Classification of "isomer"
      2) Classification of "stereoisomer" and "optical isomer"
      3) Classification of "diastereomer"

II) Naive
    A) Stereoisomers/optical isomers classified separately from enantiomers and diastereomers
    B) Stereoisomers seen as different from optical isomers
    C) Other

III) Difficulties involving mirror images and chirality
    A) Relationships between mirror images and structural and optical isomers
    B) Relationships between mirror images and geometric isomers and diastereomers

IV) The geometric isomer-diastereomer problem
    A) No relationship shown
       1) Issue is avoided
       2) No link between these concepts
       3) Geometric isomers and diastereomers both seen as types of stereoisomers
    B) faulty relationship

V) Improper relationships between structural isomers and stereoisomers
   A) Structural isomer includes some types of stereoisomers
   B) Some type of stereoisomers include structural isomers
      1) Improper relationships
      2) Improper examples

VI) Definitions too narrow
    A) Isomer too narrowly defined
    B) Stereoisomer/optical isomer too narrowly defined
    C) enantiomer/diastereomer too narrowly defined
Table 8.40. Selected Difficulties Identified from Concept Map 9.

<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA1</td>
<td>Diastereomers are optical isomers that are not mirror images.</td>
</tr>
<tr>
<td>IA1</td>
<td>Geometric isomers are a type of stereoisomer. Enantiomers are diastereomers that are nonsuperimposable mirror images.</td>
</tr>
<tr>
<td>IA1</td>
<td>Optical isomers are identical in structure but differ in mirror images.</td>
</tr>
<tr>
<td>IA1</td>
<td>Optical isomers include isomers that are not mirror images (diastereomers).</td>
</tr>
<tr>
<td>IA2</td>
<td>Diastereomers contain dissimilar chiral carbon atoms.</td>
</tr>
<tr>
<td>IA2</td>
<td>Optical isomer formed from chiral atom such as enantiomer which can be diastereomer.</td>
</tr>
<tr>
<td>IA2</td>
<td>Optical isomers are shown by absolute configuration to be diastereomers or enantiomers.</td>
</tr>
<tr>
<td>IA3</td>
<td>Diastereomer can be enantiomer.</td>
</tr>
<tr>
<td>IA3</td>
<td>Diastereomers are optical isomers that aren’t enantiomers.</td>
</tr>
<tr>
<td>IA3</td>
<td>Diastereomers can be geometric or enantiomers.</td>
</tr>
<tr>
<td>IA3</td>
<td>Enantiomers are a type of diastereomer.</td>
</tr>
<tr>
<td>IA3</td>
<td>Enantiomers are always diastereomers.</td>
</tr>
<tr>
<td>IA4</td>
<td>Diastereomer is a type of isomer and can be a stereoisomer.</td>
</tr>
<tr>
<td>IA4</td>
<td>Diastereomers are caused by more than one chiral atom.</td>
</tr>
<tr>
<td>IA4</td>
<td>Geometric isomers are classed as diastereomers. An example of a diastereomer is an &quot;optical diastereomer.&quot;</td>
</tr>
<tr>
<td>IA4</td>
<td>Isomers are structural, diastereomers, stereoisomers. Diastereomers and stereoisomers both include geometric isomers.</td>
</tr>
<tr>
<td>IA4</td>
<td>Stereoisomers can be geometric which have restricted rotation. Stereoisomers can be others which have no restricted rotation. Geometric isomers can be enantiomers or diastereomers.</td>
</tr>
<tr>
<td>IA4</td>
<td>Cis-trans isomerism cannot be found in enantiomers. Cis-trans-isomerism can be found in diastereomers. (The example given is diastereomers of 4-chloro-2-butanol.)</td>
</tr>
<tr>
<td>IB</td>
<td>Mirror image can be meso is superimposable. (Are there any other superimposable mirror images?)</td>
</tr>
<tr>
<td>IB</td>
<td>Optical isomers superimposable on mirror images are meso compounds.</td>
</tr>
<tr>
<td>IC1</td>
<td>(Describes isomers by &quot;various bonding attachments&quot; vs &quot;similar bond attachments.&quot;)</td>
</tr>
<tr>
<td>IC2</td>
<td>Stereoisomers have the same molecular formula and the same structural formula.</td>
</tr>
<tr>
<td>IC2</td>
<td>Stereoisomers that vary in spatial orientations can be enantiomers or diastereomers.</td>
</tr>
<tr>
<td>IC3</td>
<td>Diastereomers AKA epimers.</td>
</tr>
<tr>
<td>IC3</td>
<td>(Uses the term &quot;chiral diastereomers,&quot; and classifies geometric isomers separately)</td>
</tr>
<tr>
<td>IC3</td>
<td>(Uses the term &quot;optical&quot; followed by &quot;diastereomers&quot;)</td>
</tr>
<tr>
<td>IIA</td>
<td>(Enantiomers, geometric isomers, diastereomers are not classified as stereoisomers.)</td>
</tr>
<tr>
<td>IIA</td>
<td>(Optical isomers are not classes as stereoisomers.)</td>
</tr>
<tr>
<td>IIB</td>
<td>(Stereoisomers classified differently from enantiomers and diastereomers).</td>
</tr>
<tr>
<td>IIC</td>
<td>Stereoisomers have different bond angles.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Optical isomers are isomers that vary as mirror images.</td>
</tr>
<tr>
<td>IIIA</td>
<td>Optical isomers are mirror images, but optical isomers that are not mirror images are diastereomers.</td>
</tr>
</tbody>
</table>
Table 8.40 (cont.).

<table>
<thead>
<tr>
<th>IIIA</th>
<th>Structural isomers are related as mirror images.</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIIB</td>
<td>Diastereomers are distinguished by not having a mirror image.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Diastereomers are mirror images.</td>
</tr>
<tr>
<td>IIIB</td>
<td>Geometric can be cis-is superimposable on mirror image called meso compound, e.g. cis-1,2-dibromocyclopentane. (NB: This is correct in this example.)</td>
</tr>
<tr>
<td>IIIB</td>
<td>Geometric can be trans is nonsuperimposable, e.g. R,R- and S,S-1,2-dibromocyclopropane. (NB: This is correct in this example.)</td>
</tr>
<tr>
<td>IVA1</td>
<td>(Avoids the issue of geometric isomers being diastereomers.)</td>
</tr>
<tr>
<td>IVA2</td>
<td>(Geometric isomers are not seen as diastereomers.)</td>
</tr>
<tr>
<td>IVA3</td>
<td>(Geometric isomers are types of stereoisomers, but not types of diastereomers.)</td>
</tr>
<tr>
<td>IVB</td>
<td>(Diastereomers are optical isomers but not geometric isomers.)</td>
</tr>
<tr>
<td>IVB</td>
<td>Geometric isomers can be enantiomers or diastereomers or stereoisomers.</td>
</tr>
<tr>
<td>VA</td>
<td>A structural isomer can be a diastereomer, stereoisomer, or enantiomer.</td>
</tr>
<tr>
<td>VA</td>
<td>Structural isomers can be diastereomers which are either meso or nonmeso.</td>
</tr>
<tr>
<td>VB1</td>
<td>Diastereomers can be structural isomers.</td>
</tr>
<tr>
<td>VB1</td>
<td>Geometric isomers can be structural isomers.</td>
</tr>
<tr>
<td>VB1</td>
<td>Optical isomers include structural isomers.</td>
</tr>
<tr>
<td>VB2</td>
<td>(Cyclopropane and cyclobutane are given as examples of stereoisomers.)</td>
</tr>
<tr>
<td>VB2</td>
<td>(The compounds 1-pentanol and 2-pentanol are stereoisomers.)</td>
</tr>
<tr>
<td>VB2</td>
<td>(Two stereoisomers are two different dash formulas of n-butane.)</td>
</tr>
<tr>
<td>VIA</td>
<td>Isomers are compounds with same molecular formula but differ in structural formulas.</td>
</tr>
<tr>
<td>VIA</td>
<td>Isomers are either enantiomers, diastereomers, or stereoisomers.</td>
</tr>
<tr>
<td>VIA</td>
<td>Isomers can be chiral atom. (The verb was &quot;have&quot;, but was crossed out.)</td>
</tr>
<tr>
<td>VIA</td>
<td>Isomers can be stereoisomers with cis-configuration or trans-configuration. (This map contains mention of geometric isomers or that enantiomers are stereoisomers).</td>
</tr>
<tr>
<td>VIA</td>
<td>(Isomers are all classed as being alkenes.)</td>
</tr>
<tr>
<td>VIA</td>
<td>(Isomers are all classed in terms of no free rotation.)</td>
</tr>
<tr>
<td>VIB</td>
<td>(Diastereomers and enantiomers are not classed as stereoisomers.)</td>
</tr>
<tr>
<td>VIB</td>
<td>Isomer can be structural isomer, stereoisomer, enantiomer.</td>
</tr>
<tr>
<td>VIB</td>
<td>(Optical isomer and stereoisomer are unrelated concepts.)</td>
</tr>
<tr>
<td>VIB</td>
<td>(Optical isomers are enantiomers. Diastereomers are separate.)</td>
</tr>
<tr>
<td>VIB</td>
<td>Stereoisomers classed as being different from enantiomers and diastereomers. Examples of stereoisomers are cis- and trans-.</td>
</tr>
<tr>
<td>VIC</td>
<td>(Diastereomer is classed as a type of enantiomer.)</td>
</tr>
<tr>
<td>VIC</td>
<td>(Enantiomers and diastereomers are both types of isomers, but appear to be independent of each other.)</td>
</tr>
<tr>
<td>VIC</td>
<td>(Only enantiomers are described as chiral. The term isn't used to describe diastereomers.)</td>
</tr>
</tbody>
</table>

\[ a \] Items in parentheses are summarized from individual concept maps.  
\[ b \] Refers to alternative conception type identified in Table 8.39.
assigned in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the
first choice of superordinate concept for this map was "substitution" or "substitution
reaction" (62.1% and 64.4% of respondents, respectively). Analysis of concordance of
ordinal rank of these concepts for each semester gave values of Kendall's W of .6866 and
.6149, respectively, both of which are significant at the .0000 level. Results of these
calculations are given in Tables 8.41, 8.41, and 8.43.

Qualitative analysis of the concept maps yielded five major types of difficulties. First
were propositions in which the leaving group was too specific. Second were improper
conclusions regarding stereochemistry. The next two types of difficulties dealt with
improper assumption of chirality of reagents and incorrect action of the nucleophile.
Finally, the fifth type of difficulty involved incorrect attribution of mechanism or
conditions favoring mechanism. These types are listed in Table 8.44, with specific
examples given in Table 8.45.

Results of Concept Map 11. Concept map 11, which had the seed concepts
"alcohol", "alkoxonium ion", "alkene", "proton", and "elimination", was assigned in
both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of
superordinate concept for this map was "alcohol" or "alcohols" (66.1% and 75.4% of
respondents, respectively). Analysis of concordance of ordinal rank of these concepts for
each semester gave values of Kendall's W of .5593 and .4953, respectively, both of
which are significant at the .0000 level. Results of these calculations are given in Tables
8.46, 8.47, and 8.48.

Qualitative analysis of the concept maps yielded five major types of difficulties.
First were propositions that were interesting or unusual but not necessarily incorrect and
next were propositions that, while not incorrect, would be considered naive in the context
of the assigned map. The next two types of difficulties dealt with misattribution of
substituents and difficulties with mechanisms. Finally, the fifth type of difficulty
Table 8.41. Statistical Analysis of Concept Map 10.

Seed concepts: nucleophile, leaving group, racemization, inversion, substitution

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Percent of students choosing concept</th>
<th>Percent of students choosing concept</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Superordinate Concept</td>
<td></td>
<td></td>
</tr>
<tr>
<td>substitution (reaction)</td>
<td>62.1%</td>
<td>64.4%</td>
</tr>
<tr>
<td>nucleophile</td>
<td>9.2%</td>
<td>26.0%</td>
</tr>
<tr>
<td>alkyl halides</td>
<td>5.9%</td>
<td>0.0%</td>
</tr>
<tr>
<td>mechanism</td>
<td>4.2%</td>
<td>0.0%</td>
</tr>
<tr>
<td>alkyl halide reactions</td>
<td>2.5%</td>
<td>0.0%</td>
</tr>
<tr>
<td>reactions</td>
<td>2.5%</td>
<td>0.0%</td>
</tr>
<tr>
<td>nucleophilic reactions</td>
<td>1.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>organic halogen compounds</td>
<td>1.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>others&lt;sup&gt;b&lt;/sup&gt;</td>
<td>10.1%</td>
<td>6.8%</td>
</tr>
<tr>
<td>unclear choice&lt;sup&gt;c&lt;/sup&gt;</td>
<td>0.0%</td>
<td>2.7%</td>
</tr>
</tbody>
</table>

Mean rank of seed concept

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Mean rank of seed concept</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>substitution</td>
<td>1.16</td>
</tr>
<tr>
<td>nucleophile</td>
<td>2.48</td>
</tr>
<tr>
<td>leaving group</td>
<td>3.10</td>
</tr>
<tr>
<td>inversion</td>
<td>4.05</td>
</tr>
<tr>
<td>racemization</td>
<td>4.21</td>
</tr>
</tbody>
</table>

Value

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;d&lt;/sup&gt;</td>
<td>.6866</td>
<td>.6149</td>
</tr>
<tr>
<td>significance</td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

<sup>a</sup> Represents 119 concept maps from Fall, 1997 and 73 concept maps from Spring, 1998.

<sup>b</sup> Represents concepts chosen by only one participant.

<sup>c</sup> Represents maps without a clear superordinate concept.

<sup>d</sup> Represents the Kendall coefficient of concordance.
Table 8.42. Individual Statistical Comparisons of Seed Concepts from Map 10 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>substitution</td>
<td>1.10</td>
<td>nucleophile</td>
<td>1.90</td>
<td>.6341</td>
<td>.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.04</td>
<td>leaving group</td>
<td>1.96</td>
<td>.9078</td>
<td>.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.01</td>
<td>inversion</td>
<td>1.99</td>
<td>.9815</td>
<td>.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.01</td>
<td>racemization</td>
<td>1.99</td>
<td>.9540</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.31</td>
<td>leaving group</td>
<td>1.69</td>
<td>.2149</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.14</td>
<td>inversion</td>
<td>1.86</td>
<td>.5779</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.13</td>
<td>racemization</td>
<td>1.87</td>
<td>.6047</td>
<td>.0000</td>
</tr>
<tr>
<td>leaving group</td>
<td>1.23</td>
<td>inversion</td>
<td>1.77</td>
<td>.3314</td>
<td>.0000</td>
</tr>
<tr>
<td>leaving group</td>
<td>1.21</td>
<td>racemization</td>
<td>1.79</td>
<td>.3868</td>
<td>.0000</td>
</tr>
<tr>
<td>inversion</td>
<td>1.44</td>
<td>racemization</td>
<td>1.56</td>
<td>.0648</td>
<td>.0082</td>
</tr>
</tbody>
</table>

Table 8.43. Individual Statistical Comparisons of Seed Concepts from Map 10 for the Spring, 1998, Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>substitution</td>
<td>1.30</td>
<td>nucleophile</td>
<td>1.70</td>
<td>.1600</td>
<td>.0008</td>
</tr>
<tr>
<td>substitution</td>
<td>1.08</td>
<td>leaving group</td>
<td>1.92</td>
<td>.7207</td>
<td>.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.05</td>
<td>inversion</td>
<td>1.95</td>
<td>.8217</td>
<td>.0000</td>
</tr>
<tr>
<td>substitution</td>
<td>1.01</td>
<td>racemization</td>
<td>1.99</td>
<td>.9437</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.24</td>
<td>leaving group</td>
<td>1.76</td>
<td>.3835</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.12</td>
<td>inversion</td>
<td>1.88</td>
<td>.5989</td>
<td>.0000</td>
</tr>
<tr>
<td>nucleophile</td>
<td>1.14</td>
<td>racemization</td>
<td>1.86</td>
<td>.5546</td>
<td>.0000</td>
</tr>
<tr>
<td>leaving group</td>
<td>1.19</td>
<td>inversion</td>
<td>1.81</td>
<td>.4321</td>
<td>.0000</td>
</tr>
<tr>
<td>leaving group</td>
<td>1.20</td>
<td>racemization</td>
<td>1.80</td>
<td>.3937</td>
<td>.0000</td>
</tr>
<tr>
<td>inversion</td>
<td>1.46</td>
<td>racemization</td>
<td>1.54</td>
<td>.0321</td>
<td>.1336</td>
</tr>
</tbody>
</table>

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Table 8.44. Types of Difficulties Identified from Concept Map 10.

