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STUDENTS' WAYS OF UNDERSTANDING AROMATICITY AND  
ELECTROPHILIC AROMATIC SUBSTITUTION REACTIONS

A dissertation submitted in partial satisfaction of

the requirements for the degree of

Doctor of Philosophy in

Mathematics and Science Education

by

Anne Merete Duffy

Committee in charge:

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Professor Guershon Harel  
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Professor Fred Goldberg  
Professor Joanne Lobato

2006

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Chair

University of California, San Diego

San Diego State University

2006

## DEDICATION

To God. To my husband, Dan Regan. And to my girls, Holly and Jill.

All of whom provided love, support and understanding throughout the entire process of this doctoral program. I could not have done this without them by my side. I love you all very much.

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Duffy, A. & Sawrey, B.A. (2005) *Students' Ways of Understanding of Electrophilic Aromatic Substitution Reactions* Paper presented at the spring National Meeting of American Chemical Society – San Diego, CA

## ABSTRACT FOR THE DISSERTATION

Students' Ways of Understanding Aromaticity and Electrophilic Aromatic  
Substitution Reactions

by

Anne Merete Duffy

Doctor of Philosophy in Mathematics and Science Education

University of California, San Diego, 2006

San Diego State University, 2006

Professor Barbara Sawrey, Chair

Studies in organic chemistry education focus mainly on increasing students' performance. Studies from general chemistry education reveal that students' performance is not a good indicator of conceptual understanding. In support, Bhattacharyya and Bodner (2005) reveal that chemistry graduate students can produce correct answers to reaction mechanisms tasks in organic chemistry without understanding the underlying concepts behind the tasks.

This dissertation uses the constructs of Harel's DNR-based instruction (1998, 2001, in press [a]) to categorize students' ways of understanding aromaticity and electrophilic aromatic substitution reactions. DNR refers to three instructional

principles: *Duality Principle*, *Necessity Principle* and *Repeated Reasoning Principle*.

Primarily, this study applies the following constructs integral to the Duality Principle: *ways of understanding* and *ways of thinking*.

The purpose of this study is three-fold. The first purpose is to identify students' ways of understanding aromaticity and electrophilic aromatic substitution reactions and subsequently the ways of thinking that are inferred by these ways of understanding. The second purpose of this study is to provide quantitative evidence of students' beliefs (one category of ways of thinking) about learning organic chemistry. The third purpose is to show how we can help students develop more desirable ways of understanding aromaticity.

First, several ways of understanding were identified from semi-structured interviews conducted with 12 undergraduate-level students. Three ways of thinking were inferred from these ways of understanding: 1) non-referential symbolic reasoning, 2) non-referential use of terminology, and 3) beliefs about learning organic chemistry.

Second, the results of a 46-Item Likert-scale survey provided empirical evidence to support the claim that the students have a tendency towards memorization when learning organic chemistry.

Third, this study demonstrated the potential for students' developing more scientific ways of understanding aromaticity through teaching interview sessions where problem tasks were designed to perturb students existing ways of understanding.

## **CHAPTER 1: INTRODUCTION**

This dissertation is a report on Harel's DNR-based instruction (1998, 2001, in press [a]) applied to (a) qualitative evaluations of students' ways of understanding two concepts from organic chemistry—aromaticity and electrophilic aromatic substitution reactions—and (b) quantitative evaluations of students' ways of thinking associated with their beliefs in organic chemistry.

I begin with an overview of the background in organic chemistry including a definition of conceptual understanding in chemistry. Next, I delineate the problem statement, and present the research questions. I then outline the theoretical perspective of DNR-based instruction. After addressing the theoretical perspective, I discuss the significance of the study to the field of chemistry education. I conclude the chapter with an overview of the dissertation.

### **Background in Organic Chemistry**

#### **Students' Tendency Toward Memorization**

The focus of this study is student learning in organic chemistry. Typically, organic chemistry is a sophomore level course in most U.S. colleges and universities. Organic chemistry has a reputation among college students as being a difficult course and is seen as one of the major impediments for those students intending to go to professional school in the health sciences. An entire industry has evolved to assist students in obtaining the high grades required for acceptance into these professional schools. Students can purchase flash cards to memorize reactions, molecular modeling kits to view three-dimensional structure, additional problem solving texts,

computer software programs with more problems, in addition to molecular modeling capabilities, and organized study guides to improve test scores. While these products may create some desirable ways of understanding, they are primarily promoted as learning tools to increase student performance on organic chemistry exams.

Increasing student performance is also the emphasis of the majority of articles published in organic chemistry education. Chapter 2 will present a detailed description of the literature in organic chemistry education. For the present, I want to highlight that Bhattacharyya and Bodner (2005) published a study that demonstrates graduate students' lack of conceptual understanding despite performing well in organic synthesis problem solving. This study does not explicate students' understanding of organic chemistry concepts, rather it demonstrates the influence of students' tendency towards memorization on their ability to justify their solutions and propose sensible solutions to variants of traditional organic chemistry reactions.

Further anecdotal evidence on the influence of memorization on students' conceptual understanding can be found in the introduction sections of many organic chemistry textbooks. The authors advise students to avoid memorizing facts and reactions and to favor more "active" methods of learning, such as problem solving.

For example:

Students can truly learn organic chemistry only if they are actively involved in developing a practical understanding of the causes of chemical change, rather than trying to master organic chemistry through memorization...predicting reactivity from structure. Students have told me that they learned an entirely new way of thinking- or analyzing problems, sorting facts, reasoning by analogy, looking for patterns- and that consequently their approach to all of their work has changed. (Ege 1999, p. xxv)

...try to understand why each thing happens. If the reasons behind the behavior are understood, most reactions can be predicted. If you approach the class with the misconception that you must memorize hundreds of unrelated reactions, it could be your downfall....Mastering organic chemistry requires a thorough understanding of fundamentals and the ability to use these fundamentals to analyze, classify and predict. (Bruice 2001, p. xxx)

Too many students find that organic chemistry is an overwhelming parade of facts....The framework that we provide is the accessible notion that an understanding of structure will lead to an understanding of function. (Vollhardt and Schore 1999, p. xxiii)

Thus, memorizing facts will not produce the necessary understanding of the underlying organic chemistry concepts. Another theme observed in these passages is the idea that an understanding of molecular structure is foundational to understanding many other aspects of organic chemistry. Ege (1999) states that reactivity can be predicted from structure; Bruice (2001) includes an understanding of structure among her fundamentals; and Vollhardt and Schore (1999) explicitly state the value of structure for an understanding of function.

Central to these arguments is the promotion of conceptual understanding over the memorization of facts. Bhattaacharyya and Bodner (2005), however, demonstrate that organic chemistry graduate students can produce correct responses to problems via memorization without understanding the chemical concepts behind their solutions. Therefore, it is insufficient to merely *tell* students to avoid memorization. The research in this dissertation addresses the intent to develop students' conceptual understanding over the memorization of facts by applying Harel's DNR-based instruction (1998, 2001, in press [a]). The DNR system is used as a guide in this dissertation to evaluate

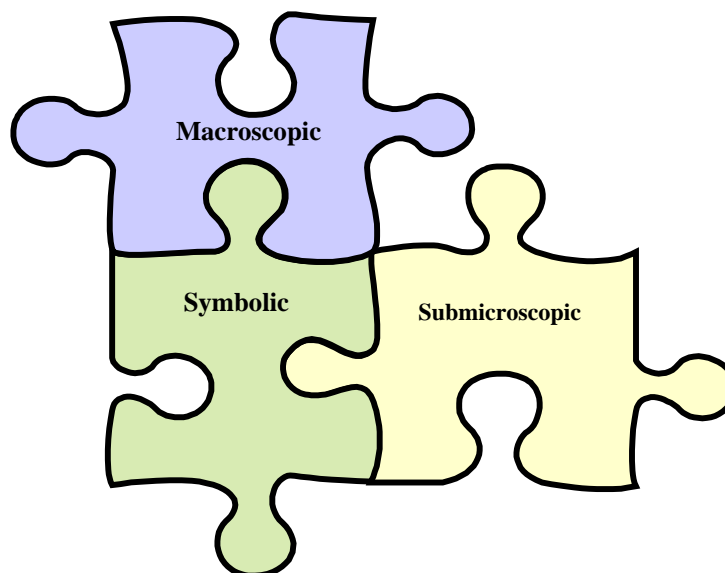
student conceptual understanding and to improve their conceptual understanding through problem solving.

### Conceptual Understanding in Chemistry

Conceptual understanding in chemistry education is multi-dimensional. Johnstone (1991) describes three levels of conceptual understanding in science education: the macroscopic level, the submicroscopic level and the symbolic level. The term “level” represents understanding at a different physical scale. The macroscopic level deals with sensory or visible phenomena, so table salt is observed as a white crystalline solid powder. The submicroscopic level represents the particulate nature of matter in various forms: atomic, ionic, molecular. For table salt at the submicroscopic level, one may understand the solid powder to be a three-dimensional array of sodium ions and chloride ions packed closely in a specific arrangement.

The symbolic level, however, functions as a bridge between the other two levels, and has no clear physical distinction (Hinton and Nakhleh 1999). Thus, table salt can be represented symbolically as NaCl, sodium chloride. The symbols, NaCl, represent both the submicroscopic and macroscopic levels. The symbolic level of understanding incorporates the majority of representations that chemists and educators use to communicate their observations and the rationales behind the observations in the other two representational levels. I have devised the following diagram to help illustrate the multi-dimensional aspect of learning in chemistry. This illustration will

be expanded to organic chemistry in a subsequent section.



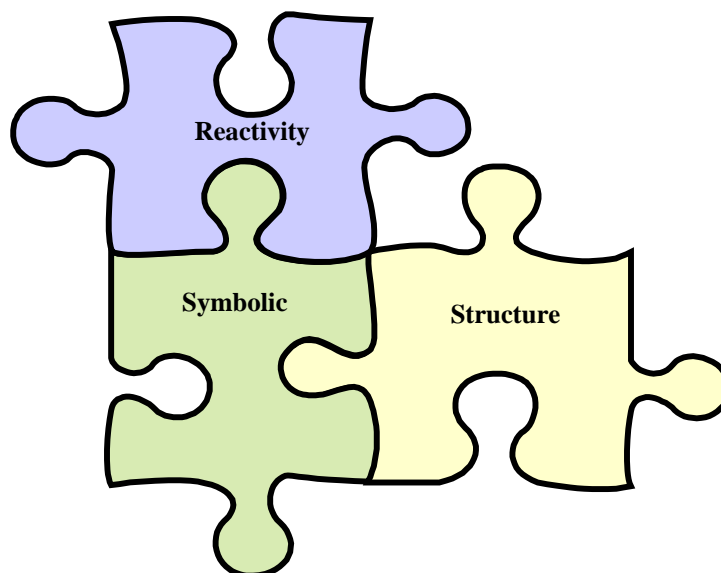
**Figure 1-1: Conceptual Understanding in Chemistry**

Figure 1-1 shows the symbol representational level as a bridge between the submicroscopic and the macroscopic representational levels. The symbolic level provides the basis by which chemists can communicate the link between the other two representational levels. In the table salt example, chemists use NaCl to represent the crystalline substance as well as the image at the particle level that is consistent with experimental observations of the structure of crystalline salt. The macroscopic and submicroscopic are different representations of the same concept represented by the symbolic representation. Thus, all pieces must be in place for a solid understanding of the chemical concept. A chemist moves easily between these three representational levels, while students have been shown to have more difficulty (Bowen and Bunce 1997; Dori and Hameiri 2003; Kozma 2003; Nicoll 2003).

Even though Figure 1-1 applies to conceptual understanding in chemistry overall, the figure can be adapted to use specific terms from organic chemistry to



illustrate the nuances of organic chemistry (See Figure 1-2).



**Figure 1-2: One Example of Conceptual Understanding in Organic Chemistry**

In Figure 1-2, “structure” represents the submicroscopic level when considering the three-dimensional structure of organic molecules. “Reactivity” is analogous to the macroscopic level, describing the actual mechanism and predicting the products of the chemical reactions. In the strictest sense, reactivity does not represent the macroscopic level in exactly the same way as defined earlier (see p. 4). Reactivity describes the interaction of molecules at the submicroscopic level encompassing both the represented entities (nucleophiles, electrophiles, etc.) and chemical processes (substitution, oxidation, etc.) that cannot be visualized. However, these entities and processes (the reactivity), underlie and account for the observable phenomena consistent with the definition of the macroscopic level. For the organic chemist, reactivity belongs in both the submicroscopic and macroscopic representational levels due to the fact that it represents both interactions at the molecular level, and observable phenomena.