I) Leaving group too specific.
   A) Leaving group is halogen or halide.
   B) Alkyl halides undergo substitution.
   C) Leaving group is alkyl halide.

II) Improper conclusions regarding stereochemistry.
   A) Relationships between mechanism and stereochemistry
   B) Nature and process of racemization and inversion.
      1) Products of inversion
      2) Product vs. process
      3) Mechanism, inversion, and racemization

III) Improper assumption of chirality of reagents.

IV) Incorrect action of the nucleophile.
   A) Nucleophile shares or donates electrons rather than electron pairs.
   B) Action of the nucleophile confused with action of the leaving group.

V) Incorrect attribution of mechanism or conditions favoring mechanism.
   A) Substitution vs elimination.
   B) Conditions favoring certain mechanisms.
   C) Mechanisms of substitution.
      1) Nature of the intermediate
      2) Nature of the transition state
<table>
<thead>
<tr>
<th>Type</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>IA</td>
<td>A halide departs and forms the leaving group.</td>
</tr>
<tr>
<td>IA</td>
<td>A leaving group is also known as a halogen and is a weak base.</td>
</tr>
<tr>
<td>IB</td>
<td>Alkyl halides can undergo nucleophilic substitution.</td>
</tr>
<tr>
<td>IB</td>
<td>Nucleophilic substitution occurs between nucleophile and alkyl halide.</td>
</tr>
<tr>
<td>IC</td>
<td>Alkyl halide is termed the leaving group.</td>
</tr>
<tr>
<td>IC</td>
<td>Nucleophilic substitution involves a negative nucleophile which replaces an alkyl halide.</td>
</tr>
<tr>
<td>IIA</td>
<td>Achiral reagent forms 50% nucleophilic substitution, 50% elimination.</td>
</tr>
<tr>
<td>IIA</td>
<td>Elimination reactions may cause inversion.</td>
</tr>
<tr>
<td>IIB1</td>
<td>R- and S- are inversions of each other.</td>
</tr>
<tr>
<td>IIB1</td>
<td>SN2 involves a nucleophile causes inversion makes a different enantiomer.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Chiral carbons form enantiomers which form racemic mixtures.</td>
</tr>
<tr>
<td>IIB2</td>
<td>Inversion favors primary halides. Racemization favors tertiary halides.</td>
</tr>
<tr>
<td>IIB3</td>
<td>SN1 is a 2-step process in which a leaving group leaves forming a carbocation intermediate which the nucleophile attacks causing inversion of configuration and racemization.</td>
</tr>
<tr>
<td>IIB3</td>
<td>Substitution can be bimolecular causes racemization because of backside attack resulting in inversion.</td>
</tr>
<tr>
<td>III</td>
<td>SN1 causing racemization favors weak bases.</td>
</tr>
<tr>
<td>III</td>
<td>SN1 mechanism forms racemic mixture is mixture of enantiomers.</td>
</tr>
<tr>
<td>IVA</td>
<td>Nucleophile donates electrons to electrophiles which then replaces a leaving group to cause nucleophilic substitution.</td>
</tr>
<tr>
<td>IVA</td>
<td>Nucleophile is a species that donates electrons.</td>
</tr>
<tr>
<td>IVB</td>
<td>Nucleophile can go through nucleophilic substitution replacing a leaving group resulting in inversion if the alkyl halide or leaving group is optically inactive.</td>
</tr>
<tr>
<td>IVB</td>
<td>Nucleophile loses halide</td>
</tr>
<tr>
<td>VA</td>
<td>Reaction may be substitution or elimination that occurs by both SN1 and SN2.</td>
</tr>
<tr>
<td>VA</td>
<td>SN1 in which nucleophile and leaving group do not depart simultaneously.</td>
</tr>
<tr>
<td>VA</td>
<td>SN2 in which nucleophile and leaving group depart simultaneously.</td>
</tr>
<tr>
<td>VB</td>
<td>SN1 where the leaving group leaves voluntarily and proceeds through a carbocation intermediate causes racemization involving primary halides.</td>
</tr>
<tr>
<td>VB</td>
<td>SN2 where the leaving group is forced out and proceeds through a transition state causes inversion involves tertiary halides.</td>
</tr>
<tr>
<td>VC1</td>
<td>Nucleophile attacks the planar carbocation; the reaction mechanisms are called SN1 and SN2.</td>
</tr>
<tr>
<td>VC1</td>
<td>SN2 the leaving group leaves and the nucleophile enters causing a carbocation intermediate.</td>
</tr>
<tr>
<td>VC2</td>
<td>SN1 in which the nucleophile enters then the leaving group departs. Proceeds through a transition state.</td>
</tr>
<tr>
<td>VC2</td>
<td>SN1 the nucleophile enters as the leaving group departs and is called transition state.</td>
</tr>
</tbody>
</table>

*aRefers to difficulty type identified in Table 8.44.*
Table 8.46. Statistical Analysis of Concept Map 11.

Seed concepts: alcohol, alkoxonium ion, alkene, proton, elimination

<table>
<thead>
<tr>
<th>Superordinate Concept</th>
<th>Percent of students choosing concept</th>
<th>Fall 1997</th>
<th>Spring 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol(s)</td>
<td></td>
<td>66.1%</td>
<td>75.4%</td>
</tr>
<tr>
<td>elimination</td>
<td></td>
<td>9.1%</td>
<td>7.2%</td>
</tr>
<tr>
<td>reactions of alcohols</td>
<td></td>
<td>5.0%</td>
<td>7.2%</td>
</tr>
<tr>
<td>dehydration</td>
<td></td>
<td>4.1%</td>
<td>0.0%</td>
</tr>
<tr>
<td>addition reactions</td>
<td></td>
<td>0.0%</td>
<td>2.9%</td>
</tr>
<tr>
<td>derivatives of water</td>
<td></td>
<td>2.5%</td>
<td>0.0%</td>
</tr>
<tr>
<td>C-H compounds</td>
<td></td>
<td>1.7%</td>
<td>0.0%</td>
</tr>
<tr>
<td>others</td>
<td></td>
<td>11.6%</td>
<td>7.2%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Mean rank of seed concept</th>
<th>Fall 1997</th>
<th>Spring 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td></td>
<td>1.23</td>
<td>1.32</td>
</tr>
<tr>
<td>elimination</td>
<td></td>
<td>2.43</td>
<td>2.48</td>
</tr>
<tr>
<td>alkene</td>
<td></td>
<td>3.73</td>
<td>3.64</td>
</tr>
<tr>
<td>proton</td>
<td></td>
<td>3.74</td>
<td>3.70</td>
</tr>
<tr>
<td>alkoxonium ion</td>
<td></td>
<td>3.88</td>
<td>3.85</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
<th>Fall 1997</th>
<th>Spring 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;c&lt;/sup&gt;</td>
<td></td>
<td>.5593</td>
<td>.4953</td>
</tr>
<tr>
<td>significance</td>
<td></td>
<td>.0000</td>
<td>.0000</td>
</tr>
<tr>
<td>degrees of freedom</td>
<td></td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents 121 concept maps from Fall, 1997 and 69 concept maps from Spring, 1998.

<sup>b</sup>Represents concepts chosen by only one participant.

<sup>c</sup>Represents the Kendall coefficient of concordance.
### Table 8.47. Individual Statistical Comparisons of Seed Concepts from Map 11 for the Fall, 1997, Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td>1.14</td>
<td>elimination</td>
<td>1.86</td>
<td>.5167</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.04</td>
<td>alkene</td>
<td>1.96</td>
<td>.8419</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.03</td>
<td>proton</td>
<td>1.97</td>
<td>.9283</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.02</td>
<td>alkoxonium ion</td>
<td>1.98</td>
<td>.9489</td>
<td>.0000</td>
</tr>
<tr>
<td>elimination</td>
<td>1.27</td>
<td>alkene</td>
<td>1.73</td>
<td>.2268</td>
<td>.0000</td>
</tr>
<tr>
<td>elimination</td>
<td>1.14</td>
<td>proton</td>
<td>1.86</td>
<td>.5642</td>
<td>.0000</td>
</tr>
<tr>
<td>elimination</td>
<td>1.15</td>
<td>alkoxonium ion</td>
<td>1.85</td>
<td>.4976</td>
<td>.0000</td>
</tr>
<tr>
<td>alkene</td>
<td>1.52</td>
<td>proton</td>
<td>1.48</td>
<td>.0020</td>
<td>.6588</td>
</tr>
<tr>
<td>alkene</td>
<td>1.52</td>
<td>alkoxonium ion</td>
<td>1.48</td>
<td>.0021</td>
<td>.6507</td>
</tr>
<tr>
<td>proton</td>
<td>1.43</td>
<td>alkoxonium ion</td>
<td>1.57</td>
<td>.0232</td>
<td>.1333</td>
</tr>
</tbody>
</table>

### Table 8.48. Individual Statistical Comparisons of Seed Concepts from Map 11 for the Spring, 1998, Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td>1.13</td>
<td>elimination</td>
<td>1.87</td>
<td>.5563</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.03</td>
<td>alkene</td>
<td>1.97</td>
<td>.9011</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.12</td>
<td>proton</td>
<td>1.88</td>
<td>.6080</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.04</td>
<td>alkoxonium ion</td>
<td>1.96</td>
<td>.8545</td>
<td>.0000</td>
</tr>
<tr>
<td>elimination</td>
<td>1.26</td>
<td>alkene</td>
<td>1.74</td>
<td>.2548</td>
<td>.0001</td>
</tr>
<tr>
<td>elimination</td>
<td>1.18</td>
<td>proton</td>
<td>1.82</td>
<td>.4447</td>
<td>.0000</td>
</tr>
<tr>
<td>elimination</td>
<td>1.18</td>
<td>alkoxonium ion</td>
<td>1.82</td>
<td>.4298</td>
<td>.0000</td>
</tr>
<tr>
<td>alkene</td>
<td>1.50</td>
<td>proton</td>
<td>1.50</td>
<td>.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>alkene</td>
<td>1.43</td>
<td>alkoxonium ion</td>
<td>1.57</td>
<td>.0232</td>
<td>.2382</td>
</tr>
<tr>
<td>proton</td>
<td>1.49</td>
<td>alkoxonium ion</td>
<td>1.51</td>
<td>.0003</td>
<td>.8909</td>
</tr>
</tbody>
</table>
Table 8.49. Types of Difficulties Identified from Concept Map 11.

I) Interesting or unusual

II) Naive
   A) References to nomenclature
   B) Statements about intermediates

III) Misattribution of substituents.
   A) alcohols as alkanes
   B) others

IV) Difficulties with mechanisms.
   A) Alkoxonium ion not related to elimination.
      1) Alkoxonium ion related to substitution.
         a) Elimination is entirely absent.
         b) Elimination simply seen as dehydration.
         b) Some aspect of mechanism of elimination is discussed.
         d) Mechanism of substitution is discussed, but not elimination.
      2) Alkoxonium ion stands alone.
         a) Alkoxonium ion forms from alcohols
            1) alkoxonium ions form from acid-base reaction or
               addition of proton
            2) method of formation of alkoxonium ion absent
         b) Alkoxonium ion not related to alcohols
   B) Formation of alkoxonium ions.
      1) Structure of alkoxonium ions.
      2) Process of formation of alkoxonium ions.
         a) alkoxonium ion formed by elimination
         b) alkoxonium ion formation not related to protons
   C) Difficulties regarding what eliminates.
      1) Protons eliminate
      2) Other species eliminate
   D) Acid-base difficulties.
      1) Conjugate acid - base difficulties
         a) acid seen as nucleophile
         b) difficulties with what species gain or lose protons
      2) Correct statement with incorrect example
   E) Other mechanistic difficulties
      1) Elimination reactions in alcohols can be E2.
      2) Substitution-elimination difficulties
      3) Wrong reaction conditions

V) Formation of incorrect products.
   A) Acid-base vs redox
   B) Other

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Table 8.50. Selected Difficulties Identified from Concept Map 11.

<table>
<thead>
<tr>
<th>Type</th>
<th>Alternative conception</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Attached note reads, &quot;This assignment reads like a recipe for the E1 dehydration reaction of an alcohol.&quot;</td>
</tr>
<tr>
<td>I</td>
<td>(Relates alkoxonium ions to ethers, RO(H)R⁺.)</td>
</tr>
<tr>
<td>II A</td>
<td>Alcohol has a change in nomenclature like an addition of the alkoxonium ion to change ethyl to ethoxy.</td>
</tr>
<tr>
<td>II B</td>
<td>Alcohol takes precedence over alkene in numbering.</td>
</tr>
<tr>
<td>III A</td>
<td>(Alcohols are weak acids and react with alkali metals to form strong bases. Alcohol not seen as weak base when alkoxonium ion formed.)</td>
</tr>
<tr>
<td>III B</td>
<td>Oxygen is produced with a positive charge making it have a dominating number of protons.</td>
</tr>
<tr>
<td>III A</td>
<td>Alcohols are alkanes e.g. R-OH in which H is replaced by OH and can form oxonium ions which are formed by hydrogen bonding.</td>
</tr>
<tr>
<td>III A</td>
<td>Carbon-hydrogen compound can be alkene e.g. amide.</td>
</tr>
<tr>
<td>III A</td>
<td>Elimination involving alcohols occurs when an alkane (e.g. 2-propanol) reacts with a H-proton (which is a catalyst) to form an alkene and water.</td>
</tr>
<tr>
<td>III B</td>
<td>Alcohol reacts with hydrogen halides through elimination reactions use hydrogen halides such as H₂SO₄, H₃PO₄.</td>
</tr>
<tr>
<td>III B</td>
<td>ROH is alkene in which hydrogen is replaced by OH.</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohol through substitution forms an alkoxonium ion. (Elimination is not related to alkoxonium ion.)</td>
</tr>
<tr>
<td>IV A</td>
<td>(Dehydration is seen as separate from elimination.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Elimination forms alkenes from a Lewis acid-Lewis base structure which loses a H₂O molecule. (Alkoxonium ion occurs in separate part of map)</td>
</tr>
<tr>
<td>IV A</td>
<td>(Alkoxonium ion is seen as intermediate in substitution but not elimination, although elimination requires H⁺ catalyst.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Reactions of alcohols can be substitution forms an alkoxonium ion as an intermediate. Reactions of alcohols can be elimination forms a double bond which is formed by removing a proton, for example H⁺. (Elimination and alkoxonium ion not seen as related.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohol plus proton gives alkoxonium ion and then carbocation. (Elimination is not related to alkoxonium ions.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohols can be added to alkoxonium ion to produce ethers. Alkoxonium ion has an extra proton. (The term 'alkoxonium ion' is not related to elimination.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohols can do elimination the alcohol plus proton equals alkene.&quot; (The term &quot;alkoxonium ion&quot; is in the branch of the map dealing with substitution.&quot;</td>
</tr>
<tr>
<td>IV A</td>
<td>(Alkoxonium ion is not linked to elimination, it just forms in an acid-base reaction.)</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohols do not form alkoxonium ions. Alcohols form alkenes when added to a proton in the reaction.</td>
</tr>
<tr>
<td>IV B</td>
<td>Alkoxonium ion is a proton.</td>
</tr>
<tr>
<td>IV B</td>
<td>Carbocation intermediate AKA alkoxonium ion which then forms alkene + water.</td>
</tr>
<tr>
<td>IV B</td>
<td>Alcohols can go through elimination to make alkoxonium ions when they eliminate S_N1.</td>
</tr>
<tr>
<td>IV B</td>
<td>Alkenes can be formed by elimination which forms an alkoxonium ion.</td>
</tr>
</tbody>
</table>
Table 8.50 (cont.).