Support for the inclusion of reactivity as part of the macroscopic level can be found in Kozma's (2003) review of several studies on the use of multiple representations for science understanding. A large part of the review consists of the use of multiple representations in organic chemistry. Kozma, Chin, et al. (2000) summarize one study of the role of representations for organic chemists in the following description:

The symbolic expressions James used simultaneously represented both the physical materials—the solutions and procedures performed on the lab bench—and the underlying chemical entities and processes—compounds and their reactions....Having made a connection between the representations and the laboratory substances, James used the material affordances of the diagrams (i.e., specific symbolic features) to think about different chemical structures and reactions that had implications for the procedures he performed on the chemical substances on his lab bench (p. 211)

For James, an organic chemist, the symbols represent the molecular structure, the observable chemical substances, and the potential for chemical reaction (the reactivity).

Students, in contrast, do not make reference to the physical materials when discussing features of the symbolic representation (Kozma and Russell 1997). Kozma and Russell conclude that students in a college chemistry laboratory course are “more likely than chemists to base their thinking on surface features than underlying chemical principles.” In other words, they are more concerned with the physical nature of the laboratory (for example, the color of a solution or correctness of the procedure) than what is happening at the molecular level. The lack of connection between the different representational levels, including the physical phenomena, constitutes one of

the main challenges in chemistry education. Thus, one cognitive objective is for students to make connections across the representational levels—to give chemical meaning to physical phenomena as well as physical meaning to symbolic representations.

### **Problem Statement and Research Questions**

One of the major problems with college students in learning organic chemistry is that these students tend to resort to a memorize-oriented approach to learning. One study (Bhattacharyya and Bodner, 2005) found that organic chemistry graduate student participants “had simply reproduced a memorized sequence of events”(p. 1406). More evidence can be found in advice given to students in the forewords of several textbooks (see examples on p.2 and 3) where the authors warn students against learning organic chemistry with an emphasis on memorization. In addition, anecdotal evidence from my own experience teaching organic chemistry reveals that students literally buy into the memorize-oriented approach through the purchase of flashcards and other memory aides associated with organic chemistry.

The data in this dissertation provides further evidence for students’ memorize-oriented approach to learning both qualitatively and quantitatively. The qualitative data demonstrates not only the presence of the memorize-oriented approach to student learning, but also demonstrates the influence that this approach has on conceptual development.

Another problem in organic chemistry education relates to the lack of research in evaluating students’ conceptual understanding. In other words, conceptual

understanding is distinct from student performance; students may do well on typical organic chemistry exams but may not have grasped the underlying concepts. This phenomenon has been well documented in general chemistry settings (Nurrenbern and Pickering 1987; Pickering 1990; Sawrey 1990), but not in organic chemistry. Organic chemistry educators have proposed teaching methods that improve student performance, student attitudes toward organic chemistry, and student retention (see Tien, Roth et al. 2002). Yet, there are very few comprehensive studies in organic chemistry education research that examine students' understanding of organic chemistry concepts. The research in this dissertation focuses on students' conceptual understanding rather than their performance.

A third problem in research studies, documented by Kozma and colleagues (Kozma and Russell 1997; Kozma, Chin et al. 2000; Kozma 2003), is the lack of connections that students make between the various representational levels in chemistry. In other words, the students' conceptual understanding in chemistry is fragmented, as they do not make connections between the symbolic representation and the macroscopic observations, or the submicroscopic interpretation, of the symbols. Clearly, it is not enough to address the students' conceptual understanding, but their way of thinking about organic chemistry must necessarily be addressed as well.

### Research Questions

The three problems listed above—memorize-oriented approach; conceptual understanding; and lack of connections—led to the development of the following research questions<sup>1</sup>:

- 1) What are students' ways of understanding aromaticity and electrophilic aromatic substitution reactions?
- 2) What are students' predominant ways of thinking associated with their beliefs about organic chemistry?
- 3) What ways of understanding aromaticity emerge among students as a result of an instructional intervention?

Thus, the purpose of this study is three-fold. The first purpose is to identify students' ways of understanding aromaticity and electrophilic aromatic substitution reactions and subsequently the ways of thinking that are inferred by these ways of understanding. The second purpose of this study is to provide quantitative evidence of students' beliefs (one category of ways of thinking) about learning organic chemistry. The third purpose is to show how we can help students develop more desirable ways of understanding aromaticity.

### Why Aromaticity and Electrophilic Aromatic Substitution Reactions?

The majority of students who take organic chemistry are expecting to go into the health care fields, and aromaticity is of relative importance for those students. (Scimone and Scimone 1996). Krygowski, Cyranski, et al. (2000) reference the

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<sup>1</sup> The questions, and the study conducted to address them, are oriented in Harel's (1998, 2001, in press [a]) DNR-based instruction theoretical framework.

concept of aromaticity as one of immense practical importance, and report that the terms “aromaticity” and “aromatic” are two of the most frequently used in the fields of chemistry, biochemistry, biology and medicine. Several reports support the claim that aromaticity is an important organic chemistry concept (Krygowski and Cyranski 2001; Balaban, Oniciu et al. 2004; Kovacevic, Baric et al. 2004).

In addition to the importance of the concept of aromaticity, the selection of this concept for study served another purpose. In the review of the literature in organic chemistry education (see chapter 2), spatial visualization is reported as an important skill in organic chemistry. Students with poor spatial visualization skills tend to struggle in organic chemistry. Choosing the concept of aromaticity creates a unique circumstance in the field of organic chemistry in that three-dimensional visualization is not nearly as important. By definition, aromatic compounds are planar, cyclic compounds that are well represented in two-dimensional media.

The concept of aromaticity has not been discussed in the chemistry education literature beyond possible teaching approaches (Glidewell and Lloyd 1986; Box 1994). This is also true for the extension into electrophilic aromatic substitution (EAS) reactions (Zanger, Gennaro et al. 1993; Nelson 2001). Incorporating EAS reactions as a topic of interest provided the bridge to the existing literature in problem solving in organic chemistry synthesis problems. Conceptual understanding of aromaticity provides the basis for the extension into EAS reactions. Therefore, not only will this study tie in ideas from the existing literature in problem solving, but it will also provide evidence of students’ ability to apply their understanding of aromaticity.

The research questions explore students' ways of understanding aromaticity and EAS reactions. In addition, I provide preliminary evidence about students' beliefs about learning in organic chemistry. I use the data from the first two research questions in the design and analysis of three teaching interview sessions whose intent is that students' develop more desirable ways of understanding aromaticity through engaging in DNR-based instruction.

### **DNR-Based Instruction and Its Fundamental Principles**

Harel's DNR-based instruction (1998, 2001, in press [a], in press [b]) is a theoretical framework designed to help students develop conceptual knowledge gradually through problem solving. Careful development, selection, and sequencing of the problems are key to the development of conceptual knowledge. The DNR system originated in mathematics education and was introduced as an instructional method for the development of students' ways of understanding and ways of thinking in mathematics (Harel 2001). Since problem solving plays a key role in the teaching and learning of organic chemistry, the DNR system can provide a new foundation for the development, selection and sequencing of problems in organic chemistry.

Harel's DNR system is composed of premises, foundational concepts, and instructional principles. The premises of DNR are the underlying assumptions about the construction of knowledge. These premises will not be individually defined in this dissertation; however, it is important to clarify that Harel's DNR system finds its underlying assumptions about learning rooted in Piaget's constructivist learning

theory. Thus, learning occurs in a series of equilibrium-disequilibrium cycles initiated by some internal perturbation.

The foundational concepts and instructional principles of Harel's DNR are defined in detail in the following sections, with examples in the context of chemistry and organic chemistry, in particular.

### The Triad of Determinants

Three foundational concepts of the DNR system, also called the triad of determinants, (Harel, in press [a]) refer to *Mental Acts*, *Ways of Understanding* and *Ways of Thinking*.

#### Mental Act

In Harel's DNR-based instruction, mental act is a term representing the actions that we carry out in our minds (Harel 2004). This is in contrast to the *physical acts* that we may carry out with our bodies. Examples of mental acts are interpreting, problem solving, explaining, generalizing, searching, proving, relating, classifying, etc. These mental acts are meant to be distinguished from analogous *physical acts*. For example, searching, as a *mental act* would refer to a mental search for something intangible (perhaps trying to remember a phone number). In contrast, searching, as a *physical act*, would refer to a search for something more tangible (perhaps looking for the car keys).

*Mental acts* are not limited to the domains of mathematics and science but are present in all facets of human reasoning. It is important to note that mental acts are not independent of each other. Any mental act may be used in conjunction with any other,



simultaneously or in sequence. Thus, one mental act may trigger the use of another. For example, in organic chemistry we often interpret some symbolic structural representation and relate it to the particular context before us. In using a specific mental act to make claims about ways of understanding and ways of thinking, we must realize that there is a subjective component associated with which mental act we attend to as researchers. In other words, attending to the *mental act* of *interpreting* in this dissertation is the lens through which the data is analyzed. Attending to another mental act may result in a different interpretation of the data.

When viewing the skeletal structure of benzene, one student may interpret the representation to be an assembly of lines with alternating double lines connected together in a ring. An interpretation of the same structure by another student may result in that student interpreting the symbolic representation as that of the three-dimensional molecular structure with the delocalized *pi* electrons above and below the ring of sigma-bonded carbon atoms. Both of these students have employed the *mental act* of interpreting the symbolic representation of benzene with different results. These different results are known as the *product of the mental act* or the *way of understanding*.

#### Ways of Understanding and Ways of Thinking

Ways of understanding, as formulated by Harel (in press [b]), refers to the products of a person's mental acts. For example, the meaning one gives to a term, or the solution provided for a problem. In the example given above, each of the students' interpretations of the symbolic representation of benzene are *products* of the *mental*

*act* of *interpreting* the skeletal structure. These products are directly identifiable in a person's statements and actions within a given context. In the context of the above example, the following situation occurred (during one of the student interviews conducted for this dissertation):

**Interviewer:** I would like you to draw the skeletal structure of bromobenzene.

**Student 6C:** [*Draws skeletal structure with alternating double bonds*]

**Interviewer:** Can you draw it another way?

**Student 6C:** Yeah. [*Draws the Lewis Structure of Bromobenzene*]

Through observations such as this, it was determined that this student held a way of understanding the symbolic representation of benzene as an assembly of ordered lines.

Ways of thinking, as formulated by Harel (in press [b]), refers to the *character* of a *mental act*. This characterization of a mental act is not directly observable, as with ways of understanding, but is inferred based on the observations of several ways of understanding in a given context. From the patterns one identifies from several ways of understanding, one may infer one or more ways of thinking. All of this is done in the context of a specific mental act.

It is also important to note that Harel classifies ways of thinking into three main categories: problem solving approaches, proof schemes, and beliefs about mathematics (Harel, in press [b]). Harel specifies that these classifications are based on the field of mathematics, even though problem solving is integral to scientists in any field of study. Yet, the nature of the problem solving act is likely to be different for different fields of science, and even a different subsection of each field. As a

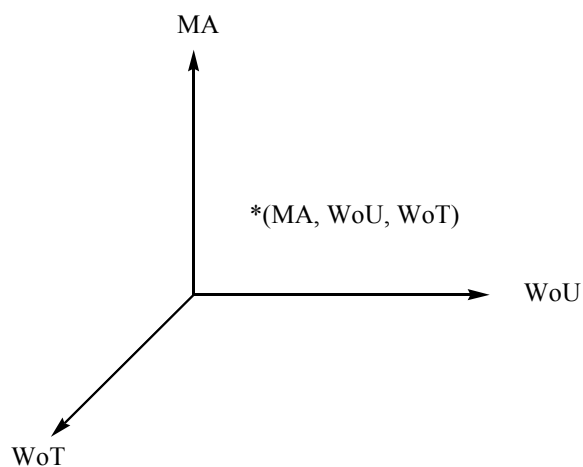
result, the problem solving approach category of ways of thinking for the mathematical-based DNR system cannot be directly applied to another field of study without further study. Thus, the application of these categories to organic chemistry education results in some modification of these categories that is beyond the scope of this dissertation.

The research in this dissertation does identify some students' ways of thinking as a result of an analysis of students' ways of understanding, but makes no attempt to formulate a classification of a specific category of *way of thinking*. The integration of the beliefs category does find a more direct analogy to science education in reference to students' beliefs about science and organic chemistry, in particular, and is discussed further in chapter 2.