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IVB2b</td>
<td>Alkoxonium ion loses an electron, and the proton gives the structure a positive charge.</td>
</tr>
<tr>
<td>IVB2b</td>
<td>Oxygen donates a proton to hydrogen which forms an alkoxonium ion.</td>
</tr>
<tr>
<td>IVB2c</td>
<td>Alcohol can go through neutralization where alkyl groups bond to oxygen forms alkoxonium ions.</td>
</tr>
<tr>
<td>IVB2c</td>
<td>Alcohols are alkanes e.g. R-OH in which H is replaced by OH and can form oxonium ions which are formed by hydrogen bonding.</td>
</tr>
<tr>
<td>IVC1</td>
<td>Alcohols contain protons that go through elimination can be E1 favors polar solvent.</td>
</tr>
<tr>
<td>IVC1</td>
<td>Alcohols contain protons that go through elimination can be E2 favors nonpolar solvent.</td>
</tr>
<tr>
<td>IVC2</td>
<td>Onium ion loses a hydrogen molecule and forms a carbocation.</td>
</tr>
<tr>
<td>IVD1a</td>
<td>Alkoxonium ion is a nucleophile or strong base. (NB: from the same map that confused alkoxonium and alkoxide ions.)</td>
</tr>
<tr>
<td>IVD1a</td>
<td>Alkoxonium ion is a nucleophile or strong base. Alkoxonium ion has an extra proton which creates a positive charge.</td>
</tr>
<tr>
<td>IVD1b</td>
<td>Alcohol is a strong base in elimination.</td>
</tr>
<tr>
<td>IVD1b</td>
<td>Alcohols are weak acids that form alkoxonium ions when reacted with metals. (NB: this is an alkoxide ion.)</td>
</tr>
<tr>
<td>IVD2</td>
<td>Addition reaction, a proton is added to an alcohol to form an alkoxonium ion. CH₃CH₂OH⁺ + HBr -&gt; CH₃CH₂OH₂ + Br⁻</td>
</tr>
<tr>
<td>IVD2</td>
<td>Alcohols can be dehydrated with acid causes loss of proton which forms conjugate base e.g. ClO₂⁻</td>
</tr>
<tr>
<td>IVE1</td>
<td>Alcohol reactions can be elimination follows E1 or E2 mechanisms.</td>
</tr>
<tr>
<td>IVE1</td>
<td>Elimination of alcohols can be E1 or E2 (and is simply seen as dehydrolation).</td>
</tr>
<tr>
<td>IVE2</td>
<td>Alcohols can eliminate SN₂ when they have H⁺ proton.</td>
</tr>
<tr>
<td>IVE2</td>
<td>In an addition reaction, water is eliminated, e.g. CH₃CH₂H₂O + Br⁻ -&gt; H₂O + CH₂Br⁺CH₂</td>
</tr>
<tr>
<td>IVE3</td>
<td>Elimination reactions of alcohol favored in strong base, alcohol solvent, bulky base.</td>
</tr>
<tr>
<td>VA</td>
<td>Alcohol goes through elimination called E1; product consists of alkene called oxidation reaction.</td>
</tr>
<tr>
<td>VA</td>
<td>Alcohol goes through substitution consists of SN₁, SN₂, react with hydrogen halides goes through reduction reaction.</td>
</tr>
<tr>
<td>VB</td>
<td>Alcohols form alkoxonium ions before forming ketones and carboxylic acids.</td>
</tr>
<tr>
<td>VB</td>
<td>Alcohols go through reactions - substitution that makes an alkoxonium ion which has proton in either SN₁ or SN₂ and makes an alkane.</td>
</tr>
<tr>
<td>VB</td>
<td>In an addition reaction, water is added to form an alkene.</td>
</tr>
</tbody>
</table>

---

Items in parentheses are summarized from individual concept maps.

Refers to difficulty type identified in Table 8.49.
involved formation of incorrect products. These types are listed in Table 8.49, with specific examples given in Table 8.50.

Results of Concept Map 12. Concept map 12, which had the seed concepts "alcohol", "aldehyde", "carboxylic acid", "oxidation", and "reduction", was the last map assigned in both the Fall, 1997, and Spring, 1998, semesters. For both semesters, the first choice of superordinate concept for this map was "alcohol" or "alcohols" (66.3% and 76.2% of respondents, respectively). Analysis of concordance of ordinal rank of these concepts for each semester gave values of Kendall's W of .4587 and .4160, respectively, both of which are significant at the .0000 level. Results of these calculations are given in Tables 8.51, 8.52, and 8.53.

Qualitative analysis of the concept maps yielded seven major types of difficulties. First were propositions that were interesting or unusual but not necessarily incorrect and next were propositions that, while not incorrect, would be considered naive in the context of the assigned map. Third were difficulties in which oxidation was confused with reduction, and fourth were difficulties involving incorrect atom count or atom motion in reactions. The next two types of difficulties dealt with hydrogen bonding and attribution of acid-base products to redox reactions. Finally, the seventh type of difficulty involved impossible redox reactions. These types are listed in Table 8.54, with specific examples given in Table 8.55.

Correlation of Concept Maps to Student Test Scores. Each of the assigned concept maps from both the Fall, 1997 semester and Spring, 1998 semester were examined for their relevance to the study of stereochemistry. Six concept maps from the Fall, 1997 semester and eight concept maps from the Spring, 1998, semester, were judged to focus primarily on stereochemistry. In the Fall, 1997 semester, these were the concept maps labeled 2, 9, 10, 11, 12, and 13 (Tables 2a, 9a, 10a, 11a, 12a, and 13a, respectively). In the Spring, 1998 semester, these were the concept maps labeled 2, 3, 4, 9, 10, 11, 12, and 13 (Tables 2a, 3a, 4a, 9a, 10a, 11a, 12a, and 13a, respectively).
Table 8.51. Statistical Analysis of Concept Map 12.

Seed concepts: alcohol, aldehyde, carboxylic acid, oxidation, reduction

<table>
<thead>
<tr>
<th>Superordinate concept</th>
<th>Percent of students choosing concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol(s)</td>
<td></td>
<td>66.3%</td>
<td>76.2%</td>
</tr>
<tr>
<td>oxidation</td>
<td></td>
<td>11.2%</td>
<td>9.5%</td>
</tr>
<tr>
<td>functional groups</td>
<td></td>
<td>7.1%</td>
<td>0.0%</td>
</tr>
<tr>
<td>aldehyde(s)</td>
<td></td>
<td>5.1%</td>
<td>0.0%</td>
</tr>
<tr>
<td>reaction(s)</td>
<td></td>
<td>0.0%</td>
<td>4.8%</td>
</tr>
<tr>
<td>esters</td>
<td></td>
<td>2.0%</td>
<td>0.0%</td>
</tr>
<tr>
<td>others&lt;sup&gt;b&lt;/sup&gt;</td>
<td></td>
<td>8.2%</td>
<td>9.5%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Seed concept</th>
<th>Mean rank of seed concept</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td>1.64</td>
<td>1.63</td>
<td></td>
</tr>
<tr>
<td>oxidation</td>
<td>2.34</td>
<td>2.38</td>
<td></td>
</tr>
<tr>
<td>aldehyde</td>
<td>3.93</td>
<td>3.42</td>
<td></td>
</tr>
<tr>
<td>reduction</td>
<td>3.10</td>
<td>3.48</td>
<td></td>
</tr>
<tr>
<td>carboxylic acid</td>
<td>3.99</td>
<td>4.11</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
<th>Fall 1997&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Spring 1998&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>W&lt;sup&gt;c&lt;/sup&gt;</td>
<td>.4587</td>
<td>.4160</td>
<td></td>
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<tr>
<td>significance</td>
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<td>.0000</td>
<td></td>
</tr>
<tr>
<td>degrees of freedom</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>

<sup>a</sup>Represents 98 concept maps from Fall, 1997 and 63 concept maps from Spring, 1998.
<sup>b</sup>Represents concepts chosen by only one participant.
<sup>c</sup>Represents the Kendall coefficient of concordance.

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Table 8.52. Individual Statistical Comparisons of Seed Concepts from Map 12 for the Fall, 1997 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td>1.25</td>
<td>oxidation</td>
<td>1.75</td>
<td>.2606</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.09</td>
<td>aldehyde</td>
<td>1.91</td>
<td>.7070</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.18</td>
<td>reduction</td>
<td>1.82</td>
<td>.4355</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.12</td>
<td>carboxylic acid</td>
<td>1.88</td>
<td>.6448</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.14</td>
<td>aldehyde</td>
<td>1.86</td>
<td>.5740</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.31</td>
<td>reduction</td>
<td>1.69</td>
<td>.2905</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.13</td>
<td>carboxylic acid</td>
<td>1.87</td>
<td>.5809</td>
<td>.0000</td>
</tr>
<tr>
<td>aldehyde</td>
<td>1.68</td>
<td>reduction</td>
<td>1.32</td>
<td>.1452</td>
<td>.0002</td>
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<tr>
<td>aldehyde</td>
<td>1.48</td>
<td>carboxylic acid</td>
<td>1.52</td>
<td>.0018</td>
<td>.6746</td>
</tr>
<tr>
<td>reduction</td>
<td>1.28</td>
<td>carboxylic acid</td>
<td>1.72</td>
<td>.2273</td>
<td>.0000</td>
</tr>
</tbody>
</table>

Table 8.53. Individual Statistical Comparisons of Seed Concepts from Map 12 for the Spring, 1998 Semester.

<table>
<thead>
<tr>
<th>First Concept</th>
<th>Relative Rank of First Concept</th>
<th>Second Concept</th>
<th>Relative Rank of Second Concept</th>
<th>W</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>alcohol</td>
<td>1.23</td>
<td>oxidation</td>
<td>1.77</td>
<td>.2958</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.14</td>
<td>aldehyde</td>
<td>1.86</td>
<td>.5564</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.16</td>
<td>reduction</td>
<td>1.84</td>
<td>.4681</td>
<td>.0000</td>
</tr>
<tr>
<td>alcohol</td>
<td>1.11</td>
<td>carboxylic acid</td>
<td>1.89</td>
<td>.7250</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.20</td>
<td>aldehyde</td>
<td>1.80</td>
<td>.3900</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.29</td>
<td>reduction</td>
<td>1.71</td>
<td>.3368</td>
<td>.0000</td>
</tr>
<tr>
<td>oxidation</td>
<td>1.11</td>
<td>carboxylic acid</td>
<td>1.89</td>
<td>.6290</td>
<td>.0000</td>
</tr>
<tr>
<td>aldehyde</td>
<td>1.48</td>
<td>reduction</td>
<td>1.52</td>
<td>.0013</td>
<td>.7856</td>
</tr>
<tr>
<td>aldehyde</td>
<td>1.28</td>
<td>carboxylic acid</td>
<td>1.72</td>
<td>.2550</td>
<td>.0001</td>
</tr>
<tr>
<td>reduction</td>
<td>1.39</td>
<td>carboxylic acid</td>
<td>1.61</td>
<td>.0505</td>
<td>.0897</td>
</tr>
</tbody>
</table>

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Table 8.54. Types of Difficulties Identified from Concept Map 12.

I) Interesting or unusual

II) Naive
   A) Discussion of non-redox reactions
   B) Discussion of structure of functional groups
   C) Discussion of formal redox definitions

III) Confusion of oxidation with reduction

IV) Incorrect atom count or atom motion in reactions
   A) Wrong numbers of hydrogen atoms gained or lost
   B) Application of incorrect redox rule
   C) Insertion/removal of incorrect atoms or ions in redox

V) Difficulties involving hydrogen bonding
   A) Attributing redox reactions to H-bonding
   B) Attributing incorrect physical properties to H-bonding

VI) Attribution of acid-base products to redox reactions.

VII) Impossible redox reactions
   A) Formally correct reactions
   B) Formally incorrect reactions
<table>
<thead>
<tr>
<th>Type</th>
<th>Alternative conception</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>A student noted, &quot;This one was difficult because everything was related in more than one way.&quot;</td>
</tr>
<tr>
<td>I</td>
<td>Alcohol reduction has no reaction.</td>
</tr>
<tr>
<td>II A</td>
<td>Alcohols generally react S\text{N}1.</td>
</tr>
<tr>
<td>II A</td>
<td>Ketone forms cyanide group is hydrolyzed into carboxylic acid.</td>
</tr>
<tr>
<td>II B</td>
<td>H\text{2}O is an ingredient of phenols, alcohols, ethers.</td>
</tr>
<tr>
<td>II C</td>
<td>Oxidation is loss of electrons results in more (+) charge.</td>
</tr>
<tr>
<td>II C</td>
<td>Oxidation is the opposite of reduction which is gain of electrons results in more (-) charge.</td>
</tr>
<tr>
<td>III</td>
<td>Alcohols can form aldehydes by reduction.</td>
</tr>
<tr>
<td>III</td>
<td>Alcohols gotten by reduced compounds, \textit{e.g.} (ketone + H\text{2} -&gt; (Pt) 2° alcohol).</td>
</tr>
<tr>
<td>III</td>
<td>Carboxylic acids which have the formula RCOOH are involved mainly in oxidation.</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohol loses H to form aldehyde.</td>
</tr>
<tr>
<td>IV A</td>
<td>Alcohols undergo oxidation in which a hydrogen is removed from a carbon-oxygen single bond.</td>
</tr>
<tr>
<td>IV A</td>
<td>Primary alcohols can undergo oxidation in which a hydrogen is removed to form a carbon-oxygen double bond.</td>
</tr>
<tr>
<td>IV B</td>
<td>Alcohol loses a double bond during reduction.</td>
</tr>
<tr>
<td>IV C</td>
<td>Alcohols can be oxidized which means that hydrogen is removed from a C-O bond then insertion of an oxygen in the remaining C-H bond.</td>
</tr>
<tr>
<td>IV C</td>
<td>Aldehyde have a carbonyl which is lost during oxidation can form carboxylic.</td>
</tr>
<tr>
<td>IV C</td>
<td>Carboxylic acid adds OH to form alcohol.</td>
</tr>
<tr>
<td>IV C</td>
<td>Oxidation of an aldehyde results in loss of H\text{+} on a carbonyl carbon.</td>
</tr>
<tr>
<td>V A</td>
<td>Alcohols can H-bond and 1° become aldehydes, \textit{e.g.} RCHO, and carboxylic acid, \textit{e.g.} RCOOH.</td>
</tr>
<tr>
<td>V A</td>
<td>Alcohols can H-bond and 2° becoming ketones, \textit{e.g.} RCOR.</td>
</tr>
<tr>
<td>V A</td>
<td>Alcohols can H-bond resulting in oxidation, losing electrons, \textit{e.g.} alkenes.</td>
</tr>
<tr>
<td>V B</td>
<td>Alcohols can H-bond to itself increasing water solubility.</td>
</tr>
<tr>
<td>V B</td>
<td>Alcohols can H-bond to water increasing melting and boiling point.</td>
</tr>
<tr>
<td>V I</td>
<td>Alcohol can be reduced by the gaining of hydrogen which would form from an alkoxonium ion.</td>
</tr>
<tr>
<td>V I</td>
<td>Primary alcohols have one alkyl group and can react by S\text{N}2 with hydrogen halides to form alkyl halides and in the process form an oxonium ion occurring by reduction.</td>
</tr>
<tr>
<td>V I A</td>
<td>Alcohol which looks like -C-OH is involved mainly in reduction.</td>
</tr>
<tr>
<td>V I A</td>
<td>Alcohols can form alkanes through reduction which is gain of electrons.</td>
</tr>
<tr>
<td>V I A</td>
<td>Carboxylic acids can undergo reduction to form alkyenes.</td>
</tr>
<tr>
<td>V I B</td>
<td>Alcohol reduction goes from alkene to alkane.</td>
</tr>
<tr>
<td>V I B</td>
<td>Alcohols oxidize into aldehydes then into ketones then into carboxylic acid finally into esters.</td>
</tr>
</tbody>
</table>

\(^a\)Items in parentheses are summarized from individual concept maps.  
\(^b\)Refers to difficulty type identified in Table 8.54.
Students were evaluated throughout both semesters by means of multiple choice tests. A total of 177 questions (from five unit tests, a midterm examination, and a final examination) were administered during the Fall, 1997, semester, and a total of 196 questions (from four unit tests, a midterm examination, and a final examination) were administered during the Spring, 1998, semester. From these tests, a total of 32 questions from the Fall, 1998 semester and 34 questions from the Spring, 1998, semester were chosen that fit best with the concepts given in each concept map.

For each concept map and its corresponding multiple choice questions, the total percent of correct responses was tabulated along with the number of questions sampled, Kendall's W for the concept map, and the percent of students who chose the most frequently occurring superordinate concept (Table 8.56). Correlation coefficients (Pearson's r) between the percent correct on related questions and Kendall's W, percent correct on related questions and percent of students choosing the most common superordinate concept, and Kendall's W and percent of students choosing the most common superordinate concept were determined using SPSS®. These data along with the corresponding significance levels are given in Table 8.57. Graphs of percent correct on related questions vs Kendall's W for both semesters are shown in Figures 8.1 and 8.2. Six of the concept maps deemed most relevant to the learning of stereochemistry (maps 2, 7, 8, 9, 10, and 11; Tables 8.56 and 8.57) were assigned in both semesters. Correlation of Kendall's W for the Fall, 1997, and Spring, 1998, semester for these six concept maps is given in Figure 8.3. The coefficient of correlation (Pearson's r) was .7918. In the absence of a model indicating the type of relationship that might exist between Kendall's W and test question percentage, possible nonlinear relationships were not investigated.