Although each way of understanding and way of thinking is the product and character, respectively, of one mental act, by definition, they may be a result of the interaction of more than one mental act. For example, in the context of determining the molecular geometry of methane ( $\text{CH}_4$ ), one may suspect that the mental act of *relating* is involved, since the conceptual understanding of chemists relates the symbolic representation to the submicroscopic and macroscopic representational levels. If a student, when solving the task, had made counting actions and stated "four bonds mean tetrahedral," we may suspect that the student was not relating the symbolic representation with any other representational level but, instead, relating the determination of molecular geometry with an act of counting. But the statement "four bonds mean tetrahedral" implies the enactment of another mental act, that of

*interpreting*. The student's interpretation that "four bonds mean tetrahedral" is a way of understanding molecular geometry. Both of these ways of understanding would result in the inference of a non-referential symbolic (NRS) reasoning<sup>2</sup>.

Harel's triad of determinants can be represented as  $(MA, WoU, WoT)$ <sup>3</sup> designating a point in a theoretical three-dimensional coordinate system as seen below in Figure 1-3:



**Figure 1-3: Triad Coordinate System**

As a result, the triad of determinants for the mental act *relating* could be represented as  $(relating, counting\ bonds, NRS)$ . Likewise, for the *interpreting* mental act, the triad would consist of  $(interpreting, "four\ means\ tetrahedral", NRS)$ . It is crucial to maintain the triad in the application of Harel's DNR-based instruction.

<sup>2</sup> Non-referential symbolic reasoning [Harel, in press [b], p. 155] is defined in Chapter 5 as one of the inferred ways of thinking.

<sup>3</sup> MA is mental act, WoU is ways of understanding, and WoT is ways of thinking

### Three Instructional Principles of the DNR System

As stated above, Harel's DNR system comprises three constructs: 1) premises, 2) concepts and 3) instructional principles. For Harel, an instructional principle is "a conception implying an effect of a teaching action on *student learning*. The teaching action may be conceived as a likelihood condition, necessary condition, or sufficient condition for the effect to take place" (Harel, in press [b]). Harel clarifies what he means by *teaching action* as "a curricular or instructional measure or decision a teacher carries out for the purpose of achieving a cognitive objective, establishing a new didactical contract, or implementing an existing one."

The three instructional principles that are foundational to DNR are the *Duality Principle*, the *Necessity Principle* and the *Repeated Reasoning Principle*. Each of these pedagogical principles is discussed separately below, including a discussion of the notion of Didactical Contract with the Necessity Principle.

#### The Duality Principle

The Duality Principle reflects the intimate association between ways of thinking and ways of understanding. The Duality Principle is formulated as:

Students develop ways of thinking only through construction of ways of understanding, and the ways of understanding they produce are determined by the ways of thinking they possess.  
(Harel, in press [a])

And the relationship between one's ways of understanding and ways of thinking is referred to as a "developmental interdependency between what the students produce and the character of their mental acts" (Harel, in press [b]). Even though the Duality Principle relates the interdependency of ways of understanding and ways of thinking,

they are not mutually dependent. In other words, there is not an exclusive one-to-one correlation between one way of understanding and one way of thinking. For example, one group of ways of understanding may lead to the identification of a particular way of thinking. Yet, another group, with some members being part of the original group and some new members, may lead to the identification of a different way of thinking. As a result, identification of several ways of understanding may lead to just a few ways of thinking, each dependent on a different set of ways of understanding.

For example, in the coordinate system representation of the triad of determinants (see Figure 1-3), one triad consists of (*interpreting*, “*four means tetrahedral*,” and *NRS*). The way of understanding “*four means tetrahedral*” can also lead to another way of thinking, defined in chapter 4, as “non-referential use of terminology (*NRT*)”. As a result, a new triad can be described with (*interpreting*, “*four means tetrahedral*”, and *NRT*).

The Duality Principle posits that ways of thinking can only change by concurrent changes in one’s ways of understanding. Harel states, “An immediate implication of the Duality Principle is that it is essential that teachers form instructional goals in terms of ways of thinking and devise and use appropriate instructional activities through which students can build ways of understanding that can potentially help them construct desirable ways of thinking” (in press [a]). The remaining two instructional principles of the DNR system, the Necessity Principle and the Repeated Reasoning Principle, attend to the nature and the composition of instructional activities.

### The Necessity Principle

The Necessity Principle is formulated in the following manner:

For students to learn what we intend to teach them, they must have a need for it, where ‘need’ refers to intellectual need not social or economic need. (Harel, in press [a])

*Intellectual need* is distinguished from *social need* (desire to please parents, teacher, etc.) or *economic need* (need to get a good grade to continue to be eligible for scholarship). *Intellectual need* refers to the internal desire to solve a problem because of the cognitive puzzlement it creates. Thus, the learner is intrinsically motivated by the problem itself. Harel (1998) distinguishes among three types of intellectual need: the *need for computation*, the *need for formulation*, and the *need for elegance*.

The *need for computation* includes the desire to obtain an unknown numeric value or “determining conditions for existence and uniqueness of solutions to linear systems” (p. 503). Organic chemistry does not involve the computation of numerical solutions. Instead, organic chemistry problems inquire about the outcome of a chemical reaction or the design of a synthetic pathway. Therefore, the *need for computation* in organic chemistry may involve a need for resolution for the problem presented.

The *need for formulation* refers to the need to communicate ideas, including the validity of a solution. In organic chemistry, part of the *need for formulation* embodies the need for students to learn the methods in representing molecular structures symbolically in order to communicate their ideas. Another part involves the need for students to justify their responses. For example, how does the student know

that he or she will obtain a certain product in a given reaction? In the *need for formulation*, the student must be able to communicate not only the solution to others, but also the reason behind the solution.

The *need for elegance* is perhaps a more advanced form of intellectual need, when the *needs for computation and formulation* are not enough to result in a satisfactory outcome of a problem. This holds true in more advanced organic syntheses where several routes may lead to the same product. The *need for elegance* results in a satisfaction with the problem solving result that goes beyond mere computation and formulation. “Classics in Total Synthesis” (Nicolaou 1996), illustrates the *need for elegance* in the total synthesis of organic molecules. Several of the natural product molecules are presented with two different synthetic pathways because the science of organic synthesis is constantly enriched through advances in technology and new developments in organic chemistry. Nicolaou and Sorensen (1996) present the first total synthesis of strychnine from Woodward and colleagues in 1954. A later chapter outlines a new synthetic route to strychnine via a tandem cyclization strategy from Overman and colleagues in 1993. Both of these synthetic pathways result in the synthesis of strychnine. However, the inclusion of the latter synthetic route is presented as an example of “a beautiful application of a tandem...cyclization strategy in the synthesis of ...strychnine (pg. 641).”

The Necessity Principle has, in theory, been a part of the organic chemistry education community as some educators have designed courses that integrate students’ interests with the desire to increase the intrinsic motivational factor in student learning



(Kelley 2001; Levy 1995; Yong 1994). However, the design of instructional activities is not sufficient to improve student learning. The environment in which these instructional activities occur has an equal if not greater influence on what the students learn. An important part of the environment is the Didactical Contract.

### The Didactical Contract

In order to create an environment in which the student not only feels compelled to solve problems but also is free to make mistakes both publicly and privately during the problem solving process, the notion of Didactical Contract comes into play.

The construct of Didactical Contract (Brousseau, 1997) is an essential element in the implementation of DNR-based instruction. This contract between the teacher and the student, as described by Brousseau (1997), is an often implicit, but sometimes explicit, agreement as to what each partner, teacher and student, will be responsible for managing. This includes the agreement of what responsibility each of them has towards the other. The Didactical Contract deals with the part of the teacher-student contract that is directly related to the content that is to be learned.

To have an effective implementation of DNR, the students must have the opportunity to explore and make mistakes when solving problems. One reason that the Didactical Contract is so important is the fact that, in a DNR-based instructional environment, students are often given problems that they have no algorithm to follow. They need to be able to explore the problems without the typical pressures of performance. The Didactical Contract has a direct influence on the implementation of the Necessity Principle. In order for the student to develop the *need for resolution*, the

*need for formulation*, and possibly the *need for elegance*, the Didactical Contract must allow for such an environment to exist.

The *need for resolution* is not unfamiliar in a typical Didactical Contract in organic chemistry. Instructors, whether they assign homework or not, preach the necessity of problem solving in order to succeed in organic chemistry. This *need for resolution*, however, is rarely an intellectual need on the part of the student. As noted at the beginning of this chapter, students tend to enter a memorize-oriented *way of thinking* resulting in their lack of real puzzlement over the problems being solved.

#### The Repeated Reasoning Principle

Designing instruction based on the Necessity Principle means that problems are designed that create in students an intellectual need for a particular way of understanding. However, it is the repeated reasoning that occurs through multiple problem solving opportunities that concludes the discussion of the three instructional principles of DNR.

Harel formulates the Repeated Reasoning Principle of the DNR-based instructional system as:

Students must practice reasoning in order to internalize, organize and retain ways of understanding and ways of thinking. (Harel, in press [a])

The use of the word “practice” refers to the need for repeated situations of reasoning in problem solving. It is repeated reasoning and not the practice of routine problems that is the important factor in solidifying conceptual knowledge. In other words, the result of one problem would not lead to a standard method for solving other problems.

By giving students several problems to reason through repeatedly they have the potential for internalizing specific ways of understanding.

*Internalization*, used in this context, refers to the idea that a specific approach for solving a problem has been attained by the student, and they are able to use this approach spontaneously in the context of the problem. For example, in organic chemistry, a student may spontaneously use the mechanism (including drawing all of the resonance structures) for electrophilic aromatic substitution (EAS) of an already substituted benzene ring to determine the product (in other words, whether the new substituent will be ortho, para or meta to the already existing substituent). The student has then internalized the process of solving subsequent EAS reactions through writing the reaction mechanism.

Educators in chemistry have also deemed that reasoning in problem solving has value for student learning. This can be seen in the development of what these educators refer to as “Problems not Exercises” (Bodner 1987; Frank, Baker et al. 1987; Browne 1999; Wilson 1986; Wilson 1987). However, the principles of DNR not only require *repeated* opportunities for reasoning to change students’ ways of thinking and ways of understanding, but the student must also be engaged in the act of problem solving.

### **Significance for the Field of Chemistry Education**

The application of Harel’s DNR-based instruction offers a significant contribution to the field of chemistry education because it provides a conceptual framework for curriculum development and instruction. In addition, the DNR system

provides a theoretical perspective with which to evaluate and categorize students' ways of understanding and ways of thinking. Ways of understanding, in the DNR system, is a neutral term, whereas the term "conceptual understanding" in chemistry carries a positive connotation. As a result, explicating the students' ways of understanding can reveal the state of students' ways of understanding, and the corresponding ways of thinking. The ultimate cognitive objective lies in development of desirable ways of thinking through changes in students' ways of understanding.

Another contribution implied in the use of the DNR system is that the focus of this study is not on student performance, but in the assessment and development of the students' ways of understanding. Students in a traditional organic chemistry lecture course<sup>4</sup> develop undesirable ways of understanding as a result of their memorize-oriented ways of thinking (see chapter 4). Students can respond correctly to organic chemistry problems while holding undesirable ways of understanding. In this dissertation, I propose that curriculum assessment should focus on students' ways of understanding rather than students' performance on exams.

Finally, the research in this dissertation prompts questions about problems posed in textbooks and on assessments. If students can respond correctly to exam questions, but have undesirable ways of understanding, then organic chemistry educators might benefit from a reevaluation of the problem tasks that students solve in the learning process.

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<sup>4</sup> The traditional organic chemistry lecture course consists of an instructor presenting relevant course material to students who follow along by taking notes, asking mainly clarification questions.

## Overview of the Dissertation

The research reported in this dissertation arose from a desire to evaluate and improve university students' conceptual understanding in organic chemistry. The absence of research in the field of organic chemistry education regarding conceptual understanding resulted in a review of literature that finds its basis in physics education research and extends into general chemistry education research.

Chapter 2 provides an overview of the literature on conceptual understanding in these fields, leading to the current state of research in organic chemistry education research. Chapter 2 also includes a discussion on the applicability of DNR-based instruction in organic chemistry. The DNR system and its relation to studies in science education, with regard to the beliefs category of ways of thinking are also discussed.

Chapter 3 outlines the methodology employed for the three phases of research. The research for this dissertation uses both qualitative and quantitative methods to answer the three research questions. Questions one and three use qualitative methods in the semi-structured problem-solving interview and teaching interviews respectively. Question two uses quantitative methods in the administration of a 46-item Likert-scale survey evaluating students' beliefs in organic chemistry.

Chapter 4 describes the results of the first research question evaluating students' ways of understanding aromaticity and electrophilic aromatic substitution reactions. Several categories of students' ways of understanding are developed and subsequently employed to identify two specific ways of thinking.