The correlation between Kendall's W and test question percentage was used as a measure of whether lack of concordance in placement of seed concepts correlates with
student knowledge and difficulties of the corresponding stereochemistry. This is further elaborated in the Discussion.
Table 8.56. Summary of Test Question Data for Each Concept Map.

<table>
<thead>
<tr>
<th>Concept Map</th>
<th>Percent Correct(^a)</th>
<th>Questions in Sample</th>
<th>Kendall’s W</th>
<th>SOC Percent(^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fall 1997</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>76.9</td>
<td>7</td>
<td>.6368</td>
<td>74.6</td>
</tr>
<tr>
<td>7</td>
<td>75.7</td>
<td>3</td>
<td>.5852</td>
<td>43.4</td>
</tr>
<tr>
<td>8</td>
<td>54.4</td>
<td>4</td>
<td>.4542</td>
<td>42.2</td>
</tr>
<tr>
<td>9</td>
<td>80.1</td>
<td>8</td>
<td>.7930</td>
<td>79.8</td>
</tr>
<tr>
<td>10</td>
<td>70.1</td>
<td>6</td>
<td>.6866</td>
<td>62.1</td>
</tr>
<tr>
<td>11</td>
<td>69.8</td>
<td>4</td>
<td>.5593</td>
<td>66.1</td>
</tr>
<tr>
<td>Spring 1998</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>72.5</td>
<td>10</td>
<td>.7155</td>
<td>91.3</td>
</tr>
<tr>
<td>3</td>
<td>71.1</td>
<td>3</td>
<td>.7380</td>
<td>88.9</td>
</tr>
<tr>
<td>4</td>
<td>89.0</td>
<td>4</td>
<td>.9703</td>
<td>79.3</td>
</tr>
<tr>
<td>7</td>
<td>71.0</td>
<td>3</td>
<td>.5125</td>
<td>65.8</td>
</tr>
<tr>
<td>8</td>
<td>64.3</td>
<td>4</td>
<td>.5637</td>
<td>75.0</td>
</tr>
<tr>
<td>9</td>
<td>66.3</td>
<td>3</td>
<td>.8771</td>
<td>93.4</td>
</tr>
<tr>
<td>10</td>
<td>60.9</td>
<td>4</td>
<td>.6149</td>
<td>64.4</td>
</tr>
<tr>
<td>11</td>
<td>44.5</td>
<td>3</td>
<td>.4953</td>
<td>75.4</td>
</tr>
</tbody>
</table>

\(^a\)Represents the total percent of correct responses from multiple choice questions corresponding to each concept map.

\(^b\)Represents the percent of students choosing the most common superordinate concept for each concept map.

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Table 8.57. Correlation Data (Pearson's r) from Concept Maps and Related Questions.

<table>
<thead>
<tr>
<th></th>
<th>Fall, 1997</th>
<th>Spring, 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kendall's W</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>Percenta</td>
<td>.8093</td>
<td>.7191</td>
</tr>
<tr>
<td>Correct</td>
<td><code>p = .051</code></td>
<td><code>p = .044</code></td>
</tr>
<tr>
<td>SOCb</td>
<td>.7689</td>
<td>.6109</td>
</tr>
<tr>
<td>Percent</td>
<td><code>p = .074</code></td>
<td><code>p = .108</code></td>
</tr>
</tbody>
</table>

\[ ^a \] Represents the total percent of correct responses from multiple choice questions corresponding to each concept map.

\[ ^b \] Represents the percent of students choosing the most common superordinate concept for each concept map.
Figure 8.1. Correlation of test question percentage with Kendall's W of corresponding concept maps, Fall, 1997, semester.
Figure 8.2. Correlation of test question percentage with Kendall’s W of corresponding concept maps, Spring, 1998, semester.
Figure 8.3. Correlation of Kendall's W scores for concept maps collected in the Fall, 1997, and Spring, 1998, semesters.
RESULTS FROM STUDENT JOURNALS

Student journals were not a productive method to probe difficulties in the learning of stereochemistry in this study. Many of the journals simply recounted lecture material as given in spite of requests to use the journals as a means for students to monitor their own learning. Occasionally some students used the journals as a tool to inform the course instructor what they liked or disliked about the lecture. Such suggestions rarely touched on stereochemical topics, and when they did occur, they were helpful in redesigning course layout and lectures, but not as a means to assess specific difficulties.

The use of clinical interviews was clearly a superior method to obtain information regarding these students' difficulties in the learning of stereochemistry.
DISCUSSION

Analysis of Student Journals. Every student who completed either semester of organic chemistry in this study also completed a student journal using the guidelines outlined in Table 3.7. The journals were collected several times during each semester and returned with appropriate written comments. Many of the students were very serious about the journals, producing lengthy and detailed entries, but in general they consisted of the students' interpretation of the lecture material. Although other researchers may have had success using journals as tools to monitor metacognition and diagnose difficulties in learning, they were not effective tools in this study. Interviews and concept maps were much more valuable to the researcher.

Analysis of Interviews. Each of the interviews given during both semesters is discussed below. The first three interviews were conducted using ten students (six from the Fall, 1997, semester and four from the Spring, 1998, semester). Nine students were interviewed for the fourth interview because one participant was ill during the Spring, 1998, semester. The analysis discusses the major categories of difficulties in the learning of stereochemistry that were revealed by the interviews.

Analysis of Interview 1. This interview was designed to probe students' understanding of valence shell electron pair repulsion (VSEPR) theory, visualization of the shapes of pi bonds, the nature of conformers, and various methods of representation of geometric and structural isomers. Although each of these topics was investigated, most of the difficulties that emerged related to students' ideas about conformers. The questions prepared for this interview are listed in Table 3.2, and the major categories of difficulties that were revealed are listed in Table 4.1.

Each of the participants claimed to be familiar with valence shell electron pair repulsion theory, either from their high school chemistry background or from their freshman inorganic chemistry course at the university level. However, only one of the ten students interviewed was able to apply the principles of VSEPR to organic structures
and make any useful predictions about the shapes of molecules using this theory. The first difficulty discussed from Interview 1 addresses this issue (Table 1, category I).

Most students were successful in their efforts to draw the shapes of pi bonds, especially pi bonds in isolation, but were less successful when attempting to draw a pi bond within a molecule, and had difficulty describing pi bond as being perpendicular to the plane of the atoms. Some students did not associate alkenes as molecules containing pi bonds (Table 1, category II).

Students frequently drew and discussed conformers as though they were types of structural isomers, and a common difficulty was the attempt to draw conformers using two-dimensional dash formulas, using the terms 'cis' and 'trans' to describe them. Students could recite the definition that conformers rotated freely around a sigma bond, but even after saying this many students would affirm that individual conformers can be isolated (Table 1, category III). A further difficulty in differentiating between conformers and structural isomers was encountered among students who failed to differentiate between rotation around a bond and rotation of an entire structure (Table 1, category V).

The final difficulty that students had in understanding the nature of conformers dealt with their reluctance to use Newman projections, which are specifically designed to depict conformers and the free rotation around a sigma bond. A common difficulty was that students could not connect the structural elements of a molecule in the proper order when drawing a Newman projection and were more inclined to place an incorrect number of bonds on an individual atom when drawing a Newman projection that when drawing other types of formulas (Table 1, category VI).

**Analysis of Interview 2.** This interview was designed to probe students' understanding of the nature of conformers, geometric isomers, and structural isomers in cyclic molecules. The questions prepared for this interview are listed in Table 3.3, and the major categories of difficulties that were revealed are listed in Table 5.1.
Many of the findings of this interview related to students' lack of understanding of what really happens in a conformer when rotation occurs around a sigma bond. Students fail to realize that it is the flexibility in a bond that allows conformers to rotate. Because of this, students will sometimes affirm that conformers can form around either the rigid double bonds of alkenes or in rigid small cyclic compounds (Table 5.1, category I). Lack of realization of what happens when rotation occurs around a sigma bond may also explain why some students will claim that two different conformations represent distinctly different, isolable species, a difficulty also noted in the first interview (Table 4.1, category III, & Table 5.1, category I). This was particularly evident when asking students to describe the difference between the 'chair' and 'boat' conformers of cyclohexane (Table 5.1, category I). This confusion will sometimes disappear when students are forced to physically handle molecular models; however, many students are reluctant to do this (Table 5.1, categories I & VI).

Another difficulty related to rotation is that students fail to recognize the difference between rotating around a bond and rotating around an entire molecule (Table 5.1, category II). This tendency was also noted in the first interview (Table 4.1, category V). Identical structures oriented differently on a piece of paper were frequently perceived as being different. Perhaps related to this difficulty is the tendency of some students to disassemble and reassemble a model when building conformers of a structure, instead of simply rotating around a bond. Simple structures, such as the staggered and eclipsed conformers of 1,2-dichloroethane presented few problems (Table 3.4, question 5); however, more complex structures such as the chair and boat conformers of 1,2-dichlorocyclohexane (Table 3.3, question 12) were more problematic. The interconversion of the 'chair' and 'boat' conformers of cyclohexane was not associated with rotation around a bond.

One student coined the phrase "living in a flat world," which is a category of difficulty used to describe the reluctance of students to associated three-dimensional
phenomena with their own two-dimensional drawings. This reluctance was observed in both of the first two interviews and will be encountered again in analysis of the third interview. Many students were reluctant to draw a ring in a perspective with the ring atoms are perpendicular to the plane of the paper and the orientation of the functional groups is emphasized. The preference of many students was to draw both the ring and its substituents in the plane of the paper: when drawn in this manner, it is not possible to distinguish between geometric isomers (Table 4.1, category VII, & Table 5.1, category II). Another difficulty students have with their own two-dimensional drawings occurs when they attempt to draw cyclohexane from a three dimensional model. Several students drew a two-dimensional diagram of cyclohexane (generally in the form of a regular hexagon) and then claim that, because it is cyclic, it doesn’t form any conformers. This occurred even after the students had built, handled, and manipulated the conformers of a three dimensional model of cyclohexane (Table 5.1, category III).

When given a set of diagrams of chemical structures and asked which pairs of structures represented isomers, students in this study generally identified the pairs of geometric isomers without difficulty. The pairs of structural isomers were more problematic, and it frequently occurred that students failed to identify pairs of structural isomers. This is perhaps because, on first inspection, it is clearer that pairs of geometric isomers contain both the same numbers and types of atoms. In contrast, when asked to build all of the isomers of a given structure, students in this study readily built the structural isomers and frequently failed to build the geometric isomers (Table 5.1, category IV).

The terms 'axial' and 'equatorial' that are properly used to describe the positions of substituents in cyclohexane conformers were sometimes used to describe the positions of the substituents in geometric isomers. In contrast, the terms 'anti' and 'gauche', which are more general terms that describe the positions of substituents in many acyclic conformers, were not used by any students in this study to describe geometric isomers.
Confusion of the terms 'axial' and 'equatorial' with 'cis' and 'trans' may be one aspect of a difficulty many students seem to have in describing substituents that are perpendicular to a cyclohexane ring. In particular, trans-1,2-disubstituted cyclohexanes in which both substituents are equatorial are sometimes described as being "neither cis nor trans", whereas when the same substituents are in an axial conformation, they are readily described as "trans." Perhaps related to this is the observation that axial substituents that are clearly perpendicular to the cyclohexane ring were readily described as being 'up' or 'down', whereas these terms were rarely applied to the equatorial substituents (Table 5.1, category V).

One further observation from the second interview that seemed relevant to most of the exercise was the reluctance of many students to build and handle models. This was noted in all of the interviews, but most of the students overcame this reluctance by the time of their last interview. However, in this second interview, students had to be encouraged to use the models, and when they did, they answered most of the questions with greater ease (Table 5.1, category VI).

**Analysis of Interview 3.** This interview was designed to probe students' understanding of the nature of chirality and chiral carbon atoms and the relationships between enantiomers, diastereomers, and meso compounds. The questions prepared for this interview are listed in Table 3.4, and the major categories of difficulties that were revealed are listed in Table 6.2.

Some of the difficulties revealed in the third interview are similar to those discussed for the second interview. This interview revealed further difficulties involving rotation around bonds and rotation of entire molecules. Some students built models of acyclic molecules containing only sigma bonds, manipulated the models by rotating around each bond and, despite the evidence of the models in their hands, concluded that rotation around at least one bond was impossible. These structures were then described as being geometric isomers rather than conformers. This difficulty was more prevalent when
structures contained substituents such as halogens and less prevalent when the model was simply a hydrocarbon. A related conclusion, reached after building and interconverting models of the chair and boat forms of cyclohexane, was that these conformers actually represent geometric isomers (Table 6.2, category I).

The second interview revealed a molecule drawn 'upside down' is sometimes perceived as being different a different structure (Table 5.1, category II). The corresponding difficulty from the third interview is that chiral structures drawn 'upside down' represent enantiomers, or mirror images (Table 6.2, category I). Another difficulty involving rotation of entire molecules is that students sometimes fail to rotate a model through an appropriate angle when attempting to draw its enantiomer (Table 6.2, category I).

Most of the interviewees had difficulty representing and recognizing mirror images of structures. A mirror image that is rotated or translated was frequently not recognized as the mirror image. In contrast, if the frameworks of two structures were drawn as mirror images, they were sometimes perceived as being mirror images even when they had different substituents attached to the chiral center (Table 6.2, category II).

Several other difficulties involving chirality were detected. An achiral atom drawn using three-dimensional drawing conventions was frequently perceived as chiral. When the students built models corresponding to the drawings, they then expressed surprise that the models were superimposable. Even telling a student that an atom was achiral did not insure that the student would not be concerned with its configuration when analyzing a structure (Table 6.2, category II).

Many of the difficulties in nomenclature, or naming chiral molecules, were caused by difficulties in numbering the parent chain. Of particular interest is the difficulty these students had in recognizing the parent chain when structures were drawn using three-dimensional conventions. Several students focused on the chiral atom and named each
substituent attached to this atom instead of searching for the longest chain of carbon atoms (Table 6.2, category III).

The category entitled "Living in a flat world" was again used in analysis of the third interview. In the second interview, this category included the difficulties encountered by students in representing the three-dimensional nature of cyclic structures (Table 5.1, category III). In the third interview, this category also includes difficulties encountered by students who analyze drawings of three-dimensional acyclic structures. When presented with a structure such as 2,2-dibromo-3-chlorobutane in which the portion of the molecule not directly attached to the chiral atom is drawn using a dash formula, it was common for students to ask whether a portion of the molecule was really planar (Table 3.4, question 11B). A related difficulty is the tendency of some students to redraw complex structures in a form that does not show the stereochemistry (e.g., a dash, Kekule, or condensed formula) when the stereochemistry of the molecule is important to the exercise (Table 6.2, category IV).

Students in this study frequently had difficulty aligning a three-dimensional model with its two-dimensional representation on paper (Table 6.2, category VI). Perhaps in part because of this, these students often resorted to 'rote rules' when comparing structures. The rule most frequently used and abused is one that states that, in order to draw the enantiomer of a structure containing exactly one chiral center, one can simply exchange the position of any two substituents on that chiral center. Exchanging another pair of substituents on the same chiral center then reproduces the original structure.

This rule was sometimes used when comparing geometric isomers instead of enantiomers, with the result that two representations of the same trans isomer oriented differently were described as different structures. Another difficulty arose when comparing diastereomers. Some students would exchange the positions of substituents on two different chiral atoms and claim that they had reproduced the original structure.
(Table 6.2, category VI). Misapplication of rote rules that were perceived to work in a specific situation to a different inappropriate situation was a common source of difficulty.

Finally, some students are reluctant to rotate around either sigma bonds or entire molecules in order to make it easier to compare two structures. This is particularly apparent when using complex structures (Table 6.2, category VII).

Analysis of Interview 4. This interview was designed to probe students' understanding of the stereochemical consequences of chemical reactions at chiral sites. Reactions with the $S_N1$, $S_N2$, and E2 mechanisms were probed. The questions prepared for this interview are listed in Table 3.5, and the major categories of difficulties that were revealed are listed in Table 7.1.

With the exception of alkenes, one of the first planar chemical species encountered by students in this study was the planar carbocation that forms in the $S_N1$ mechanism. Thus, it is one of the first species that can be easily drawn on a flat surface. Some students preferred to draw this intermediate on a flat piece of paper and others drew it perpendicular to the plane of the paper. Students who chose the latter method in general had less difficulty drawing and explaining the formation of an equimolar mixture of enantiomeric products when the carbocation formed from a chiral reactant. Approach of the nucleophile from either side appeared to be equally likely to most of these students. In contrast, students who drew the carbocation intermediate in the plane of the paper were much more likely to claim that approach of the nucleophile must be more likely from one side than from the other (Table 7.1, category IA).

Students in this study had less difficulty with the $S_N2$ mechanism in which inversion of configuration occurs, perhaps in part because only one product forms. However, several students did not associate approach of the nucleophile from the backside with inversion of configuration (Table 7.1, category IB).

The E2 elimination of hydrogen halide to form an alkene was much more difficult than the $S_N1$ and $S_N2$ substitution reactions for most students, and statements indicating
that students felt that elimination reactions were more difficult than substitution reactions were common. Several students focused on the atoms that were eliminated instead of those that remained when predicting the products of an elimination reaction. Because the atoms that are eliminated in an E2 elimination must be antiperiplanar, students who did this always predicted that the trans isomer would form. Other students would build a model or draw a diagram in which one hydrogen was antiperiplanar to the halide leaving group but eliminate a different hydrogen atom in the gauche position. Still other students attempted to eliminate halide and hydrogen from the same carbon atom instead of removing a vicinal hydrogen atom. Only when asked where the double bond would form and how many bonds needed to form on each carbon atom would these students reexamine the reaction (Table 7.1, category IC).

The category 'Rote rules and reorientation' that emerged from the fourth interview (Table 7.1 category II) is related to the category 'Difficulties with rote rules' that emerged from the third interview (Table 6.2, category VI). The rote rule in question states that an enantiomer of a compound containing exactly one chiral center is formed when any two substituents attached to that center are exchanged. Students who used this rule were reluctant to reorient any chiral molecules by rotation in order to facilitate viewing a mechanism. An example of the difficulty that this causes is that students would fail to placed the incoming nucleophile 180 degrees from the leaving group when examining the S\(\text{N}2\) mechanism (Table 7.1, category IIA).

A third category emerging from the fourth interview was entitled "What students say vs. what they do." In this interview, several contradictions between what students said and what they did were encountered; this situation was much more common in this fourth interview than in either of the first three. Some of these contradictions may stem from memorized dicta such as "Elimination occurs anti." Students will affirm that this is true in the E2 elimination of hydrogen halide, but when given either a diagram or a model, will fail to orient the structure so that hydrogen and halogen are antiperiplanar. Similarly,
students will affirm that "back-side attack causes inversion of configuration," but when demonstrating the SN2 mechanism using either models or drawings, they may simply remove the leaving group and attach the nucleophile, with the result that the configuration is retained rather than inverted (Table 7.1, category III).

The final category of difficulty noted in the fourth interview deals with bond making and bond breaking. Several different but related difficulties about both elimination and substitution are noted here; among the most interesting are the following. Some students tried to illustrate the E2 elimination by eliminating only one atom (halogen) without eliminating any hydrogen atom. Others eliminated both hydrogen and halogen but failed to introduce a double bond, instead describing the product as an alkane.

In describing substitution, several students said that the S_N1 and S_N2 mechanisms are "really the same." Other students attempted to build the nucleophile into the reactant, and were unsure that the nucleophile began as a separate species.

Analysis of Concept Maps. Each of the concept maps assigned during both semesters is discussed below. At some times during each semester, concept maps were assigned covering material that did not primarily related to stereochemical topics. In the hope that each set of concept maps would divulge some type of information relating to the learning of stereochemistry, each set was analyzed. Finally, the results of those concept maps deemed most appropriate to the learning of stereochemistry were compared with corresponding test results.

Analysis of Concept Map 1. Concept map 1, which had the seed concepts 'alkane', 'alkene', 'alkyne', 'hydrocarbon', and 'multiple bond', was assigned as the first concept map in both the Fall, 1997, and Spring, 1998, semesters. The corresponding lecture material covered the structure of hydrocarbons and the differences between alkanes and alkenes. Because hydrocarbons are three-dimensional, this material might be considered to be the students' first introduction to stereochemistry, although use of this term did not occur for several more lecture periods. It was anticipated that this concept map would not
be too difficult for the students; however, some interesting information did emerge from this first set of concept maps. A large majority of students in both semesters chose 'hydrocarbon' as the superordinate concept (88.2% and 95.1% of students in the Fall, 1997, and Spring, 1998, semesters, respectively), and indeed alkanes, alkenes, and alkynes are all types of hydrocarbons. The overwhelming choice of 'hydrocarbon' as the superordinate concept is reflected in the mean rank of this term among the seed concepts (1.09 and 1.00 in the Fall, 1997, and Spring, 1998, semesters, respectively, Table 1a).

The Kendall coefficient of concordance (W) for the ranks of the five seed concepts was unexpectedly low (.6030 and .6368 for the Fall, 1997, and Spring, 1998, semesters, respectively). Further examination of the data reveals that the terms 'alkene' and 'alkyne' are virtually tied in rank (Tables 1a, 1b, 1c). Statistically, the term 'multiple bond' ranks significantly higher than both the terms 'alkene' and 'alkyne', but W for each pair is low (Tables 1a, 1b, 1c). Further examination of the individual concept maps reveals that they fall into two broad categories. A majority of the students classified the hydrocarbons by the types of bonds they contained (generally single or multiple bonds) and gave 'alkane' as an example of a compound containing only single bonds, and 'alkene' and 'alkyne' as examples of compounds containing multiple bonds. A sizable minority of students classified the hydrocarbons instead as being either alkanes, alkenes, or alkynes, and at a lower level of their maps then classified alkenes and alkynes as compounds containing multiple bonds. This apparent dichotomy in the way students classified hydrocarbons may be responsible for the somewhat low value for W obtained for concept map 1.

A simple enumeration of superordinate concepts does not reveal these two different methods of organizing these concepts. The lower-than-expected value of W lead to an examination of the maps, revealing the two methods of classification. When using either method, the concepts 'alkene' and 'alkyne' were viewed as being examples of compounds containing multiple bonds. The mean ranks of these two concepts were
virtually tied in both semesters (Table 8.1), and no statistically significant difference existed between these ranks (Table 8.2).

The second most common superordinate concept found in this set of maps was 'alkane', and this term was chosen by only 4.7% of the students in the Fall, 1997, semester, and by no students in the Spring, 1998, semester (Table 1a). Four students produced maps that read, "'Alkane' is a 'saturated hydrocarbon' and a base for 'alkenes'"; and three of these maps are so similar to each other and different from the rest that the suspicion arises that three of the students may have worked together. Calling an alkane a base for an alkene may seem unorthodox, but given the possibility of catalytic dehydrogenation (which was discussed in their lecture), it seems unfair to call it incorrect. Nevertheless this does not appear to be the most sophisticated way to view these two concepts. One student produced a map that read "An 'alkane' is a 'hydrocarbon' that can also be an 'unsaturated compound'"', which is clearly incorrect.

One student used 'unsaturated compounds' as the superordinate concept, producing a map that read, in part, "'Unsaturated compounds' can be 'alkynes' having no 'single bonds' that are found in 'saturated compounds'". However, even the simplest alkenes and alkynes contain single bonds. The alkyne acetylene, H:C:::C:H, contains two single bonds and one multiple bond. The idea that alkenes and alkynes do not contain single bonds occurred in several other maps. This same map also contained the statement that "'Hydrocarbons' are 'saturated alkanes'"; leading to question whether this student would accept the existence of 'unsaturated alkanes.'

Many students attempted to incorporate the terms 'sigma bond' and 'pi bond' into this concept map. In doing so, some awkward 'concepts' such as 'one sigma and one pi bond,' or 'one sigma and two pi bonds' were sometimes encountered.

**Analysis of Concept Map 2.** Concept map 2, which had the seed concepts 'conformer', 'equilibrium', 'staggered', 'eclipsed', and 'rotation', was assigned as the second concept map in both the Fall, 1997, and Spring, 1998, semesters. The lecture
material corresponding to this concept map dealt with the nature of conformers and the continuous interconversion between the eclipsed and staggered conformers that occurs in acyclic hydrocarbons and related compounds by rotation around sigma bonds.

In both semesters, the term 'conformer' was chosen by a large majority of students as the superordinate concept (74.6% and 91.3% of students in the Fall, 1997, and Spring, 1998, semesters, respectively), and the relatively high values for W (.6368 and .7155, respectively) indicates a good deal of agreement regarding relative placement of the seed concepts. In the Fall, 1997, semester, 13.8% of students chose either 'isomer' or 'isomerism' as the superordinate concept, with far fewer students (2.5%) making this choice in the Spring, 1998 semester. Another indication that students agreed on placement of seed concepts in this concept map is the agreement in choice of superordinate concept. In the Fall, 1997, semester, 74.6% of subjects chose 'conformer' as the superordinate concept, and 91.3% of subjects chose this superordinate concept in the Spring, 1998, semester (Table 8.6). Most students appeared to find this material relatively easy (with the exception being use of the term 'equilibrium' as noted below); 76.9% of the test questions in the Fall, 1997, semester were answered correctly and 72.5% of the test questions in the Spring, 1998 semester were answered correctly.

With one exception, there was a statistically significant difference in the ranks of each pair of seed concepts in this set of maps (Tables 8.11 & 8.12). The single exception was the pair of terms 'structural isomer' and 'stereoisomer'. Most students classified each as an example of an isomer, and they therefore were placed on the same rank in most of the concept maps.

The concept maps produced at this point in the semester appeared to be considerably more sophisticated than the first set of maps, with fewer of what might be termed 'grammatical errors' occurring within the maps. Nevertheless, some important difficulties emerged. Many students had difficulty using the term 'equilibrium', which
may be reflected in the mean rank of this concept in both the Fall, 1997, and Spring, 1998, semesters (4.20 and 4.44, respectively, Table 8.6).

**Analysis of Concept Map 3.** Concept map 3, which had the seed concepts 'isomer', 'structural isomer', 'stereoisomer', 'geometric isomer', and 'conformer', was assigned only in the Spring, 1998, semester. The lecture material corresponding to this concept map introduced the terms 'stereoisomer' and 'geometric isomer', discussed the idea that the geometric isomer is one type of stereoisomer, and elaborated on the differences between structural isomers, geometric isomers, and conformers. The mean relative rankings of the seed concepts 'stereoisomer' and 'geometric isomer' indicates that many students classified geometric isomers as types of stereoisomers; this is confirmed by examination of the individual concept maps submitted. However, this relationship was not always as clear in subsequent concept maps. The high value of Kendall's W obtained (.7380) and the choice of 'isomer' or 'isomerism' by a large majority of the class (88.9%, Table 8.11) indicate a good deal of agreement among the class regarding relative placement of the seed concepts. Students performed fairly well on related multiple choice questions (71.1% correct, Table 8.56).

Relatively few difficulties in the learning of stereochemistry emerged from this assignment, but some that were observed are noteworthy. The idea that conformers form from rotation around single bonds and geometric isomers form from rotation around double bonds is very interesting, as is the idea that geometric isomers only occur in cyclic molecules (Table 8.14, category IVA). The number of 'grammatical errors' in this map appears to be decreasing, but the propositions "isomer is a molecular formula" and "Newman diagram is example of alkane" (Table 8.14, category IIA) appear to be of this type.

**Analysis of Concept Map 4.** Concept map 4, which had the seed concepts 'reaction', 'substitution', 'elimination', and 'addition', was assigned only in the Spring, 1998, semester. The lecture material corresponding to this concept map introduced the
three major types of reactions (substitution, elimination, and addition) that were discussed during much of the remainder of the semester. The value of Kendall’s W obtained in analysis of this concept map (.9703, Table 8.15) was the highest of any map studied. The seed concept 'reaction' was assigned as the superordinate concept by 79.3% of students, again indicating a good deal of agreement regarding the structure of this concept map.

The remaining three seed concepts were essentially tied for the second rank position (Table 8.15). There was no statistically significant difference between the terms 'substitution' and 'addition' at the 5% level, and although the differences were significant for the pairs 'substitution' and 'elimination'; and 'addition' and 'elimination', the values of Kendall’s W for these latter pairs were small (0.0649 and 0.0519, respectively, Table 8.16). This corresponds well with the lecture material that categorized elimination, substitution, and addition with major reaction types.

The number of types of difficulties elucidated from this concept map was small; however, one type of difficulty noted in this map was consistently seen both in this map and in concept map 10 (Tables 8.42 & 8.43). This is the confusion of atoms with substituents. Several concept maps were submitted that stated that atoms were added across double bonds, eliminated to form double bonds, or substituted for other atoms. In the data analysis, propositions that confused atoms with substituents were said to have "narrow focus," and another example of narrow focus in concept map 4 involved catalysis. Many students produced propositions that stated that elimination requires a catalyst, although they had covered the mechanism of dehydrohalogenation in which there is no catalyst present (Tables 8.17 & 8.18).

**Analysis of Concept Map 5.** Concept map 5, consisting of the terms 'carbocation', 'carbanion', 'free radical', 'nucleophile', and 'electrophile', was assigned during both the Fall, 1997, and Spring, 1998, semesters. The lecture material corresponding to this concept map covered material related to the mechanisms of organic chemistry and the
types of intermediates produced. Kendall's W for these concepts was .5203 and .2508 for the Fall, 1997, and Spring, 1998, semesters, respectively (Table 8.19). The latter value of W was the lowest obtained in the analysis of any concept map. Thus, it appears that there existed considerable disagreement among the students regarding proper placements of the seed concepts in this map. This is verified by looking at the choice of superordinate concept; only 68.9% of students chose the concept 'intermediates' in the Fall, 1997 semester, and only 65.4% of the students chose this term in the Spring, 1998, semester (Table 8.19). Except for the term 'intermediates', none of the superordinate concepts noted were chosen from the list of seed concepts (Table 8.19).

The mean ranks of the seed concepts 'carbocation', 'carbanion', and 'free radical' were very close in both semesters (Table 8.19), and no statistically significant difference was noted between them (Tables 8.20 & 8.21). Examination of individual concept maps revealed that most students classified these three terms as being examples of reaction intermediates. The mean ranks of the terms 'nucleophile' and 'electrophile' were also very close (Table 8.19), and again no statistically significant difference between them was observed (Tables 8.20 & 8.21). Examination of the concept maps revealed that, in many cases, 'carbanion' was linked to the term 'nucleophile,' and 'carbocation' was attached to the term 'electrophile'. The term 'nucleophile' is more general than the term 'carbanion' (all carbanions are nucleophiles, but the converse is not true), and the term 'electrophile' is more general than the term carbocation. Although few of the maps had propositions involving these terms that were formally incorrect, a more sophisticated concept map would appear to rank the terms 'electrophile' and 'nucleophile' above the more specific terms 'carbocation' and 'carbanion'.

Some important difficulties in learning organic chemistry emerged from this concept map, but none was directly related to the learning of stereochemistry. Several students equated free radicals with either nucleophiles or electrophiles, perhaps indicating a fundamental problem with Lewis structures and calculation of formal charge. Many of
the difficulties identified involved the improper use of charges and the relationships between Lewis acid and bases, nucleophiles and electrophiles, and carbanions and carbocations (Tables 8.22 & 8.23).

**Analysis of Concept Map 6.** Concept map 6, consisting of the terms 'reaction intermediate', 'carbocation', 'carbanion', 'free radical', 'homolytic cleavage', and 'heterolytic cleavage', was only assigned during the Fall, 1997, semester. Like concept map 5, the lecture material corresponding to this concept map covered material related to the mechanisms of organic chemistry and the types of intermediates produced. However, this concept map and the corresponding lecture are intended to address the manner by which these intermediates are produced. Because few difficulties in the learning of stereochemistry were identified from this concept map and the value of Kendall's W was very high (.8308), this concept map was not assigned during the Spring, 1998, semester.