Chapter 5 presents the results of the survey data that identified quantitatively memorize-oriented learners in the seven principal components. In addition, chapter 5 includes a discussion of the results, including the limitations of the survey results, as well as suggestions for further research associated with the survey.

Chapter 6 portrays, in detail, the emerging ways of understanding the concept of aromaticity for two of the five student participants in the constructivism-based teaching interviews. The chapter concludes with a summary of the results for each of the remaining three students' teaching interviews focusing on the influence their ways of thinking in organic chemistry had on the development of their ways of understanding aromaticity.

The final chapter offers a summary of the major findings, and discusses the significance of those findings relative to the field of chemistry education. A reconceived framework for conceptual understanding in chemistry education is suggested based on the findings of this research. The instructional implications relevant to educators in organic chemistry are discussed. The chapter concludes with suggestions for further research based on the results of this study.

## **CHAPTER 2: REVIEW OF LITERATURE**

### **Introduction**

The goal of this literature review is to set the present study in the context of the current research literature. One context of this study is in the field of organic chemistry education. Because this field of research is in its early stages, the review of literature will also encompass relevant literature from general chemistry education and physics education research. Therefore, the review of literature will start by introducing the impetus from physics education that led to a change in thinking in the field of general chemistry education regarding students' conceptual understanding.

In order to place this research in the context of research already conducted in the field of organic chemistry education, an overview of the three main themes within the field of organic chemistry education research—spatial visualization and molecular geometry, problem-solving in organic synthesis and teaching effects on performance—are included. Following the general overview of research in organic chemistry education, a detailed discussion of conceptual understanding research in organic chemistry education is also incorporated.

Upon discussing the current state of the literature in conceptual understanding in chemistry education, Harel's DNR-based instruction, as the theoretical framework of this study, is discussed in terms of its applicability to chemistry education and specifically its relationship to organic chemistry. This chapter concludes with a discussion of the literature on ways of thinking associated with beliefs about learning

in physics education, with further justification for the use of DNR-based instruction in this study.

### **Conceptual Understanding in Physics Education**

The research in physics education has produced a large number of papers looking at students' conceptual understanding. Rather than present a comprehensive review of the literature on conceptual understanding in physics education, this section instead highlights the overall field, based on recent review article from physics education, presents a description of an exemplar study in physics education, and discusses how research in conceptual understanding in physics education influenced the chemistry education research community.

In the empirical studies portion of their overview of physics education research, McDermott and Redish (1999) chose to highlight research in which the investigations focused on the student as the learner, presented a clear theoretical perspective with explicitly stated goals, and provided evidence that the data was collected carefully and systematically. Despite these strict standards for inclusion, McDermott and Redish still listed 114 studies that were conducted evaluating students' conceptual understanding in a variety of content areas of physics education research. The majority of the studies were in the area of mechanics, where work in physics education research on student conceptual understanding began to be published in and around 1980 (Trowbridge and McDermott 1980; Trowbridge and McDermott 1981). McDermott (2001) acknowledged that the research, the first of its kind published in the *American Journal of Physics*, began in 1973. In the mid-1980s, that



work was followed by publications on new instructional strategies addressing the issues from the previous research on conceptual understanding.

After beginning the research on conceptual understanding in the area of mechanics, other areas of physics education followed, including electricity. McDermott and Shaffer (1992) reported the findings from a long-term investigation on students' understanding of DC circuits. This research found precedence in the researchers' concern that students' success on quantitative problems was an unreliable measure of their conceptual understanding. They began their investigation with individual student interviews, classroom observations and analysis of student work on homework and exams. Later, they extended their investigation by examining student progress over time and, ultimately, through questions on tests administered to a large body of students to estimate persistence in the former case and prevalence in the latter. McDermott and Shaffer identified a number of student difficulties which they grouped into three main categories: "an inability to apply formal concepts to an electric circuit, an inability to use and interpret formal representations of electric circuits, and an inability to reason qualitatively about the behavior of the an electric circuit" (p. 995).

Using the specific difficulties identified under each category, they later developed two types of curriculum (Shaffer and McDermott 1992). One of the curricula consisted of tutorial materials for instructors to use with any standard introductory physics textbook (McDermott, Shaffer et al. 1998). The tutorials were designed for use in small groups of three or four students working collaboratively on worksheets guiding them through the reasoning required to develop and apply

important physics concepts. The other type of curriculum, a set of laboratory-based instructional modules called *Physic by Inquiry*, focused on the development of material towards preparing prospective and practicing physics teacher to teach physics at the pre-college level (McDermott 1996; McDermott 1998).

As noted in the example above, qualitative research presented the problem of specific student difficulties in their conceptual understanding, despite success on quantitative problems. In 1985, Halloun and Hestenes published a paper in physics education that became one of the driving forces for an assessment of the state of conceptual understanding in chemistry education. Halloun and Hestenes (1985) report the results of a multiple choice instrument, the Mechanics Diagnostic Test, that later evolved to the Force Concept Inventory (FCI) (Hestenes, Wells et al. 1992) This paper provided compelling evidence that many students could perform well on quantitative exam questions but had serious conceptual understanding difficulties.

### **Conceptual Understanding in General Chemistry Education**

Although the research in this dissertation focuses on students in organic chemistry, the papers published in general chemistry education research far exceed those in organic chemistry education research. As a result, the field of conceptual understanding in general chemistry education research provided a basis for the research in organic chemistry learning. The purpose of this section is to situate the field of chemistry education research in between the content-based studies of physics education research and those beginning to emerge from organic chemistry education. This issue of conceptual understanding versus students' performance in general

chemistry provided the link between chemistry and physics education research. The research in conceptual understanding of two general chemistry concepts, covalent bonding and molecular structure, provided the background from general chemistry that was most relevant to the studies in organic chemistry education.

#### Conceptual Understanding and Student Performance on Exams

Physics education researchers provided a quantitative tool to identify a widespread problem of students' lack of conceptual understanding despite their ability to perform well on quantitative examination questions. Before the development of a similar quantitative chemistry-based probe on student understanding, a key study presented supporting information that chemistry educators faced a similar issue. Yaroch (1985) found that nine of fourteen high-achieving students interviewed could correctly balance chemical equations but could not explain the physical meaning behind the equations.

Although the above-mentioned and earlier studies had provided observations from chemistry educators regarding the lack of student understanding in a variety of topics in chemistry, the extent of the problem did not begin to be apparent to the field of chemistry education until Nurrenbern and Pickering (1987) published an article on research questioning whether students' ability to solve chemistry problems correctly portrayed students' understanding of molecular concepts. They developed and administered a multiple choice test and found that students were able to solve quantitative problems correctly, without demonstrating an equivalent understanding of the conceptual basis behind the problem. This study has been repeated and expanded

in the years following (Pickering 1990; Sawrey 1990; Nakhleh 1993; Nakhleh and Mitchell 1993; Zoller, Lubezky et al. 1995; Nakhleh, Lowery et al. 1996). Along with a similar study published around the same time on students' understanding of the particulate nature of matter (Gabel, Samuel et al. 1987), this indicated that many students succeeded in solving problems by executing algorithms without exhibiting comparable understanding of the chemical concepts underlying the problem. These studies provided a basis for many researchers investigating students' conceptual understanding qualitatively for a variety of chemical concepts (Smith and Metz 1996; Pinarbasi and Canpolat 2003; Sanger 2005) and quantitatively in a variety of academic venues (Lin, Kirsch et al. 1996 ; Stamovlasis, Tsaparlis et al. 2004; Stamovlasis, Tsaparlis et al. 2005).

During the same time period and immediately following the study by Nurrenbern and Pickering, there was an effort in chemistry education research to identify students' misconceptions<sup>5</sup>. Conceptual understanding in chemistry education referred to the desired and accepted chemistry concepts from the community of chemists. Any deviation from the desired conceptual understanding was referred to as misconceptions, preconceptions, alternative conceptions or alternative frameworks (Nakhleh 1992; Taber 2001). While most of the research identifying misconceptions in general chemistry occurred in the 1980's and early 1990's (see Nakhleh, 1992 and Mulford, 2002), chemistry educators continued to report findings of misconceptions even in recent literature (Nicoll 2001).

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<sup>5</sup> The term "misconceptions" will refer to all variations relating to the identification of student conceptions that are not consistent with the conceptual consensus of the scientific community.

As the field of chemistry education developed, many researchers avoided merely conducting deficit studies to identify student misconceptions but instead used existing research and their own findings with the purpose of improving student understanding in chemistry.

### Conceptual Understanding of Covalent Bonding

The concept of chemical bonding, and more specifically covalent bonding, is one of the fundamental concepts from general chemistry that plays a key role in organic chemistry (Spencer 1992). This section will present the research that has been conducted in chemistry education focusing on conceptual understanding of covalent bonding.

Peterson and Treagust (1989) published a study that identified several misconceptions in covalent bonding and molecular structure. Nearly 25% of Grade 12 General Chemistry students in Australia believed that there existed equal sharing of the electron pair in all covalent bonds, regardless of differences of electronegativity. Additionally, these students identified the location of the electron pair in a covalent bond to be exactly halfway between two atoms, disregarding the physical characteristics of the atoms in question<sup>6</sup>.

Taagepera, Arasasingham et al. (2002) used the instrument developed by Peterson and Treagust (1989) with organic chemistry students in the United States. The study with the U.S. organic chemistry students showed similar results as with the Australian students: 30% of the students in the U.S. held the same beliefs of equal

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<sup>6</sup> A more scientific understanding of the location of the electron pair in a covalent bond considers the influence of each atom's electronegativity resulting in the probability of the electron pair being located closer to the more electronegative atom.

sharing with an exact location of the electron pair between the two atoms regardless of electronegativity. These same findings were also observed recently in the U. S. with general chemistry college students (Nicol 2001) in a qualitative study investigating students' conceptions of bonding. Given that the concept of covalent bonding is one of the foundational concepts of organic chemistry, one may suspect that the unscientific understanding of the covalent bond has an effect on students' development of knowledge in organic chemistry.

Coll and Taylor (2002) interviewed 30 students in Australia and New Zealand regarding their understanding of chemical bonding. The students ranged in their academic levels from seniors in secondary school, to undergraduates, to beginning graduate students. For covalent bonding, the researchers focused their investigation of students' understanding of iodine,  $I_2$ , and chloroform,  $CH_3Cl$ . Both senior secondary students and undergraduates demonstrated the same incorrect beliefs that the electron pair in a covalent bond is shared equally, and located directly between two atoms. The graduate students also demonstrated inconsistencies in their understanding of covalent bonding. While recognizing the difference in electronegativities, the graduate students still claimed that the four bonds in chloroform were equal. While the graduate students and undergraduates focused on fulfilling the *Octet Rule*—emphasizing that each atom had a full set of eight electrons—as the primary justification for covalent bonding, the secondary school seniors demonstrated a greater variety of responses on what was being shared in a covalent bond. In addition, the secondary school students

were not consistent with their use of terminology and their construction of symbolic representations:

Most of the students said that the bonding in  $I_2$  was covalent, but were not then able to say what the term actually meant. For example, Anne said that the bonding in molecular iodine is 'pure covalent' and her drawing of the bonding of  $I_2$  simply consisted of two 'I' symbols with no links between the symbols. (p. 180)

The overall finding of the study by Coll and Taylor (2002) was that students developed a robust understanding of covalent bonding as equally shared electrons based on fulfilling the Octet Rule as a justification of the sharing of electrons. Emphasis on the Octet Rule resulted in students' ignoring the physical meaning of the covalent bond, while employing the Octet Rule as a problem solving heuristic, in order to draw correct Lewis Dot structures. Here is a clear example of students' ability to respond correctly in drawing the Lewis Dot structure with unscientific understanding of the foundational concept of covalent bonding. Thus, students' performance is not an adequate indication of their conceptual understanding.

Harrison and Treagust (2000) examined the conceptual development of covalent bonding using a variety of different analogical models in chemistry teaching.

For Harrison and Treagust an analogical model:

...refers to concrete, abstract and mixed concrete-abstract representations of scientific objects and theories that are used by textbooks, teachers and students. In this study, "analogical model" is preferred to "model" because a model can be a *way* to do something as well as being a *representation* of a familiar or nonobservable entity. (p. 355)

In other words, an analogical model referred to the representation of a non-observable entity, and not a method for solution. In their study, Harrison and Treagust used a variety of analogical models with secondary students including symbolic representations of electron density distributions, Lewis Dot Structures, space-filling models sets, Ball-and-Stick models sets, balloons, Spring-and-Ball representations, and skeletal structure models of organic compounds. Using these analogical models in a small class environment in Australia, they reported the development of deep conceptual understanding consistent with the chemistry community of the Grade 11 students. Among their conclusions, they recommended introducing multiple analogical models in the early stages of chemistry learning and providing students with time for practice and discussion about the models.