The mean ranks of the concepts 'carbocation', 'carbanion', and 'free radical' were very close in this map (Table 8.24), and no statistically significant difference existed between them (Table 8.25). This relationship was discussed above in the analysis of concept map 5. The mean ranks of the concepts 'homolytic cleavage' and 'heterolytic cleavage' were also very close (Table 8.24) and again no statistically significant difference existed between them (Table 8.25). The mean ranks of these latter two terms were lower than the ranks of the concepts 'carbocation', 'carbanion', and 'free radical', and these differences were statistically significant (Tables 8.24 and 8.25). Examination of individual concept maps shows that most students focus on the intermediates and categorize the process using the intermediate produced. Thus, the intermediate (carbocation, carbanion, or free radical) is placed at a higher level in the concept map than the process by which it is formed (homolytic or heterolytic cleavage). Only a small minority of students focus on the process and categorize the intermediates using the process whereby it is formed.
Concept Map 7. Concept map 7, consisting of the terms 'enantiomer', 'physical properties', 'chemical properties', 'plane-polarized light', and 'racemic mixture', was assigned during both the Fall, 1997, and Spring, 1998, semesters. The lecture material corresponding to this concept map can be considered an introduction to optical isomerism, covering the nature of enantiomers, their chemical and physical properties, and the nature of their interaction with plane-polarized light.

The test questions intended to address this material were not in general too difficult for the students. For the Fall, 1997, semester, 75.7% of the questions related to this material were answered correctly, and for the Spring, 1998, semester, 71.1% of these questions were correctly answered (Table 8.56). However, an examination of Kendall's W (.6862 and .5125 for the Fall, 1997, and Spring, 1998, semesters) indicates considerable disagreement among the students as to how this map was constructed, and this is confirmed by the disagreement in choice of superordinate concept. The most common choice for superordinate concept was enantiomer (or its plural, enantiomers), and was chosen by 43.4% and 65.8% of students in the Fall, 1997, and Spring, 1998, semesters, respectively (Table 8.28). A slight but significant difference was noted in the mean ranks of the terms 'chemical properties' and 'physical properties' in the Fall, 1997, semester (Tables 8.26 and 8.27). This difference was not significant in the Spring, 1998, semester (Tables 8.26 and 8.28). Examination of the concept maps from the Fall, 1997, semester reveals that this difference appears to be caused, at least in part, by the efforts made by some students to show the differences between chemical and physical properties of enantiomers. With the exception of the rotation of plane-polarized light, physical properties of enantiomers are identical. Chemical properties are identical when enantiomers react with achiral compounds but can vary when enantiomers react with chiral compounds. In order to accommodate these ideas, some students were required to place the term 'chemical properties' on a lower level of the concept map.
This concept map generated more different difficulties than any of the maps that preceded it. Some of these, such as the propositions 'enantiomers have chemical properties' and 'enantiomers have physical properties' were classified as naive. Naive propositions first occurred in appreciable numbers in concept map 7, and they recurred in the next two concept maps, numbers 8 and 9. Maps 10 through 12 had remarkably fewer naive propositions. The three concept maps labeled 7, 8, and 9 appear to lie at the heart of the most difficult stereochemical material.

When using these naive propositions, it appears that some students were simply trying to incorporate these terms into their concept maps without being formally incorrect. Other propositions indicated that students could not distinguish between chemical and physical properties. An example is 'chemical properties such as boiling point' (Table 8.30). Other students confused structure with chemical or physical properties in propositions such as "Chemical properties of enantiomers include R-(-) and S-(+)", "Enantiomer has a chemical property of chiral carbon", and "Enantiomers have physical properties like nonsuperimposable mirror images" (Table 8.30). Several students equated optical isomers with enantiomers, not realizing that 'optical isomer' is a broader term (Table 8.30). Because the term 'diastereomer' had not yet been introduced as another type of optical isomer, this confusion is understandable.

The confusion of the term 'atom' with 'functional group' noted in concept map 4 is most probably related to the confusion of the term 'atom' with 'molecule' noted here. Propositions such as "A chiral atom has one pair of enantiomers", "Chiral carbons can be a racemic mixture", and "Chiral carbons can be a racemic mixture" indicate a lack of differentiation between atoms and molecules (Table 8.29).

This concept map also generated some very interesting statements. The statement "Enantiomers have identical stabilities therefore chemical properties are the same", was clearly written by a thoughtful student (Table 8.30). Although the chemical properties of enantiomers can differ when reacting with chiral molecules, it is difficult to criticize this
Another interesting statement is, "Enantiomers almost always need chiral atoms" (Table 8.30). Some very unusual pairs of enantiomers do exist that do not contain chiral atoms (March, 1977), but this was not discussed in either the lecture or the text. It is interesting to speculate how this proposition was generated by the student.

**Analysis of Concept Map 8.** Concept map 8, consisting of the terms 'enantiomer', 'racemate', 'mirror image', 'inversion', and 'absolute configuration', and 'resolution', was assigned during both the Fall, 1997, and Spring, 1998, semesters. The lecture material corresponding to this concept map covered the nature of the tetrahedral carbon atom and chirality, absolute configuration around a chiral atom and its relationship to the rotation of plane-polarized light, inversion of configuration in substitution reactions, and the process of separation (resolution) of enantiomers in a racemic mixture.

The test questions designed to assess this material were difficult for each class. Students in the Fall, 1997, semester received an average grade of 54.4% on these questions, and students in the Spring, 1998, semester received an average grade of 64.3%. In addition, there was considerable disagreement among students regarding placement of concepts in the corresponding concept maps. Kendall's W for the mean ranks of the six seed concepts had values of .4542 and .5637 for the Fall, 1997, and Spring, 1998 semesters, respectively. The most commonly chosen superordinate concept in both semesters was 'enantiomer' (or its plural); 42.2% of students in the Fall, 1997, semester and 75.0% of students in the Spring, 1998, semester used this as the superordinate concept. As a whole, these data seem to indicate that this was particularly difficult material for students to assimilate.

Like concept map 7 discussed previously, this concept map generated a large number of difficulties as well as some particularly interesting statements. The students who constructed the propositions "Absolute configuration is asking, 'What is the shape of the actual molecule,'" and "Absolute configuration is their position in space," obviously tried to express the meaning of absolute configuration clearly in their own words (Table 8.35).
The student who wrote "One chiral atom implies one pair of enantiomers" appears to have grasped the relationship between chirality and mirror images.

Several students generated propositions that were classified using the term 'naive', and, as in concept map 7, it is suspected that these propositions were included solely because the student needed to use the assigned seed concepts. Examples are "Chiral atoms form enantiomers", "Diastereomers involve inversion" and "Optical isomerism involves mirror images" (Table 8.35).

Some creative views of absolute configuration generated by this concept map have already been discussed. Many other students were not as successful in integrating this seed concept into a map. Propositional statements such as "Inversion results in absolute configuration", "A carbon atom attached to four different functional groups rotates to form absolute configuration", and "Enantiomers have 2 different absolute configurations; each is called a racemate" all indicate that the authors of these propositions do not realize that absolute configuration is used to describe the chirality of a structure (Table 8.35). The latter statement indicates that the concept 'racemate' was also troublesome, and several propositional statements incorrectly used this term as well. Racemates were sometimes seen as single compounds rather than equimolar mixtures of enantiomers. This hypothetical compound was often described as being achiral because it does not rotate plane polarized light (Table 8.35). One student described a racemate as a "salt of racemic acid," (Table 8.35) employing a rule for naming the salt of a carboxylic acid through the addition of the suffix '-ate' (Bailey and Bailey).

Another important category of difficulties derived from this concept map involved the relationships between types of isomers (Table 8.34). Many students stated that "Enantiomers are not diastereomers"; however, enantiomers can be viewed as specific types of diastereomers. Other students viewed diastereomers as specific types of enantiomers, and, in addition, many students proposed that geometric isomers can be enantiomers (Table 8.35). Part of this difficulty may emerge from the fact that chemists...
themselves have not developed good terms to delineate the two types of commonly
encountered diastereomers: geometric isomers and what might be termed 'optical
diastereomers.' This issue is encountered again in analysis of concept map 9.

Finally, the meaning of chirality was difficult for many students (Table 8.34).
Included here is the proposition that "Optical isomers without mirror images are
diastereomers" and "Enantiomers can be achiral reagents" (Table 8.35). These two
statements appear to relate to difficulties in the realization of the 'left-and-right
handedness' of chiral structures. Another example is "Optical isomers are identical in
structure." The idea that two structures can contain the same atoms connected in the same
order with the same bond angles and yet be different (e.g. mirror images of each other)
appeared to elude the authors of these propositions.

Analysis of Concept Map 9. Concept map 9, consisting of the terms 'isomer',
'structural isomer', 'stereoisomer', 'enantiomer', and 'diastereomer', was assigned
during both the Fall, 1997, and Spring, 1998, semesters. The lecture material
corresponding to this concept map introduced the stereochemistry of compounds
containing more than one chiral center and reinforced the relationships among the types of
isomers previously introduced. Students in the Spring, 1998, semester performed more
poorly on the test questions designed to evaluate this material (66.3% correct) than did
students in the Fall, 1997, semester (80.1% correct); this discrepancy may in part be
caused by the different questions asked of the classes in each semester (Table 8.56).

The seed concept 'isomer' was chosen to be the superordinate concept by most of the
students in both the Fall, 1997, semester (79.8%) and the Spring, 1998, semester
(93.4%) (Table 8.36). Not only did students constructing this map largely agree on the
choice of superordinate concept, they also appeared to agree regarding the relative
placement of the seed concepts as measured by Kendall's W (.7930 and .8771 for the
Fall, 1997, and Spring, 1998, semesters) (Table 8.36).
As in concept maps 7 and 8, analysis of concept map 9 revealed several naive propositions. In many maps, stereoisomers were classified separately from enantiomers and diastereomers; however, both enantiomers and diastereomers are types of stereoisomers. In some of these maps, it is clear that the map's constructor is indicating that enantiomers and diastereomers are not related to stereoisomers (Tables 8.39 & 8.40).

Comparison of concept map 8 (Tables 8.31-8.35) and concept map 9 (Tables 8.36-8.40) might indicate that students have less difficulty relating various types of isomer to each other (concept map 9) than in describing the properties of isomers (concept map 8). However, some of the difficulties originally noted in concept map 8 (Tables 8.34 & 8.35) appeared to recur in concept map in slightly different guise (Tables 8.39 & 8.40). Both sets of maps revealed propositions in which students had difficulties describing the relationships between types of isomers. In addition, the relationship between enantiomers, diastereomers, and chirality gave difficulty in both maps. The difficulty that diastereomers do not have a mirror image occurs in concept map 8, (Tables 8.34 & 8.35) and is repeated in concept map 9 (Tables 8.39 & 8.40).

Because structural isomers and stereoisomers are two different types of isomer, it was anticipated that the mean ranks of these two concepts would be tied, or very close, in the students' maps. However, in both semesters, there was a small but significant difference in the placement of these two terms (p < .0075 and p < .0067 for the Fall, 1997 and Spring, 1998 semesters, respectively. Table 8.38). In both semesters, the mean rank of the concept 'structural isomer' was slightly higher. It's mean rank in the Fall, 1997 semester was 2.72, whereas the mean rank of the concept 'stereoisomer' was 2.84. This difference was even larger in the Spring, 1998 semester. The mean rank of 'structural isomer' was 2.54 and that of 'stereoisomer' was 2.83 (Table 8.36). Examination of the individual concept maps revealed that several students classified isomers as being either 'structural isomers' or 'optical isomers', and then classified 'stereoisomers' as types of optical isomers.
Concept map 9 revealed an interesting issue that is termed the 'geometric isomer - diastereomer problem' (Tables 8.39 & 8.40). Diastereomers are defined as "stereoisomers which are not enantiomers" (March, p. 104), and thus geometric isomers (that are caused by hindered rotation around a bond) are a type of diastereomer. However, the term 'diastereomer' is most commonly applied to a different type of structure, one that contains two different chiral sites but may not have any hindered rotation around a bond. This important distinction gave many students difficulty, and some students resorted to the method used in their lecture to distinguish between these two types of diastereomers. Diastereomers caused by the presence of two different chiral sites in a molecule were termed 'chiral diastereomers.'

In some concept maps, the geometric isomer - diastereomer problem was avoided by omitting the term 'geometric isomer', which was not one of the seed concepts. In others, no link was placed between the terms 'geometric isomer' and 'diastereomer.' In still others, a faulty relationship was noted, such as "Geometric isomers can be enantiomers or diastereomers or stereoisomers" (Tables 8.39 & 8.40).

Analysis of Concept Map 10. Concept map 10, which had the seed concepts 'nucleophile', 'leaving group', 'racemization', 'inversion', and 'substitution', was assigned as the second concept map in both the Fall, 1997, and Spring, 1998, semesters. The lecture material corresponding to this concept map dealt with the stereochemical consequences of first- and second-order nucleophilic substitution (racemization at a chiral center and inversion of configuration at a chiral center, respectively).

The test questions that evaluated these concepts were somewhat difficult. In the Fall, 1997, semester, the response rate was 70.8% correct, and in the Spring, 1998, semester, this rate was only 60.9% correct. Some discrepancy existed in both semesters regarding the choice of superordinate concept for this concept map, with the most prevalent concept, 'substitution' (or 'substitution reaction') being chosen by only 62.1% of students in the Fall, 1997, semester and 64.4% of students in the Spring, 1998, semester.
The second most common choice, 'nucleophile', was chosen by 9.2% and 26.0% of student in the Fall, 1997, and Spring, 1998, semesters, respectively (Table 8.41). Kendall's W for the placement of seed concepts in this map had a value of .6866 and .6149 for the Fall, 1997, and Spring, 1998, semesters, respectively.

It was anticipated that the concepts 'racemization' and 'inversion' would be placed at the same level in most of the concept maps because these are the two processes that can occur at a chiral carbon atom during a substitution reaction. In the Fall, 1997 semester the concept 'inversion' had a mean rank of 4.05 compared to a mean rank of 4.21. In the Spring, 1998 semesters, these same concepts had mean ranks of 4.10 and 4.19, respectively (Table 8.41). Although the differences are small, for the Fall, 1997, semester the difference is significant ($p < .0082$, Table 8.42). One hundred nineteen concept maps were analyzed in the Fall, 1997, semester, and of these maps, sixteen placed the concept 'inversion' at a higher level in the map, and six placed the term 'racemization' higher. The maps in which the concept 'inversion' was higher that the concept 'racemization' fell into two categories. The first category consisted of maps in which a concept involving the $S_{N}1$ mechanism was linked to the term 'racemization', placing this concept at a lower level in the map. The second category consisted of maps in which the terms 'inversion' and 'retention' combine to yield the term 'racemization', again placing the term 'racemization' at a lower level. This is what occurs in the $S_{N}1$ mechanism. No clear pattern emerged in the six concept maps in which 'racemization' was placed at a higher level than 'inversion'.

Although the test questions for this map may have been somewhat difficult, the number of difficulties identified in this map were relatively few. In contrast to the previous three maps, none of the propositions was categorized as 'naive' (Table 8.44). Like concept map 4, this assignment revealed several propositions that confused atoms with leaving groups (Tables 8.44 & 8.45).
Analysis of Concept Map 11. This was the last concept map assigned that appeared to be related to the learning of stereochemistry. It consisted of the seed concepts 'alcohol', 'alkoxonium ion', 'alkene', 'proton', and 'elimination'. The related lecture material covered the mechanism of the dehydration of alcohols to form alkenes. One student noted, "This assignment reads like a recipe for the E1 dehydration reaction" (Table 8.50).

Students did poorly on the test questions related to this material, with success rates of 69.8% and 44.5% in the Fall, 1997 and Spring, 1998 semesters, respectively. The values of Kendall's W for relative placement of the seed concepts were also low (.5593 and .4953 in the Fall, 1997 and Spring, 1998 semesters, respectively, Table 8.46). Only 66.1% of students in the Fall, 1997 semester chose 'alcohol' as the superordinate concept, with 75.4% of students in the Spring, 1998, semester choosing this same superordinate concept. Taken together, these three criteria all seem to indicate that this material was difficult for students. In a manner similar to propositions encountered in maps 7, 8, and 9, several students produced propositions that were categorized as 'naive'. References to nomenclature of alcohols are examples (Tables 8.49 & 8.50).

Because the alkoxonium ion is an intermediate in the synthesis of an alkene from an alcohol by an elimination reaction, it was anticipated that this concept would rank fairly high among the five seed concepts. This was not so. In both semesters, it averaged last among the five seed concepts (Table 8.46). Examination of the individual concept maps revealed that several students did not seem to know what to do with this term.