The above studies provided evidence on students' conceptual understanding of covalent bonding when the students emphasized problem solving heuristics in the Octet Rule and analogical models. Even though these studies focused on the concept of covalent bonding, the relevance for organic chemistry education was in the influence that the available representations had on students' development of concepts. By extension, the limitations of the various representations were also observed in the development of students' understanding of molecular geometry.

#### Conceptual Understanding of Molecular Geometry

The concept of molecular geometry provides the necessary foundation for organic chemistry students in their understanding of molecular structure. High school and college students are introduced to the concept of molecular geometry in general



chemistry based on three general models. The first and most prevalent model is Valence Shell Electron Pair Repulsion (VSEPR) developed in the early 1960s with slight modifications in recent years (Gillespie 1963; Gillespie, Spencer et al. 1996; Gillespie 2000). The main posit of VSEPR is based on a localized electron pair approach where repulsive interactions between electron pairs in the valence shell of the central atom determine the geometry of the molecule about the central atom and its three-dimensional structure.

The second model students are introduced to is the Valence Bond model in conjunction with hybridization, where the arrangement of hybrid atomic orbitals explains the overlap of shared electrons in conjunction with the molecular geometry (Pauling 1960). Although hybridization theory aids in explaining the molecular geometry and the equivalence of bonds, it is not based on physical phenomena but on mathematical derivations of quantum mechanical wave equations. As a result, chemistry educators have raised some debate about its use in teaching molecular geometry to general chemistry students (Gillespie 2004).

The third model to explain molecular geometry is Molecular Orbital (MO) theory. This model is also based on mathematical calculations of quantum mechanical wave equations. One difference between hybridization theory and MO theory is that the existence of molecular orbitals has been demonstrated using photoelectron spectroscopy (McQuarrie 1983). MO theory is a powerful concept that is mainly used in general chemistry to explain the paramagnetism of oxygen gas. It is relatively

complex and, therefore, the model least favored by chemistry educators in explaining and predicting molecular geometry.

Based on evidence from the chemical bonding domain by Harrison and Treagust (2000), one would expect introducing general chemistry students to multiple models for molecular geometry could strengthen their conceptual development. Because two of the models are based on complex mathematical operations, chemistry educators often emphasize VSEPR theory over the other two models. This has been supported by recommendations in the general chemistry education literature (Desseyn 1985; Gillespie, Spencer et al. 1996; Gillespie 2004). Simplifying the concept for students would appear to chemistry educators as beneficial. However, it may not create a strong conceptual basis for chemistry students, based on the results presented by Harrison and Treagust who found that presenting students with multiple models resulting in deep conceptual understanding of covalent bonding in Grade 11 Australian students

Sawrey and Duffy (2000) supported this claim in an unpublished study where they conducted problem solving interviews with 12 university general chemistry students in order to explore the students' understanding of molecular geometry using VSEPR theory. All of the students interviewed relied on the algorithmic nature of VSEPR theory and often did not extend their understanding to the actual three-dimensional shape or the relative effects of differential electronegativities. Their neglect of the three-dimensional shape was even more apparent based on their interpretations of two-dimensional representations. When dichloromethane was

represented in two different orientations on paper, most of the students claimed that the molecule did have a dipole moment in one representation (where both chlorine atoms appeared on one side of the molecule) and did not have a dipole moment for a second representation (where each chlorine appeared to be above or below the central carbon atom)<sup>7</sup>. Although organic chemists rely more heavily on hybridization and MO theory than on VSEPR theory, incorporating these elements did not change the responses that organic chemistry students gave to the same probes given to the general chemistry students mentioned above.

### **Overview of Research in Organic Chemistry Education**

The methods of predicting and explaining molecular geometry about a central atom introduced in general chemistry are extended to more complex molecules in organic chemistry. Thus students are no longer asked to determine the simple geometry about one central atom, but to manufacture a global outlook of electron distributions throughout an entire molecule, where the geometry about multiple atoms must be accounted for. This broader focus of electron distribution in a larger molecule is the focus of the development of students' ideas of molecular structure.

#### Spatial Visualization and Molecular Structure

In organic chemistry, students are often asked for the first time in a chemistry context to visualize the molecular structure in three dimensions. In addition, students are also required at times to manipulate molecular structures mentally in order to predict the correct conformation of the product molecule. The following studies look

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<sup>7</sup> Dichloromethane does have a dipole moment given the tetrahedral nature of the geometry about the central carbon atom.

at the concepts of stereochemistry<sup>8</sup> with regard to students' spatial ability and students' understanding of molecular structure.

Stereochemistry is a difficult topic for many organic chemistry students. Not only are students introduced to the concepts associated with stereochemistry (for example, chirality) but they are also required to manipulate a two-dimensional representation of a three-dimensional structure mentally, in order to name structures, solve problems using three dimensional structures, and show the three-dimensional products of reactions between structures. Early research in spatial ability, and its role in organic chemistry performance, showed a positive correlation between spatial ability and performance in organic chemistry (Small and Morton 1983; Pribyl and Bodner 1987). Many articles on the topic of stereochemistry focus on improving teaching of stereochemical concepts (Weininger 1984; Rozzelle and Rosenfeld 1985; Woolley 1985; Brand and Fisher 1987; Barta and Stille 1994; Mezl 1996; Collins and Easdon 2001; Lujan-Upton 2001). All of these studies focused on improving students' performance on problems associated with stereochemical concepts rather than improving student conceptual understanding.

The nature of the difficulty associated with stereochemical concepts was explored by Ferik et al. (2003), who investigated the achievement of students from 13-25 years of age, using different representations of molecular structure, and differing the requirements for manipulating the structure in three-dimensional space, either by

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<sup>8</sup> Stereochemistry is the study of the three-dimensional structure of molecules. Stereochemical principles are important in both isomerism and the reaction mechanisms. Implicit in all reaction mechanisms, the three-dimensionality is often only highlighted when particular reaction occurs at or generates a stereocenter, a chiral carbon atom.

rotation, reflection or both. They found that a larger portion of the students from all ages could solve the tasks correctly using concrete or pseudo-concrete photographs of molecular models or computer generated molecular models. However, use of more abstract representations (schematic or stereochemical formulas) proved more difficult for all age groups, especially for the primary school children.

Not only did the type of representation affect student performance, but the degree of mental manipulation of the molecular model had an even greater influence on their performance. Students who were capable of solving a problem using a given representation lowered their success rate by at least one half when required to both rotate and reflect the molecule. In general, student performance correlated positively with education level, type of representation, and spatial relations skills. Thus, the representations the student used, and their ability to visualize and manipulate the molecular structure, played a key role in successful performance of problem tasks in stereochemistry.

Understanding of molecular structure also proved to be key in understanding many concepts in organic chemistry. Both Schmidt (1996) and Gonzalez (1998) suggested the use of molecular model kits to help develop and solidify organic chemistry concepts. In fact, molecular model kits had also been suggested as an approach to improve visualization skills (Nelson, Williamson et al. 1996). However, a recent study investigating interpretations that students developed using molecular model kits, suggested that undergraduate general chemistry students developed inaccurate mental images of how atoms were arranged in various molecules as a result

of the use of the molecular modeling kit (Nicoll 2003). Additionally, these students did not pay attention to bonding concepts when building models, due to the fact that most model kits did not allow for flexibility in, for example, number of bonds. Since chemical bonding proved to be another difficult concept for students to master (Peterson and Treagust 1989; Henderleiter, Smart et al. 2001; Coll and Taylor 2002; Taagepera, Arasasingham et al. 2002; Teichert and Stacy 2002), the use of molecular model kits should occur with the knowledge of their limitations, as shown by Nicoll (2001), and time for discussion with students about the limitations of the models, as suggested by Harrison and Treagust (2000).

#### Problem-Solving in Organic Synthesis

Understanding molecular structure is a key component to understanding the chemical reactions that students encounter in an organic chemistry course. How we represent the molecules also plays a key role in organic chemistry students' understanding and their ability to problem solve. Problem solving in organic chemistry takes on increasing difficulty as the year-long undergraduate introductory course in organic chemistry proceeds. The more organic reactions that are introduced to the students, the more tools the students have to solve the organic synthesis problems. Typical organic synthesis problems often ask students to design a synthetic pathway from the starting reagents to final products. Most of the research assesses problem solving on organic synthesis problems with an emphasis on the representations or processes used when problem solving.

Bowen (1990) investigated the representational systems that graduate students employed in order to solve organic synthesis problems. In this study, representational systems were defined as a “collection of structures and processes that allow a problem solver to construct a solution and communicate it to others” (p.351). The overall goal of this study was to identify the representational systems used by the students and their predominance of use. Bowen identified seven representational systems used by the graduate students with the “verbal,” “pictorial,” and “methodological” representational systems being used most frequently. The *verbal* representational system was the means used by the students to communicate their problem-solving processes orally. The *pictorial* representational system, predominant in organic chemistry, communicated molecular structure and synthetic pathways via a well-defined system of structural representations and curved-arrows to show electron flow in organic reaction mechanisms. Students used the verbal and pictorial representations in every organic synthesis problem-solving situation.

The *methodological* representations were the preferred systems used to solve over half of the problem solving situations. These methodological representations were defined as *known methods* inherent in organic synthesis, as well as retrosynthetic analysis. For example, a well-known method of creating six-membered rings with diverse functionality and controlled stereochemistry is the Diels-Alder reaction. Bowen concluded that the graduate students were more likely to use reactions to solve the tasks in a “guess and check” mode, rather than focusing on underlying conceptual principles of organic chemistry.

In only one-third of the problem-solving situations did the students use the “principles-oriented” representational system. This representational system included principles of molecular structure, thermodynamics, kinetics, and acid/base chemistry. The “principles-oriented” representational system was mainly used when students recognized that their “guess and check” method failed to result in the desired product. The study focused on students’ relative correctness in problem solving based on their use of the various representational systems and not their interpretation of the problem or the representational systems themselves.

The interpretation of the structural representational systems while problem solving in organic chemistry was considered in another study (Bowen and Bodner 1991). The interpretations occurred in what Bowen and Bodner referred to as the *preparation phase* of problem solving. However, the interpretation described was limited to the graduate students identifying functional groups on both reactant and product structures, followed by a search for an appropriate set of reactions to obtain the correct conversion from reactant to product. In one task, students were asked to pick one of three molecules to synthesize and explain why it was chosen. The students tended to reject molecules that required consideration of stereochemistry because they were deemed more difficult. The exact nature of the difficulty was not explored in that study.

Bodner and Domin (2000) focused on the limitations that a given representation invoked on undergraduate students’ ability to solve an organic chemistry problem successfully. They argued that the symbolic representations had



two separate meanings for instructors and students. For the instructor, the symbols represented a physical reality. For students, the symbols were merely “letters and numbers and lines”(p. 25) with no physical meaning. As a result, several students did not recognize a pentavalent carbon<sup>9</sup> in one molecular structure as erroneous. Bodner and Domin concluded that students’ understanding of the symbolic representations, as well as their ability to manipulate these representations mentally, affected their success in problem solving.

### Teaching Effects on Performance

Overall, the majority of the literature in organic chemistry education maintains the goal of increasing student performance on organic chemistry exam problems. Performance on exams in organic chemistry may be used as an indicator for successful implementation of some new teaching strategies, but new teaching strategies are often suggested with little or no effective evidence. The studies in organic chemistry education illustrated earlier represent the small fraction of studies focusing on student understanding. Most research studies in organic chemistry education use mainly quantitative data, measuring changes in student performance based on instructional intervention which range from distance-education (Kurtz and Holden 2001), student-directed learning (Katz 1996), promoting active learning (Harvey and Hodges 1999; Zoller 1999), or implementation of cooperative learning situations (Black and Deci 2000; Tien, Roth et al. 2002; Carpenter and McMillan 2003).

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<sup>9</sup>A pentavalent carbon is one with five covalent bonds associated with one carbon atom. This is nonsensical, since carbon is tetravalent.

One instructional approach that has attained some degree of notoriety in organic chemistry education, is the implementation of *Peer-Led Teach Learning* (PLTL) as a supplement to the traditional lecture (Tien, Roth et al. 2002). The PLTL instructional model (Sarquis, Dixon et al. 2001):

...requires active engagement of the students with specifically constructed material and with each other. Undergraduate students who recently completed the course take on the role of peer leader to facilitate group work for a team of six to eight students. The peer leader is not a teacher or an answer giver; the role of the leader is a guide and a mentor.(p. 607)

The student groups worked on problems that were developed by the course instructor with an emphasis on ideas, reasoning, and conceptual understanding, not just obtaining the correct answer. The peer leaders were trained to promote metacognitive strategies. Tien et al. (2002) quantitatively evaluated the influence of PLTL on student performance, retention, and attitudes in a first-semester organic chemistry course over an eight-year time span. These researchers also assessed the role of the leader and the actual activities qualitatively through student and leader surveys, leader interviews, and peer leader reflective journals.

The quantitative study consisted of an experimental and control group comparison of student performance based on a discussion section using the PLTL model (years 1996-1999), and the more typical graduate teaching assistant discussion (years 1992-1994) sections.<sup>10</sup> The results showed that PLTL improved student performance and retention with a positive correlation between PLTL section

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<sup>10</sup> 1995 was the pilot study year in which some discussion sections followed the traditional TA approach while others used the PLTL model. 1995 was omitted due to a possible volunteer effect.

attendance and course grade. Student attitudes, based on a 33-item Likert-scale survey, revealed that students rated the PLTL sessions as the most important aid to their learning.

In the qualitative component to the PLTL study, the researchers interviewed the peer leaders to gain insight into what actually happened in the PLTL sessions. Peer leader journal entries supplemented the interviews. The peer leaders suggested three reasons for the success:

- 1) The PLTL sessions were a community of learners working together on common tasks.
- 2) The PLTL sessions provided students with the opportunity to negotiate and refine their understanding of ideas and concepts.
- 3) The PLTL sessions provided modeling of expert thinking skills by the peer leaders sharing problem-solving strategies with the students.

Although these results seem encouraging, the researchers focused on student performance on exams and used the increase in student performance and retention as an indication of student understanding and development of problem-solving skills. However, evidence exists that performance on organic chemistry assessments does not necessarily indicate that students understand the underlying concepts.

### **Conceptual Understanding in Organic Chemistry**

Assessments in organic chemistry have changed little over the years. This is best seen through reviewing the end-of-chapter problems in a popular textbook first published in 1959, Morrison and Boyd's "Organic Chemistry". Although Morrison

and Boyd are credited with changing how organic chemistry is taught (Borman 2005)—by using a mechanistic approach<sup>11</sup>—their problems have changed little since 1959. As seen in the general chemistry and physics education literature, students will focus on obtaining the correct answer over understanding the conceptual basis (Lythcott 1990). Students can use the mechanistic approach in solving organic chemistry problems, but will focus on getting the correct response, just as the general chemistry students. This problem is evident in a recent study on how students use the organic chemistry reaction mechanisms (Bhattacharyya and Bodner 2005).

#### Concepts versus Algorithms: Analogs in Organic Chemistry

In organic chemistry, there are few algorithmic calculations as compared to general chemistry. There are, however, several problem-solving heuristics that students misuse in the same fashion as the mathematical algorithms in general chemistry. Bhattacharyya and Bodner (2005) demonstrated that an organic chemistry analog exists for students solving reaction mechanism problems. The researchers reported their findings of a study in which they conducted problem-solving interviews with fourteen graduate students. The graduate students were asked to write reaction mechanisms for problems with two to four step variants of traditional mechanisms. These graduate students were well versed in the reactions of organic chemistry and knew what the correct product would be in a given reaction. Upon observing the students writing the mechanisms for these reactions, two significant results emerged.

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<sup>11</sup> A mechanistic approach to learning organic chemistry implies that students learn organic chemistry through an understanding of the postulated organic reaction mechanisms—a detailed account of how the reactants interact to form the products.

The first result demonstrated that students used the curved arrows typical of reaction mechanisms in a heuristic formalization without the physical meaning of representing the “how” and “why” of a reaction mechanism. The students limited their focus on the starting materials, known intermediates, and reaction products rather than the process of the reaction—the main purpose of the reaction mechanism. As a result, their mechanisms were little more than connect-the-dots exercises with little meaning given to any individual step in the process.

This “connect-the-dots” mentality created a second important finding also consistent with the literature in general chemistry. The students emphasized obtaining the correct answer with little regard for the underlying concepts behind their response. Their justification included the response: “It gets me to the product”(p.1405). This mentality, or way of thinking, resulted in students blindly focusing on obtaining the correct answer (product) rather than focusing on the process of getting the answer. The mechanisms presented by the students were mainly based on memorized components at various points in the process. Therefore, the students had a tendency to propose nonsensical mechanisms, forming unlikely intermediates, to arrive at a correct reaction product structure. The students did not exhibit a global view of molecular structure but focused only on certain memorized traits that they knew were important to get to the next step and ultimately to the final product. Thus, the overarching result was that organic chemistry graduate students focused more on getting the correct answer in lieu of creating viable pathways in order to obtain the correct answer. These

students simply reproduced a memorized sequence of events producing correct answers without exhibiting the conceptual understanding behind their responses.

The students in this study were graduate students in a field heavily reliant on organic chemistry where they would be expected to be able to predict the correct product for most typical organic reactions. In fact, most of the studies in organic chemistry problem solving have come out of the Bodner group, and have used graduate students as research subjects (Bowen 1990; Bowen and Bodner 1991; Bodner and Domin 2000). Similar studies with undergraduate students have not been conducted.

These types of studies are rare in the field of organic chemistry education research. Rather than focus on improving student performance, the study evaluates the students' understanding. It is not a deficit study focusing on students' misconceptions, but on the actual processes that students use to solve these problems. In essence, Bhattacharyya and Bodner (2005) examined what students focus on and how, and whether they gave meaning to various representation systems.

This qualitative research field is wide open in organic chemistry education, especially for research in undergraduate students' conceptual understanding. A general evaluation of problem solving in organic chemistry crosses many conceptual domains making it difficult to study the conceptual understanding of undergraduate students. The expectation is that undergraduate students will not only exhibit some of the same problems as graduate students, but also exhibit problems unique to the undergraduate population.

It is important to note that most of the studies highlighted in this chapter's review of literature, especially those evaluating students' conceptual understanding, find their underlying theoretical perspective in constructivism. From a constructivist view of learning, students develop knowledge through a series of assimilations, perturbations and accommodations (von Glasersfeld 1995). The knowledge constructed may not be compatible with the conceptual ideal from the specific education community. In other words, students develop conceptual schemes based on their unique experiences and backgrounds. These schemes are personal representations of a concept that resides in the mind of each individual learner, and may not conform to the concept agreed upon within a specific community. Since these conceptual schemes are individual constructs within the mind of the learner, they cannot be explored directly because they exist as a learner's own private cognitive representation. What can be explored through direct observation of behavior and statements during problem solving are the products of the learners' mental acts, the students' ways of understanding, one of the main constructs of DNR-based instruction.

### **DNR-Based Instruction and Chemistry Education**

#### Constructivism in Chemistry Education

Constructivism is of great interest in chemistry education. The constructivist issue has been the topic of an online symposium in the Journal of Chemical Education (2001) and as the theoretical foundation for books for chemistry educators (Herron 1996; Wink and Gislason 2002). Even Piaget's cognitive developmental theory continues to appear in current literature in chemistry education (Shibley, Milakofsky

et al. 2003). Chemistry educators have often shunned the notions of radical constructivism (von Glasersfeld 1995), due mainly to the idea that knowledge may not represent reality, in favor of other forms of constructivism such as social constructivism (Ernest 1990; Ernest 1994; Gabel 1999), human constructivism (Lowery Bretz 2001) or contextual constructivism (Cobern 1993). Even well-known chemistry educators who have supported a Piagetian constructivism in the past (Bodner 1986) have begun to modify their constructivist beliefs (Bodner, Klobuchar et al. 2001). Despite the turn from radical constructivist perspective, chemistry educators continue to believe that learners are active interpreters of their environment (rather than a blank slate in which knowledge needs to be imparted) constructing their own ideas about the world around them (Bunce 2001; Nakhleh 2001; Samarapungavan and Robinson 2001; Townes 2001; Wink 2001). Thus, constructivism is still currently used as a foundational learning theory in the development of new instructional methodologies in chemistry education (Browne and Blackburn 1999; Blakely 2000; Coll and Taylor 2001; Taber 2001; Teichert and Stacy 2002).

#### Chemistry Education and Harel's DNR

Despite a widely accepted view of learning from a constructivist perspective, there is still an active philosophical debate about how much of the constructivist perspective educators should adopt (see Bodner, Klobuchar et al. 2001; Scerri 2003). The existence of such a debate distracts from the real issue of improving student learning. Since constructivism is a learning theory and not a teaching theory, all of the different teaching methods apply to the student as an active interpreter of knowledge



in any environment. Yet, in order to enhance learning, a teaching theory should also take into account the students' original conceptions and expand upon them. This, in essence, is what Harel's (1998, 2001, in press [a]) DNR-based instruction takes into account and, thereby, offers a theoretical framework for producing activities that can lead to more scientific ways of understanding.

Based on Johnstone's (1991) three representational levels of conceptual understanding, chemistry educators' ideas of conceptual understanding in chemistry implies a positive connotation not present in Harel's neutrally-based *ways of understanding*. (The research questions in this dissertation look at students' ways of understanding.)

The following example from organic chemistry supports the compatibility of organic chemistry education with the constructs of Harel's DNR-based instruction.

Students coming into an organic chemistry course know that the course has a reputation for being difficult because of the many new terms, ideas and reactions that the students are responsible for learning (Seymour and Hewitt 2000). If a student entering the course holds the way of thinking that learning organic chemistry means memorizing all of the reactions that they encounter, then this will influence the way that they understand the new organic chemistry concepts. When solving problems, this student will focus on the content that he or she needs to commit to memory in order to solve the problem successfully. Thus, the ways of thinking influence ways of understanding. The reverse is also true; namely, ways of understanding influence ways of thinking. Regardless of whether or not the textbook or the instructor tells the

students not to emphasize memorization as a learning strategy in organic chemistry, the students' experiences problem solving in organic chemistry will reinforce their ways of thinking.

The Duality Principle explains that how a student comes to understand organic chemistry is more influential on their ways of thinking than a direct verbal suggestion by an instructor or the foreword of a textbook. A student who solves problems from the textbook with a focus on memorizing will find the memorize-oriented way of thinking reinforced as they continue to successfully (to some degree, at least) solve problems. Likewise, quiz and midterm problems can also reinforce students' memorize-oriented ways of thinking, especially when the volume of information can more easily be committed to memory. As the course proceeds, the strategy of memorizing proves more burdensome, thus resulting in students either dropping the course or completing the course with a very weak knowledge base.

The nature and sequence of problems can have a profound influence on students' learning. In most organic chemistry textbook, problems are set in order of difficulty (Ege 1999; Bruice 2001) with more challenging problems labeled "team problems" (Vollhardt 1999) or "challenge problems" (Wade 2002) located as the last problems at the end-of-chapter problem set. Students solving the "easier" problems early in the problem set may choose to stop solving problems or rely on the study guide to show them the answers as they reach the more challenging problems. Typically students will solve the same type of problem in clusters. These problem clusters give the students skill practice that reinforces the memorize-oriented way of

thinking because they use their memory of how they solved the previous problem to solve new problems. These problems, in essence, are not real problems for the students. In other words, the problems do not pose situations of real puzzlement for the students.

Harel's DNR provides the theoretical framework from which chemistry educators can identify students' ways of understanding and ways of thinking and can help students develop more desirable ways of understanding and ways of thinking.

### Ways of Thinking in Science Education

This section focuses on one of Harel's ways of thinking categories: "beliefs about mathematics" (or in this study, "beliefs about science"). The analogous definition in science would be associated with students' beliefs about what they believe science is, how they believe scientific concepts emerge, and the intellectual and practical benefits of science.

Pintrich et al. (1993) posit that the "individual's goals, intentions, purposes, expectations [and] needs" (p.168) are as important as the cognitive strategies in conceptual development. In their review of the literature, Pintrich et al. highlight the importance of interest, and personal and situational beliefs in their relationship to students' engagement in learning activities.

In their study comparing deep versus surface approaches to learning science, Chin and Brown (2000) discuss, as part of their rationale for their study, the issue that not only does prior knowledge affect students' ability to learn, but their motivation, expectations and epistemological beliefs do, as well. Of particular relevance to this

dissertation is that student expectations and epistemological beliefs affect student learning. Ways of thinking, as formulated by Harel, influences student understanding as illustrated above by both Pintrich et al. (1993) and Chin and Brown (2000).