A variety of difficulties were identified from this concept map (Tables 8.49 & 8.50). Most of these involved difficulties in describing the mechanism of elimination instead of difficulties related to the learning of stereochemistry.

Analysis of Concept Map 12. Concept map was assigned relatively late in each semester (after most of the important stereochemical material had been covered). The seed concepts assigned were 'alcohol', 'aldehyde', 'carboxylic acid', 'oxidation', and
'reduction', and the corresponding lecture material covered reactions of alcohols, and in particular their oxidation to aldehydes and carboxylic acids. The term 'alcohol' or its plural was the most common choice as the superordinate concept, but the percentages of students choosing this concept were only 66.3% and 76.2% in the Fall, 1997 and Spring, 1998 semesters, respectively (Table 8.51). Kendall’s W was also surprisingly low (.4587 & .4160 for the Fall, 1997 and Spring, 1998 semesters, respectively, Table 8.51). This concept map generated relatively few difficulties, and none related to the learning of stereochemistry (Tables 8.54 - 8.55). Examination of the individual concept maps revealed the cause of the low values for Kendall’s W. Because the lecture material had emphasized oxidation of alcohols, a sizable number of students used 'oxidation' as the superordinate concept. These concept maps, although usually excellent, generally had a much different structure than those that used 'alcohol' as the superordinate concept. One student noted, "This one was difficult because everything was related in more than one way" (Table 8.55).

Comparison of Concept Maps and Interviews. Eight of the concept maps assigned (numbered 2, 3, 4, 7, 8, 9, 10, and 11) and all four of the interviews were designed to directly relate to the learning of stereochemistry. The major types of difficulties related to the learning of stereochemistry that were derived from both the interviews and the concept maps (Tables XX - XX) were tabulated, unitized, and categorized according to the methods of Lincoln and Guba (1985). Four major types of difficulties emerged from this analysis; each of these was further subdivided. In addition, a category of interesting or unusual conceptions that were not necessarily incorrect was added. These type of difficulties and their sources (concept maps or interviews) are given in Table 10.1.

Summary of Results from This Study. The four major types of difficulties tabulated above in Table 10.1 are entitled 'Focus' (type I), 'Naive' (type II), 'Processes' (type III), and 'Shapes' (type IV). Each of these types contains statements derived from both the interviews and the concept maps; however, some important distinctions can be made.
Table 10.1. Major Types of Difficulties Emerging from This Study.

<table>
<thead>
<tr>
<th>Type of Difficulty</th>
<th>Selected Examples</th>
<th>Category</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>I) Focus</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A) Chemical entity too specific</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Leaving group too specific</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2) Catalyst too specific</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3) Nucleophile or electrophile too specific</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4) Use of 'atom' for 'molecule', 'functional group', or 'substituent'</td>
<td>Concept Map 4</td>
<td>III</td>
</tr>
<tr>
<td>B) Narrow focus on isomer type</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Concept Map 9</td>
<td>VI</td>
</tr>
<tr>
<td></td>
<td>Interview 2</td>
<td>IV</td>
</tr>
<tr>
<td><strong>II) Naive</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A) Issues of optical isomerism</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Optical isomerism involves mirror images</td>
<td>Concept Map 8</td>
<td>II</td>
</tr>
<tr>
<td>2) Diastereomers involve inversion</td>
<td>Concept Map 8</td>
<td>II</td>
</tr>
<tr>
<td>B) Classification of isomers</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Stereoisomers classified differently from optical isomers</td>
<td>Concept Map 9</td>
<td>II</td>
</tr>
<tr>
<td>2) Stereoisomers classified differently from enantiomers and diastereomers</td>
<td>Concept Map 9</td>
<td>IV</td>
</tr>
<tr>
<td>3) The geometric isomer-diastereomer problem</td>
<td>Concept Map 9</td>
<td>IV</td>
</tr>
<tr>
<td>4) Confusion of the structure with its formula</td>
<td>Concept Map 2</td>
<td>IV</td>
</tr>
<tr>
<td></td>
<td>Concept Map 3</td>
<td>II</td>
</tr>
<tr>
<td>C) Nomenclature</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Use of nomenclature rules in order to include a seed concept</td>
<td>Concept Map 11</td>
<td>II</td>
</tr>
<tr>
<td>2) Misattribution of functional groups</td>
<td>Concept Map 11</td>
<td>III</td>
</tr>
<tr>
<td>3) Misapplication of nomenclature rules</td>
<td>Interview 1</td>
<td>IV</td>
</tr>
<tr>
<td></td>
<td>Interview 3</td>
<td>III</td>
</tr>
<tr>
<td></td>
<td>Interview 4</td>
<td>III</td>
</tr>
<tr>
<td>**D) Rote rules and reorientation</td>
<td></td>
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<tr>
<td></td>
<td>Interview 4</td>
<td>III</td>
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<tr>
<td></td>
<td>Interview 3</td>
<td>VI</td>
</tr>
<tr>
<td></td>
<td>Interview 4</td>
<td>III</td>
</tr>
<tr>
<td>**III) Processes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A) Molecular motion</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Rotation in conformers</td>
<td>Concept Map 2</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>Concept Map 3</td>
<td>III</td>
</tr>
<tr>
<td></td>
<td>Interview 2</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>Interview 2</td>
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<td></td>
<td>Interview 3</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>Interview 4</td>
<td>III</td>
</tr>
<tr>
<td>2) Equilibrium and conformer extremes</td>
<td>Concept Map 2</td>
<td>II</td>
</tr>
<tr>
<td></td>
<td>Concept Map 2</td>
<td>III</td>
</tr>
<tr>
<td>3) Rotation of whole structures</td>
<td>Interview 1</td>
<td>V</td>
</tr>
<tr>
<td></td>
<td>Interview 3</td>
<td>VII</td>
</tr>
<tr>
<td></td>
<td>Interview 4</td>
<td>III</td>
</tr>
</tbody>
</table>

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Table 10.1 (cont.).

B) Bond breaking and bond formation

1) Reactions
   a) Addition
   b) Substitution
   c) Elimination

2) Mechanisms
   a) Charges of intermediates
   b) Progress of the mechanism
   c) Stereochemical consequences

IV) Shapes

A) Orientation of substituents within molecules
   1) Geometric isomers
   2) "Living in a flat world"

B) Methods of Representation
   1) \( \pi \) bonds
   2) Conformers
   3) Models vs. paper representations

C) Chirality, absolute configuration, and orientation of substituents on a single atom

D) Order of connection

E) Shapes and properties of substances

<table>
<thead>
<tr>
<th>Concepts</th>
<th>Interview</th>
<th>Concept Map</th>
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</thead>
<tbody>
<tr>
<td>Addition</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Substitution</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Elimination</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Charges of intermediates</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Progress of the mechanism</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Stereochernical consequences</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Geometric isomers</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>&quot;Living in a flat world&quot;</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>( \pi ) bonds</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Conformers</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Models vs. paper representations</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Chirality, absolute configuration, and orientation of substituents on a single atom</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Order of connection</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Shapes and properties of substances</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>
regarding the types of information derived from each source. Because over two hundred students submitted concept maps in this study and only ten students were interviewed, it is perhaps not surprising that examination of the concept maps yielded a wider variety of difficulties in the learning of stereochemistry than did examination of the interviews. Nevertheless, this study seems to indicate that qualitative differences in the types of information about the learning of stereochemistry derived from these sources can be observed.

The first major type of difficulty (Table 10.1, type I), entitled 'Focus', deals with propositions or statements in which students used a specific chemical term when a general term would be preferred. All of the entries in which the chemical entity was deemed too specific were found in the concept maps; none of these difficulties emerged from examination of the interviews. Statements indicating that a substituent must be an atom or that halide must be the leaving group were common in the concept maps, but were not observed in the interviews. However, both the concept maps and the interviews produced propositions or statements in which the students focused on only one type of isomer. When using models to examine different types of isomers, students generally built only structural isomers until prodded further. Apparently, when given the individual pieces of a models kit, students in this study found it easiest to simply connect the pieces in a different order, producing a set of structural isomers. However, when asked to use these same models to build a set of geometric isomers, students then had difficulty finding the related structural isomers. Their focus tended to be on one type of isomer or the other. Given a set of drawings representing a mixture of structural and geometric isomers, students would much more readily identify pairs of geometric isomers despite their initial preference to build models of structural isomers.

The second major type of difficulty (Table 10.1, type II) is entitled 'Naive'. Most of the propositions in this type were derived from the concept maps. Inclusion of naive propositions in concept maps appears to occur when a student does not know how a
given seed concept relates to other concepts in the map. When this occurs, the student can look up the definition of the seed concept and force it into the map. Perhaps because most of the interview material did not require the use of definitions of stereochemical terms, these types of naive statements were not observed in the interviews. One important type of naive statement that occurred in the concept maps is termed the 'geometric isomer-diastereomer problem' (Table 10.1, type IIB3). This problem occurs because the term 'diastereomer' includes both geometric isomers and isomers caused by the presence of two chiral centers in a structure. There is no separate chemical term to describe this latter type of isomer, which caused several students to include naive statements about diastereomers in their concept maps.

Only when using chemical nomenclature were naive statements found in both the concept maps and the interviews. However, one important type of difficulty classified as naive was found only in the interviews. This is the type entitled 'Rote rules and reorientation' (Table 10.1 type IID), and included any difficulties that students encountered when applying rote rules. The most common rote rule giving rise to difficulties states that one can form the enantiomer of a compound containing exactly one chiral center by exchanging the positions of any two substituents attached to that chiral center. A student applying this rule does not have to visualize the mirror image of the chiral structure being studied. Use and misuse of this rule did not appear in any concept maps, but was the source of several difficulties described in the third and fourth interviews.

The third major type of difficulty (Table 10.1, type III) is entitled 'Processes,' and lists difficulties involving any of the dynamic changes that occur within or between chemical entities. This type is subdivided into 'Molecular motion' and 'Bond breaking and formation'. 'Molecular motion' includes difficulties experienced with rotation in conformers, conformer extremes and equilibrium, and the rotation of entire structures. Both concept maps and interviews revealed difficulties in describing rotation within
conformers. In particular, both concept maps and interviews revealed examples of students who thought of conformers solely in terms of one specific type of conformer: the 'chair' and 'boat' forms of cyclohexane. Analysis of concept maps also showed that some students occasionally equated conformers with structural isomers, and concept maps were an excellent tool to determine if students could relate the definition of the term conformer with other definitions (Table 9, type IIIA1). Use of the concept map was also the only method that revealed many students' lack of understanding of the equilibrium that exists between conformer extremes (Table 9, type IIIA2). However, the difficulties associated with the idea that rigid molecules do not have conformers only appeared through analysis of the interviews (Table 10.1, type IIIA3).

Under the heading 'Bond breaking and bond formation' are difficulties associated with chemical reactions and the mechanisms of these reactions (Table 10.1, type IIIB1). Both concept maps and interviews were useful tools for investigating students' difficulties involving chemical reactions. A recurring theme in analysis of the concept maps was use of the term 'atom' when a more general term such as 'molecule', 'substituent', or 'leaving group' would be preferred. This tendency was observed many times in analyzing the concept map 4 dealing with reactions (Tables 8.17 & 8.18) but not at all when analyzing the interviews, reinforcing the idea previously introduced that the concept maps are an excellent tool when investigating definitions of terms and their relationships to one another. The concept maps also were useful when investigating student difficulties in predicting reaction products. Perhaps because the interviews were more narrowly constructed to emphasize investigation of stereochemistry, this particular difficulty was not as prevalent in the interviews.

Both concept maps and interviews were also useful when investigating student difficulties with reaction mechanisms (Table 10.1, type IIIB2). The concept maps revealed several difficulties experienced by students when determining the charges on chemical intermediates. Because the charges were indicated in the problems designed for
the interviews, this difficulty did not appear in the interview analysis. Some of the
difficulties revealed by the concept maps, such as confusion of an intermediate for the
product, again appear to be misuse of a definition. Some of the key difficulties revealed
from the interviews occurred less frequently in the concept maps. Examples include
insistence that there must be a preference of the nucleophile for one side of a planar
carbocation, lack of association of a planar carbocation intermediate with formation of a
racemic product in the S_N1 mechanism, and lack of association of approach of the
nucleophile from the back side with inversion of configuration in the S_N2 mechanism
(Table 10.1, type III B2). Each of these difficulties appeared in several concept maps, but
were major themes of the fourth interview. One important difficulty from the fourth
interview, unwillingness of students to rotate around a bond to give a molecule the proper
orientation for E2 elimination, did not appear in any concept maps.

The last major type of difficulty (Table 10.1, type IV) is entitled 'Shapes'. Several
of the concept maps revealed difficulties in recognition of the structural features of
geometric isomers. This was an important difficulty revealed in the first interview (Table
10.1, type IVA). In addition, the interviews revealed that some students preferred to
"live in a flat world," in particular, they were unwilling to draw cyclic structures in a
manner that would illustrate the perspective of the substituents (Table 5.1, type III), and
tend to revert to drawing planar dash formulas when presented with complex structures,
particularly those containing more than one chiral atom (Table 6.2, type IV). These
difficulties were not readily apparent from examination of the concept maps, perhaps in
part because students were given wide latitude in their choice of examples and could
exclude more complex structures from their concept maps. Similarly, difficulties in
representing shapes of pi bonds and conformers were detected almost exclusively through
the use of interviews (Table 10.1, type IVB).

Both the concept maps and the interviews were effective tools for investigating
students' difficulties regarding chirality, absolute configuration, and orientation of
substituents on a single atom (Table 10.1, type IVC). The third interview revealed that some students will not investigate whether two structures represent mirror images unless they are plainly drawn as such. The importance of drawing the frameworks of two molecules as mirror images is so important that two structures containing different substituents were sometimes perceived as mirror images when the frameworks were drawn as such (Table 6.2, type IIA). An analogy might be to claim that a red woolen glove and a green cotton glove are mirror images of each other because one fits the left hand and the other the right. The third interview also revealed that most of the students interviewed would worry about the chirality of an achiral atom if it was drawn in three dimensions, and that stating that such an atom is achiral did not necessarily divert students' attention from it. Although the concept maps did not reveal the difficulties described above, they were useful in revealing difficulties describing the types of molecules that exhibit chirality and their relationships to each other.

Both the concept maps and the interviews were useful in determining student difficulties related to the order of connection of atoms within molecules (Table 10.1, type IVD). Concept maps were particularly useful when examining difficulties students had in relating structural isomers to other isomer types, whereas the first two interviews yielded information regarding students' failures to recognize two or more structures as being structural isomers. Finally, the concept maps provided a means for recognition of student difficulties relating chemical and physical properties of substances to chirality of molecules, although it should be mentioned that none of the interview questions addressed this issue.

The information gained from the concept maps and the interviews in many areas appears to be complementary. The concept maps were an excellent tool to detect difficulties students had in relating stereochemical terms to one another, definitions of terms, the relationships between structure, stereochemistry, and chemical and physical properties. In addition, concept maps divulged many interesting and unusual strategies.
and ideas developed by students; a sampling of these is given in Table 10.2. Perhaps because the interviews were more tightly focused on given topics, fewer of these interesting and unusual ideas emerged.

<table>
<thead>
<tr>
<th>Source Category</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>CM1</td>
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<tr>
<td>I</td>
<td>CM3</td>
</tr>
<tr>
<td>I</td>
<td>CM3</td>
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<tr>
<td>I</td>
<td>CM8</td>
</tr>
<tr>
<td>I</td>
<td>CM9</td>
</tr>
</tbody>
</table>

### Table 10.2. Sample of Some Interesting and Unusual Propositions Derived from Concept Maps.

1. Hydrocarbons are derived from decayed organic matter.
2. Recognition of a relationship between geometric isomers and stereoisomers.
3. Conformers vary in the distances between attached atoms.
4. Enantiomers differ in chemical properties (drug effects).
5. Relation of absolute configuration to positions of atoms in space.
6. One chiral atom implies one pair of enantiomers.
7. Resolution can be performed by mechanical means.
8. Interesting methods to classify stereoisomers.

Although the concept maps were an excellent tool to examine the types of difficulties described above, they were much less successful tools for examination of difficulties that students encountered when translating or rotating entire molecules, rotating around bonds, or inverting configurations. In examining these difficulties, the interview was a much more successful technique.

One could speculate that of the four major categories of difficulties identified in this study, the two that appear to be fundamentally most problematical 'processes' and 'shapes'. Difficulties involving focus, especially those that entail misapplication of definitions, may perhaps be addressed by simply addressing these definitions more forcibly in lecture. The same can perhaps be said of the 'naive' difficulties. However,
difficulties involving processes and shapes that were dealt with extensively in the classroom appear to be more resistant to change.

A concept map summarizing these four types of difficulties is given in Figure 10.1.

![Diagram: Concept Map of Difficulties in Learning Stereochemistry]

**DIFFICULTIES IN LEARNING STEREOCHEMISTRY**

- **NAIVE**
  - **USE OF**
    - **ROTE RULES**
  - **et al.

- **NARROW FOCUS**
  - **ISOMER TYPE**
  - **et al.

- **PROCESSES**
  - **MOLECULAR MOTION**
  - **et al.

- **SHAPES**
  - **CHIRALITY AT A SINGLE ATOM**
  - **et al.

Figure 10.1. Concept map summarizing the results of this study.

**Critical Junctures in the Learning of Stereochemistry.** The question remains whether concept maps can be used to determine critical junctures in the learning of stereochemistry. In an attempt to answer this question, the values of Kendall's W for each relevant concept map were compared to the results of related multiple choice questions given on class examinations. Another indicator examined was the relationship between the percentage of students choosing the most common superordinate concept on these same concept maps and the results of the same multiple choice questions. The concept maps in this study deemed most appropriate to the learning of stereochemistry were those labeled 1, 2, 3, 4, 7, 8, 9, 10, and 11 (Table 3.5). Concept maps 5 and 6, dealing with mechanisms, and concept map 12, dealing with oxidation of alcohols, were not included because, although a few interesting difficulties related to stereochemistry were discovered upon examination of some of these maps, they were not primarily related
to the learning of stereochemistry. Concept map 1 was omitted from the analysis because at the time it was assigned, students had little experience with concept mapping.

Results of these comparisons for the Fall, 1997, and Spring, 1998, semesters are given in Tables 8.56 and 8.57; graphical comparisons of the relationships between Kendall's W for each concept map and the related test question percentages for the Fall, 1997, and Spring, 1998, semesters are shown in Figures 8.1 and 8.2.

For both semesters, the correlation between Kendall’s W and test question percentage was higher than the correlation between percent choosing the most abundant superordinate concept and test question percentage (Table 8.57). Although the correlation between Kendall’s W and test question percentage (r = .8093) for the Fall, 1997, semester was not significant at the 95% level, it was very close (p < .051). Correlation between percent choosing the most abundant superordinate concept and test question percentage for the Fall, 1997, semester was lower (r = .6617) and was not significant at the 95% level (p < .152, Table 8.57).

Correlation between Kendall’s W and test question percentage for the Spring, 1998, semester was slightly lower (r = .7191), but because more concept maps were included in the sample, this correlation was significant at the 95% level (p < .044). Correlation between percent choosing the most abundant superordinate concept and test question percentage for the Spring, 1998, semester was not significant (p < .573, Table 8.57).

These results indicate that, in this study, examination of concept maps may provide a method to determine which aspects of stereochemistry are most difficult for students and constitute a critical juncture in its learning. When used with caution, Kendall’s W may be one tool to aid in the identification of these critical junctures. The concept map with the lowest value of W (.4542) was map 8 in the Fall, 1997, semester. The value of W for the same map in the Spring, 1998, semester was .5637. The corresponding test questions had relatively low scores as well (54.4% and 64.3% for the respective
semesters, Table 8.56). A large number of types of difficulties were associated with this map (Tables 8.34 & 8.35).

Inspection of Tables 8.56 and 8.57 reveals that Kendall’s W was also low for concept map 7 (.5852 and .5125 for the Fall, 1997, and Spring, 1998, semesters, respectively, Table 8.56). Like concept map 8, the number of types of difficulties revealed by this map was large (Tables 8.29 & 8.30). However, students performed much better on the related test questions (75.7% and 71.0% for the Fall, 1997, and Spring, 1998, semesters, respectively, Table 8.56).

One other concept map with a low values of W was map 11 (.5593 and .4953 for the Fall, 1997, and Spring, 1998, semesters, respectively). Like concept map 8, students also performed poorly on the related test questions (69.8% and 44.5% in the Fall, 1997, and Spring, 1998, semesters, respectively, Table 8.56). Examination of the types of difficulties associated with this concept map, however, reveals that most of them were related to mechanisms rather than stereochemistry (Tables 8.49 & 8.50).

Based on these data, it appears that a critical juncture in the learning of stereochemistry occurred when the material associated with concept map 8 was presented to the classes. This is the introductory material on optical isomerism, and represented the students’ early encounters with enantiomers and their relationships to each other, absolute configuration and inversion of configuration.

Concept map 7 also deals with enantiomers and their physical and chemical properties. Although the data do not as strongly support the conclusion that it represents a critical juncture, with the implication that it is a point at which "students must possess a certain framework of understanding of previous concepts in order to master new material" (Trowbridge & Wandersee, 1994), it clearly represented a point at which students had difficulty, and this material is closely related to that from concept map 8.

Like maps 7 and 8, concept maps 9 and 10 also dealt with stereoisomers. Map 9 investigates the relationships between various types of isomers and map 10 investigates
the relationships between stereochemistry and mechanisms. Kendall's W was higher for both map 9 (.7930 and .8771 in the Fall, 1997 and Spring, 1998 semester, respectively, Table 8.56) and map 10 (.6866 and .6149 in the Fall, 1997 and Spring, 1998 semester, respectively, Table 8.56). Students also performed better on the related multiple choice questions for these two maps than they did on the questions related to concept map 8. It is speculated that students needed to master the material from concept map 8 regarding the nature of enantiomers before they could master these topics, but once this material was assimilated, they were prepared for the remainder of the stereochemical material.

Concept maps 2, 3, and 4 also appear to be directly related to learning stereochemistry. Although several individual difficulties were gleaned from examination of these concept maps, as a whole the results do not indicate that a critical juncture in the learning of stereochemistry occurred when the material related to these concept maps was presented to the students. Concept map 2 dealt with conformers and the process of rotation around sigma bonds, concept map 3 involved the definitions of various types of isomers, and concept map 4 addressed various reaction types. Kendall's W for these three maps ranged from a low of .6368 (map 2, Fall 1997) to .9703 (map 4, Spring 1998), and students performed well on the corresponding test questions, ranging from a low of 71.1% (map 3, Spring 1998) to a high of 89.0% (map 4, Spring 1998). These data apparently do not support the presence of a critical juncture at these points.

Stability of Kendall's W for Concept Maps. The values of Kendall's W for the concept maps assigned in the Fall, 1997, semester were plotted vs. values of Kendall's W for the same concept maps assigned in the Spring, 1998, semester (Figure 8.3). Only values of W for maps related to the learning of stereochemistry were included (maps 2, 7, 8, 9, 10, and 11; Tables 8.56 and 8.57). Pearson's r had the value .7918 for these points, which is significant at p < .05. This correlation provides one measure of the stability or generalizability of this type of data from one semester to another.
Addressing the Research Questions of This Study. Three research questions were outlined at the beginning of this study. A summary of the results and conclusions addressed by these questions follows.

The first research question asked, "How effective are concept maps as tools for the identification of difficulties and critical junctures in the learning of stereochemistry?" Twelve sets of concept maps were assigned to over two hundred students in this study. Fifty three different major types of difficulties encountered by students in one semester of organic chemistry were identified through these concept maps; of these, 39 difficulties were derived from the seven concept maps deemed most relevant to the learning of stereochemistry. Most of these major types were subdivided into two or more categories. These numbers indicate that concept maps can be an effective tool for the identification of difficulties in the learning of stereochemistry. Whether it can be said that these difficulties are in fact alternative conceptions cannot be answered by the results of this study. The duration of time over which these ideas were formed, how stable these difficulties may have been, or how useful they may have been to students in the past are all factors in determining whether these difficulties should be termed 'alternative conceptions'. None of these factors could be measured in this study.

The question of whether concept mapping is an effective tool for the identification of critical junctures in the learning of stereochemistry was addressed above. The evidence of this study indicates that, with the set of concept maps assigned, several points that might be termed 'critical junctures' were identified in this study.

The second research question was, "What types of difficulties encountered in the learning of stereochemistry can be identified through interviews of students?" The third research question asked, "How do the difficulties in the learning of stereochemistry that are identified by interviews correspond to those identified through concept mapping?" These two issues can be readily addressed together.
The four main types of difficulties encountered in the learning of stereochemistry that were identified through both interviews and concept maps are outlined in Table 10.1. These types of difficulties were named "Focus", "Naive", "Processes", and "Shapes." Each of these types occurred both in the interviews and the concept maps.

The category entitled 'Focus' dealt with those difficulties encountered by students when they used chemical terms that were too specific. Many of these difficulties emerged from the concept maps; however, the interviews were most fruitful when looking for those difficulties involving focus on only one type of isomer.

The category entitled 'Naive' consisted primarily of propositions obtained from the concept maps, and involved statements such as "optical isomerism involves mirror images" or "conformers have equilibrium" in which the student appears to simply be using a seed concept because it was assigned with no clear idea of its real relationship to other concepts. Although most of these 'naive' difficulties encountered by students were derived from the concept maps, the naive difficulties that students encounter when applying rote rules to reorient structures were derived exclusively from the interviews.

The category entitled 'Processes' involved any difficulties derived from either molecular motion (rotation within molecules, conformer extremes, and rotation of entire structures) or bond breaking and bond making, and the category called 'Shapes' involved difficulties regarding the orientation of substituents within molecules, students' representations of molecular shapes, chirality, order of connection, and the relationships of shapes of molecules to their properties. Most of these difficulties were common to both the interviews and the concept maps. Difficulties involving rotation of entire molecules were only noted in the interviews, as were difficulties in representing pi bonds and conformers. Difficulties involving absolute configuration and chirality and shapes and properties of substances were noted only in the concept maps.

**Suggestions to the Practicing Teacher.** Several students interviewed in this study were reluctant to pick up and handle molecular models, even when these models were
placed in front of them and they were told that they were welcome to use them. When they finally did pick up the models they were often unwilling to take the models apart, break and make bonds, and form new structures. When these students finally did pick up and handle these models they often had fewer difficulties. Thus, at least in the case of these students, it was not enough to simply tell them to use molecular models. They needed encouragement several times. By the end of the last interview, all of the subjects interviewed looked more readily to the use of molecular models to solve their problems.

Table 10.1 identifies 'Processes' as one category of difficulty in learning stereochemistry. Even after being shown models of conformers and rotation around sigma bonds in their lecture, students found that these concepts were difficult. It is suggested that many students would benefit by building models of conformers, demonstrating free rotation around their bonds, drawing various representations of the models in their hands, and describing this process using chemical terms such as 'staggered', 'eclipsed', 'gauche', 'anti', 'boat', 'chair', and 'equilibrium.' Similarly, difficulties in visualization of entire structures might well be alleviated by having students build models of simple molecules, rotate the entire structure, and draw representations of these structures from different perspectives. This might be especially helpful for students who have difficulty identifying and distinguishing between structural and geometric isomers.

The dynamic model previously described (Figures 3.3 - 3.6) was very popular with students. Many of them came to the front of the room after class especially to see this model, and many of them commented about how helpful it was in visualizing the $S_N1$ and $S_N2$ mechanisms. Some other students made special trips to the office of the instructor and asked to use this model. Because the model is easily made, it might be profitable to have several of these available for use in groups. It is suggested that students be required to draw and describe in writing the shapes of their intermediates and transition states from various perspectives while using this model.
The dynamic model described above is very specific in purpose. Its sole function is to illustrate and differentiate between the SN1 and SN2 mechanisms; it is of no value in demonstrating elimination reactions. Comments such as "I don't like eliminations" were common. Suggestions for a type of model other than commercially available 'static' models that could be used to demonstrate the E1 and E2 elimination mechanisms might be welcomed by both teachers and students.

The 'static' models, however, are excellent tools for representing and examining optical isomers such as enantiomers and diastereomers. Their weakness is in representing inversion of configuration and racemization; the model depicted in Figures 3.3 - 3.6 is far superior for this purpose. Nevertheless, it is suggested that each student should be required to use models to represent chiral structures, view them from several perspectives, draw dash-and-wedge diagrams, Fischer projections, and Newman projections of the models from various perspectives, and write descriptions of what they observe.

Concept mapping was a very popular technique in this study; students' comments about its use were almost always favorable. The difficulties under the headings 'Focus' (Table 10.1) were derived almost exclusively from the concept maps. As an example, many students used the term 'atom' when the term 'functional group' or 'substituent' would be preferred. Other students implied that a catalyst must be the hydrogen ion. A brief writing assignment, perhaps as small as a paragraph, that forced students to clarify their thoughts might alleviate many of these issues involving narrow focus. As an alternative, once a concept map is submitted and examined, students could be asked to rework them to eliminate potential problems. This approach might be especially effective in dealing with the difficulties called 'Naive' (Table 10.1).

When analyzing the concept maps, it was not difficult to separate the seed concepts by level and analyze them using SPSS™. Because versions of SPSS™ are now available for use on personal computers, the type of analysis of concept maps using
Kendall's W could be done by most teachers using concept maps. When done with caution, this may provide a viable tool to diagnose critical junctures in many classes and disciplines. Knowledge of critical junctures provides the practicing teacher a guideline as to where to focus his or her efforts in teaching. As a suggestion, student workers could be trained to analyze and enter the concept map data into the computer if the teacher's time were limited.

If the material represented by concept map 8 represents a critical juncture in the learning of stereochemistry, then it is suggested that this material is both particularly difficult and particularly important. Some suggestions for teaching this material include the use of polarizing filters placed on an overhead projector to demonstrate both the nature and the rotation of plane polarized light, the demonstration of chirality of molecular structures using an actual mirror, demonstration of inversion of configuration and racemization using dynamic models similar to those illustrated in Figures 3.3 - 3.6, and the use of actual chiral substances in lecture demonstrations. For example, (R)-(−)-carvone and (S)-(−)-carvone are enantiomers that are responsible for the odors of spearmint and caraway seed oil, respectively (Solomons, 1996). Structures of these molecules are given in Figure 10.2. Their molecules are mirror images that differ only in the configuration around their one chiral atom, and are sensed differently in humans because the nose contains chiral receptors. A demonstration of the odors of these compounds coupled with actual models of their structures, reflection of one structure in a mirror, and a discussion of the chirality of the odor receptors in the nose might be an effective method to present this material.

Finally, it is hoped that the tables of difficulties outlined in this study might provide the practicing teacher a useful guide as to what types of difficulties will be encountered by students in learning stereochemistry.

**Suggestions for Further Research.** This study diagnosed and categorized many of the difficulties encountered by students who study stereochemistry. It does not claim to
be all-inclusive. Students at other institutions and students in other types of organic chemistry classes may be expected to yield different results. The course studied here was a one-semester organic chemistry class geared primarily toward students in the agricultural sciences, nursing, dietetics, and other related fields. Students in the typical two-semester organic chemistry sequence designed for majors in chemistry, engineering, and biological sciences may experience difficulties that are very different from those outlined in this study.

![Figure 10.2. Enantiomers of carvone. The first structure is (S)-(+)–carvone and the second is (R)-(−)-carvone.](image)

Use of Kendall’s W to measure concordance of seed concepts within concept maps did not occur to this investigator until after the data had been collected. Therefore, after the courses had ended, the test questions that were used for comparison to Kendall’s W were chosen from a pool of all of the test questions administered. Were this study to be repeated, it would be preferable to write both concept maps and test questions to correspond to the objectives of each lecture period. It may be anticipated that the correlation between Kendall’s W and test question percentage might be higher were this procedure followed. In addition, a cluster analysis of hierarchical levels of seed concepts by student might reveal hidden patterns causing artificially low values of W similar to the pattern discussed for concept map 1.
The suggestions for teachers outlined above have not been quantitatively researched. A pretest-posttest study of students taught using these suggestions might be of interest. This study was not designed to investigate conceptual change, but its results may be valuable to such a study in which a pretest-posttest strategy might be constructively employed. Nor could this study ultimately categorize the difficulties encountered as 'alternative conceptions' because it could not determine the ultimate source of these difficulties.
REFERENCES


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VITA

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DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: Gary Lester Lyon

Major Field: Curriculum and Instruction

Title of Dissertation: College Students' Understanding of Stereochemistry: Difficulties in Learning and Critical Junctures

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Date of Examination:
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