In a study from physics education, Hammer (1994) presented a framework of students' beliefs based on several interviews with university six students while they were enrolled in an introductory physics course. The framework contained the following three categories of students' beliefs:

1. Beliefs about the *structure of physics knowledge* as (a) a collection of isolated pieces or (b) a single coherent system.
2. Beliefs about the *content of physics knowledge* as (a) formulas or (b) concepts that underlie the formulas.
3. Beliefs about *learning physics*, whether it means (a) receiving information or (b) involves an active process of reconstructing one's understanding. (p.151)

These *categories of beliefs* are closely aligned with the beliefs distinguished in Harel's DNR. Harel (in press [a]) distinguishes between three characteristics of one's views of mathematics. In the case of this dissertation, the three characteristics are views of organic chemistry associated with (a) what organic chemistry is, (b) how organic chemistry is created, and (c) the intellectual and practical benefits of organic chemistry. These align well with Hammer's (1994) three categories (see Table 2-1).

**Table 2-1: Harel vs. Hammer Beliefs**

<b>Harel Analogy</b>	<b>Hammer Analogy</b>
What is organic chemistry?	Structure of organic chemistry knowledge
How is organic chemistry created?	Beliefs about learning organic chemistry
What are the intellectual and practical benefits?	Content of organic chemistry knowledge

For Hammer, the *structure category* is associated with *pieces versus coherence scheme* while the *content category* is associated with *formulas versus concepts scheme*. In organic chemistry, the *content category* is associated with *reactions versus concepts* where students who emphasize learning the reactions can lose track of the underlying concepts. The *structure category*, in organic chemistry, is also associated with *pieces versus coherence*. Thus, students view the *structure* of organic chemistry along a continuum, with one belief being a coherent system of knowledge, and the other belief being *pieces* of information that need to be memorized.

Hammer's study provided a significant portion of the background for a quantitative study on students' expectations in introductory physics (Redish, Saul et al. 1998). Redish et al. developed a 40-item Likert-scale survey intended to measure students' attitudes and beliefs (what they refer to as "expectations") about introductory physics. They administered the survey to college introductory physics students before and after instruction as well as to instructors. They found that there was a great discrepancy between the expectations of students and those of instructors; but, more interestingly, they found that students' expectations deteriorate rather than improve after the first term of introductory physics.

Harrison and Treagust (2001) demonstrated the influence that motivation had on two secondary school chemistry students' conceptual change in chemistry education. One of the students, who had a high achievement level in chemistry, was resistant to change in his conceptual understanding because his learning was motivated by achievement and the apparent belief that the "accumulation and reiteration of

information in a systematic way constituted scientific thinking”(p.76). This directly related to his beliefs about “what science is” and is therefore an example of a way of thinking consistent with Harel’s definition.

Although these studies acknowledge and document the influence that ways of thinking have on student understanding, they do not offer a coherent set of principles to address this issue in student learning. Harel’s DNR provides a conceptual framework from which to develop curricula that will address this direct influence of ways of thinking and ways of understanding using a constructivist-based view of learning.

### **Conclusion**

The review of research in this chapter focused on conceptual understanding in chemistry education demonstrating that students can perform well without scientific understanding. In addition, students’ understanding in general chemistry of concepts foundational to organic chemistry (such as molecular geometry and covalent bonding) is relatively weak. The research in conceptual understanding in organic chemistry is scarce; the research that has been conducted in the field focuses on problem solving in organic synthesis, spatial visualization, and teaching effects on performance.

The theoretical framework for this study uses Harel’s DNR-based instruction from mathematics education. The present study maintains a constructivist foundation of student learning, with the ability to account for both ways of thinking and ways of understanding through empirical evaluation of students’ interpretations.

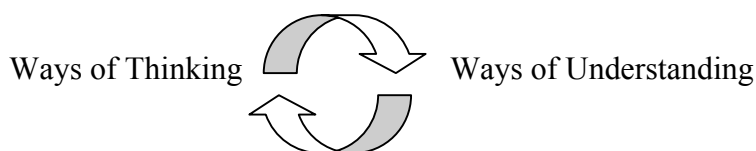
The first purpose is to identify students' ways of understanding aromaticity and electrophilic aromatic substitution reactions demonstrating that performance does not imply that students hold scientific ways of understanding. The second purpose of this study is to provide quantitative evidence of students' beliefs (one category of ways of thinking) about learning organic chemistry. The third purpose is to show how we can help students develop more scientific ways of understanding aromaticity.

## CHAPTER 3: METHODOLOGY

This dissertation explores students' ways of understanding the organic chemistry concepts of aromaticity and electrophilic aromatic substitution reactions (EAS) informed by Harel's (1998, 2001, in press [a]) DNR-based instruction (see chapter 1). The data was collected in three phases with each phase coinciding with one of three research questions. In this mixed-method study, Phases I and III were qualitative in nature while Phase II was quantitative. This chapter presents the general research perspective, an overview of the research setting, and the methodology used in each of the three phases.

### General Research Perspective

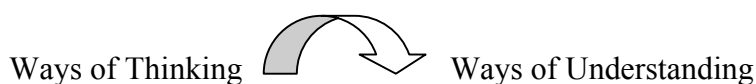
The focus of this dissertation was to determine students' ways of understanding the concepts of aromaticity and electrophilic aromatic substitution (EAS) reactions. Using the identified ways of understanding, the students' ways of thinking could be inferred. The organization of the data collection and analysis was influenced by the constructs of the Duality Principle. As stated in chapter 1, Harel formulated the Duality Principle as the interdependency of ways of understanding and ways of thinking. Students' ways of understanding influence their ways of thinking and, conversely, students' ways of thinking influence their ways of understanding.



**Figure 3-1: Duality Principle Illustrated**



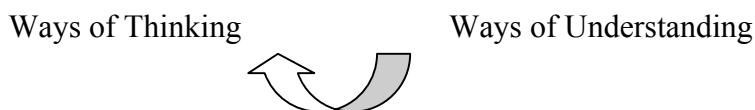
The phases of this study were directly related to one direction of the Duality Principle. The goal of Phase I was to answer the first research question of this study addressing students' ways of understanding aromaticity and EAS reactions. An additional goal of Phase I was to infer a limited number of ways of thinking from the identified ways of understanding. In this way, I explored the influence of ways of thinking on ways of understanding (see Figure 3-2).



**Figure 3-2: WoT Influences WoU**

The results of Phase I were used to inform both Phases II and III. Phase II, the quantitative component of this study, examines organic chemistry students' predominant ways of thinking associated with beliefs about learning in organic chemistry. A 46-Item Likert-scale survey was used to assess the prevalence of certain beliefs held by these students.

Phase III focuses on students' emerging ways of understanding and how they were influenced by their ways of thinking. In this phase of the study, I also examined the influence of ways of understanding on ways of thinking (see Figure 3-3).



**Figure 3-3: WoU Influences WoT**

## **Overview of the Research Setting**

This research was conducted at a large, publicly-funded university in southern California. Based on the data for the incoming freshmen of 2002, the average high school GPA of the study participants was 3.94, while the average SAT I and SAT II scores were 1239 and 1252, respectively. The participants in this study were organic chemistry students, typically in their sophomore year of college, majoring in biology, bioengineering, chemistry or other science-related fields. The age and ethnicity breakdown of the students in the organic chemistry course sequence reflected that of the entire undergraduate student population. Students selected for participation in this study represented the diversity of the student body population as much as possible. Background surveys and the Phase II surveys were distributed with the consent of the instructor, generally, at the end of the lecture period.

For the qualitative phases, the interviews (Phase I) and teaching interview sessions (Phase III) were conducted in private. The sessions were videotaped with the camera focused on the student's written work. Upon completion of the sessions, each participating student received two movies tickets valued at approximately eight dollars as compensation.

### **Phase I Methodology**

#### Recruitment of Participants

The recruitment background survey (see Appendix 1) was distributed to students enrolled in the second of the three quarter organic chemistry sequence during second summer session of 2003. During this quarter, the topics of aromaticity and

EAS reactions were presented to the students in a typical lecture format.

Approximately 250 students were enrolled in the course. A total of 28 students filled out the background survey. Nine students and two undergraduate teaching assistants from this course were interviewed in the fall quarter of 2003. The participants were selected based on availability and willingness to participate.

Students in the summer course used the text "Organic Chemistry: Structure and Reactivity: Fourth Edition" by S. Ege (1999). As a result of the sequencing of this text, the two topics of interest to this study were presented in the last few lectures of the course. Consequently, student volunteers were unwilling to be interviewed before the final exam and generally unavailable after the final; therefore, the interviews were conducted during the fall quarter of 2003. Inviting the students to participate in the fall resulted in an initial enlistment of only five participants. These five interviews were conducted approximately eight weeks after the completion of the summer session course. A greater effort to recruit students produced six additional volunteers: two undergraduate teaching assistants and four student volunteers. Due to the timing, these new recruits were interviewed close to the end of the fall quarter, nearly 10 weeks after the end of the summer session course. Two of these students were no longer enrolled in the organic chemistry sequence.

A second round of interviews was conducted using volunteers from the second quarter of the organic chemistry sequence held in winter quarter 2004. Students were recruited from two of the three lectures. Approximately 350 students were given the recruitment background survey, with over forty respondents.

Students in the winter 2004 course used the text “Organic Chemistry: Structure and Function: Fourth Edition” by Vollhardt and Schore (2003). Because of the sequencing of this text, the topics of aromaticity and EAS reactions were covered in the middle of the quarter. As a result, student volunteers were asked to conduct their interviews a few days after the second exam, in which they were tested on the topics in question. Students were recruited based on their first exam score, which they reported on the background survey. Invitations by e-mail were sent to ten “A” students from each of the two lectures. Five from each course agreed to be interviewed. A total of ten students were interviewed in the second round of data collection. All the interviews took place within a week of the second exam.

Performance in the course became important for selecting students for the second round of interviews because it became clear from the first round of interviews that performance correlated with interview quality. The quality of the interview was based on students’ ability to contribute much information for analysis of their ways of understanding. Lower performing students were not able to engage in the interview tasks because they said that they did not remember the content.

As previously stated, students participating in the first set of interviews were selected mainly based on availability. Any student who had filled out a background survey and still wanted to participate in the study in the fall (nearly one month after completing the summer session course) was recruited. Two of the students in the study had a final grade of “C”, two had a “B”, two an “A-”, two an “A” and one an “A+”. The lower the grade, the lower the quality of the interview, because these students

were more likely to reply, “I don’t remember” to questions involving the interview tasks. Table 3-1 provides a summary of the recruited students for Phase I:

**Table 3-1: Phase I Student Recruits**

<b>Student #</b>	<b>Term</b>	<b>Grade</b>	<b>Gender</b>	<b>Analyzed</b>
1C	SS03	B	F	N
2C	SS03	B	F	N
3C	SS03	A-	F	N
4C	SS03	A-	M	N
5C	SS03	C	F	N
6C	SS03	TA	M	Y
1B	SS03	A	M	N
7C	SS03	C	F	N
8C	SS03	A+	M	N
2B	SS03	A	M	N
9C	SS03	TA	M	Y
3B	W04	A	F	Y
4B	W04	A	F	Y
5B	W04	A	F	Y
6B	W04	A	M	Y
7B	W04	A	F	Y
8B	W04	A	F	Y
9B	W04	A	F	Y
10B	W04	A	M	Y
11B	W04	A	M	Y
12B	W04	A	M	Y

In Table 3-1, the designation of B or C in the Student# column was coordinated with either the course enrolled in or the highest organic chemistry course completed. Most of the students from summer session 2004 enrolled in the third quarter of the three quarter organic chemistry sequence and were designated as “C” with their student number. (The number designated the order of the interviews. Student 1C was interviewed before student 2C, etc.) Students 1B and 2B were recruited in summer session 2003 but did not go on to enroll in the subsequent organic chemistry course. They were the first of the students from the second quarter to be interviewed; yet their

interviews were concurrent with the summer session interviewees, and not with the winter 2004 recruits.

Another important factor from the first interviewees was that the time delay between when the topic was tested and the interview also influenced the quality of the interview. The longer the amount of time between the exam in which the topics were tested and the interview, the less likely the student was able to provide useful information in response to the interview questions. The quality of the answers thus depended on two factors—grade and time delay. A low grade and a long delay resulted in answers which held little value to this study. (Students responding with “I don’t know” too frequently provided little if any valuable data for identifying students’ ways of understanding aromaticity and EAS reactions.)

As a result of the first set of interviews, measures were taken to gain more valuable interview data for the second set of interviews. These measures included recruiting high performing students in the second quarter organic chemistry course from two different instructors, conducting the interviews immediately after the midterm exam that included the topics and attending all of the lectures for both instructors that presented the topics of aromaticity and electrophilic aromatic substitution reactions.

### Data Collection

Subjects in Phase I were asked to participate in a one hour semi-structured clinical interview (Bernard 1988; Ginsberg 1997). The goal of the interview was to elicit the student’s ways of understanding the concepts of aromaticity and electrophilic

aromatic substitution (EAS) reactions. The interview tasks were designed to provide evidence of students' ways of understanding these topics, as well as providing evidence for students' ability to apply their ways of understanding in novel problem situations. Novel problems consisted of problems that the student would not have encountered through reading the text or attending lecture. The interview protocol was developed through assessment of textbooks, past exam questions, and informal pilot-study interviews with past students enrolled in the second quarter of the organic chemistry sequence. The interview protocol (see Appendix 2 and 3) was designed to begin with problems that were familiar to the students from their reading and lectures, while the novel material appeared in the second half of the interviews.

Based on students' responses from the interview questions, probing questions were posed to clarify students' responses, and, when needed, to obtain further information regarding the students' ways of understanding. Thus, the interview protocol was the guide for each interview, but the student responses provided the basis for the exact line of questioning. Ginsberg (1997) described this as creating and testing hypotheses about students' ways of understanding in real time.

Along with the videotaped recording of the interviews, the collected data included the students' work—either on the blank sheets of paper available or on the interview sheets (see Appendix 3) provided from the protocol. In addition to the blank paper and black Sharpie pens, students were provided with any of the following upon request: a Periodic Table, access to their textbook (for the first batch of interviews

only), pens in other colors, and a molecular modeling kit. In addition to student work, the researcher wrote brief summary notes after each interview.

### Data Analysis

Data analysis for Phase I had two purposes: first, to inform the development of tasks for the teaching interviews in Phase III, and second, to answer the first research question identifying students' ways of understanding aromaticity and electrophilic aromatic substitution reactions. The first part of the analysis was based on an informal evaluation of the data. All the videotaped data for the second round of interviews were transcribed, while only interviews of the teaching assistants from the first round were transcribed. A total of 12 interviews were transcribed. Based on a review of the transcripts, student work, and author's notes, an informal analysis was made of students' ways of understanding aromaticity and EAS reactions. In this part of the analysis, no attempt was made to categorize or classify ways of understanding formally, but rather, to search for patterns in the data that could be used to inform task development for the teaching interviews in Phase III. For example, I found that students did not know the origin of Hückel's Rule<sup>12</sup> came from, and what  $N$  represented. Consequently, I designed a task for Phase III intended to lead the student to derive Hückel's Rule from molecular orbital diagrams of several aromatic compounds.

Following the preliminary analysis, a more formal analysis was conducted involving a grounded theory (Strauss and Corbin 1994, 1998) approach. The

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<sup>12</sup> Hückel's Rule requires the number of pi electrons in a monocyclic conjugated system to fit the formula  $4N + 2$  for the compound to be designated as aromatic.



transcripts were coded via an open-coding (Strauss and Corbin 1998, p. 101) in which categories emerged about students' ways of understanding aromaticity and EAS reactions. The mental act of interpreting was the focus during this analysis. Emerging categories of ways of understanding were then compared across several students' results and refined as more data was analyzed. These emerging categories were validated by inter-rater reliability as two transcripts were coded independently with similar results. The final identification of the categories of ways of understanding resulted in the identification of two distinct categories of students' ways of thinking. Final determination of a set of categories for students' ways of understanding aromaticity and EAS reactions were then used to re-analyze all twelve transcribed interviews in order to generate a consistent and thorough analysis.

#### Summary of Methodology for Phase I

Phase I was designed to answer the question, "What are students' ways of understanding aromaticity and electrophilic aromatic substitution reaction?" The qualitative interview data was collected in two rounds, with analysis emphasizing the second round of interviews in order to develop categories of ways of understanding. The data from the first round, although not very helpful in developing the categories, provided indisputable evidence of the inability of students to sustain viable ways of understanding due to the presence of non-referential symbolic reasoning way of thinking. Phase I informed the development of tasks for the teaching interviews in Phase III and the quantitative component to this study in Phase II.

## **Phase II Methodology**

### The Instrument Design

The goal of Phase II was to examine students' predominant ways of thinking associated with their beliefs about learning in organic chemistry. The Phase II survey was developed with significant parallels to the Maryland Physics Expectation survey (MPEX) (Redish, Saul et al. 1998). The probes in the MPEX survey were modified, with permission, for the organic chemistry course population in this study, and thus, did not have all of the same clusters as the MPEX and chemistry equivalents. Seven probes, which also applied to an organic chemistry population, were taken directly from the MPEX survey (Items 1,2,9, 19, 23,24, and 25). An additional 16 probes (Items 3,5,7,8,10,12,14,15,16,17,18,21,25,27, and 28) were slightly modified from the MPEX survey, often replacing the word "physics" with "organic chemistry". The remaining 17 probes were developed based on students' responses to a study habit and general course survey administered over three quarters by one of the organic chemistry instructors at the same university where this study was conducted. Finally, the survey included direct suggestions from several organic chemistry instructors.

In addition to utilizing the MPEX survey, student responses on course surveys, and instructor feedback, the Phase II survey items were also aligned with ways of thinking associated with beliefs according to Harel's DNR (1998, 2001, in press [a]), and Hammer's (1994) epistemological beliefs (see the following Table 3-2).

**Table 3-2: MPEX, Harel and Hammer Analogies**

<b>MPEX Analogy</b>	<b>Harel Analogy</b>	<b>Hammer Analogy</b>
Independence	How is organic chemistry created?	Beliefs about learning organic chemistry
Coherence	What is organic chemistry?	Structure of organic chemistry knowledge
Content	What are the intellectual and practical benefits?	Content of organic chemistry knowledge

The probes in the Phase II survey were labeled as either desirable or undesirable based on students' agreement with the probe. Table 3-3 shows the distribution of the probes using the MPEX analogies listed above.

**Table 3-3: Survey Item Distribution Across Categories**

<b>Category</b>	<b>Desirable</b>	<b>Undesirable</b>
Independence	1, 2, 5, 13, 26, 28, 29, 34, 35, 36, 40	4, 6, 16, 19, 23, 31, 32, 33, 38
Coherence	10, 11, 14, 20, 37, 39	8, 9, 18, 22
Concepts	25, 30	3, 7, 12, 15, 17, 21, 24, 27

One version of the Phase II survey was distributed in two discussion sections of the third quarter of the organic chemistry sequence in spring 2003 with a total of 45 surveys completed. (The pilot study survey was slightly longer in that students were given room after each probe to make comments.) Based on feedback from students (both from interviews and pilot-study data) and instructors, modifications were made to several survey items. (In order to maintain direct consistency with the MPEX survey items, MPEX items were not modified. For example, one student felt that Item 1 (“To understand most of the basic ideas in this course, I read the text, work most of the problems, and pay close attention in class”) provided too many variables to

warrant complete agreement or disagreement. The question was not changed mainly due to the results of pilot-study data that showed student agreement with Item 1 and with no other significant student comments.)

Items were modified and validated in several rounds, based on feedback from several chemistry professors, informal interviews of students prior to the study, Phase I students during the first round of interviews, and feedback from pilot-study data. The final survey consisted of 46 Items with 40 Items consisting of the Likert-scale probes of students' beliefs and an additional six items consisting of demographic probes (see Appendix 4).

#### Data Collection

The final version of the Phase II survey was administered in Fall 2003 to organic chemistry students in the third quarter of the three quarter sequence of organic chemistry. With permission from the instructor, 120 surveys were distributed at the beginning of one lecture. The students were told about the study and that participation was voluntary. Students were given approximately 15 minutes to complete the survey. A total of 102 surveys were completed.

#### Data Analysis

Survey responses were manually entered using (JMP IN Version 4.0) statistical software. Responses were coded, with "strongly agree" given a value of 1, "agree" given a value of 2, "neither" given a value of 3, "disagree" given a value of 4, and "strongly disagree" given a value of 5. Frequency distributions for each probe were analyzed. Items with mean values between 2.75 and 3.25 were deemed neutral

responses (“neither in favor of, agree, nor disagree”). Items with a mean value less than 2.75 were viewed as items that students generally agreed with, while items with a mean response value of 3.25 were viewed as items with which students generally disagreed. In addition, items with mean values less than 2 were categorized as items where students held strong agreement.

In addition to the frequency distributions, the data was treated with principal component analysis to reduce the number of variables and to detect structure in the relationships between variables. A scree plot was employed to obtain seven principal components from the 13 that had eigenvalues greater than one. The structure of the data was explored by extracting 3-13 factors using Varimax (orthogonal) rotation, studying the patterns and loadings of various survey items. Only rotated loadings with a magnitude greater than 0.5 were considered as contributing factors. The stability of the loadings was compared manually since the number of factors varied. A consistent pattern of loadings emerged after rotating seven factors.

The seven principal components (designated PCA1, PCA2, PCA3...PCA7), were characterized based on the loading patterns of the rotated factor analysis. In addition, the magnitudes of the eigenvectors in the 40 x 40 Correlation Matrix were considered when insufficient evidence was revealed in the rotated factor analysis.

### Phase II Summary

The quantitative data of Phase II was designed to answer the research question, “What are students’ predominant ways of thinking associated with their beliefs about learning organic chemistry?” A 46-Item Likert-scale survey was designed and

administered to students in the third quarter of the organic chemistry sequence. In addition to frequency distributions for each item, principal component analysis was conducted on the 40 items probing student beliefs.

### **Phase III Methodology**

#### The Experimental Design

This section presents the basic teaching experiment methodology, followed by a discussion contrasting the teaching experiment methodology (Steffe, Thompson et al. 2000) with the teaching interviews employed in this study<sup>13</sup>.

In a teaching experiment, the researcher acts as both the teacher and researcher modifying the teaching episodes in order to help facilitate the development of specific knowledge through a student-driven learning environment. One of the main components of the teaching experiment methodology is the testing of research hypotheses about student learning. The research hypotheses formed prior to the teaching experiment inform the development of the initial tasks and a hypothetical learning trajectory (Bowers, Cobb et al. 1999). During a teaching experiment, the teacher/researcher formulates hypotheses about student learning based on the interactions with the student(s) and tests these hypotheses during the interaction. Immediate evaluation of the teaching sessions from videotaped data and researcher notes generates new hypotheses, and informs the development of tasks for a subsequent session.

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<sup>13</sup> The research design of Phase III was based on the teaching experiment methodology but was referred to as *teaching interviews* because of the variations that distinguish these sessions from teaching experiments.

Both of these hypothesis generation techniques were used in this study. The hypothetical learning trajectory (see chapter 6) was informed by the results of Phase I, Harel's DNR instructional principles, as well as literature in organic chemistry on the concept of aromaticity (Krygowski, Cyranski et al. 2000; Gomes and Mallion 2001; Krygowski and Cyranski 2001; Balaban, Oniciu et al. 2004; Kovacevic, Baric et al. 2004). While the initial tasks and the hypothetical learning trajectory were developed prior to the study, it was the ongoing hypothesis generation and testing that continued to guide the teaching interviews once they had begun. Some of these hypotheses were generated in one session and tested in that same session, while others were generated after reflection on the session and tested during the subsequent sessions.

This study deviated from the traditional teaching experiment methodology in two important ways. The teaching experiment, by design, would require an observer to be present during the teaching session (in many cases, this person would operate the camera). Input from the Phase I interviews indicated that some students would find having another person in the interview room intimidating; therefore, in order to work one-on-one with the students, videotaped sessions and field notes were used in place of an observer. Since Phase III data was collected over a very short time span, the problems in the six tasks were generated in advance and modified based on the hypotheses generated for each individual student. In other words, a bank of problems were developed for each task that could be used depending on the hypotheses generated during the teaching sessions.

Another deviation from the traditional teaching experiment method was the short duration of the experiment. Each student spent between four and six hours in the teaching sessions; yet, a typical teaching experiment occurs over a period of weeks or even years. This longitudinal aspect is a distinguishing characteristic of teaching experiments (Cobb & Steffe, 1983, p. 87).

In Phase III, the researcher chose to focus on the development of the concept of aromaticity and not EAS reactions due to time constraints. Three teaching interview sessions were chosen to attempt to mimic the number of typical lectures devoted to the concept. Due to the nature of the hypothesis generation and testing, the sessions were scheduled to last for one and a half hours each, nearly doubling the amount of typical “in-class” time for fifty-minute class periods.

As a result of the variations from the characteristics of the typical teaching experiment methodology, the methodology in Phase III of this study was referred to as *teaching interview* sessions. The design of the teaching interviews was grounded in the teaching experiment methodology. The development of tasks was based on a hypothetical learning trajectory. The generation of hypotheses about the students’ developing ways of understanding aromaticity occurred in both real-time and between sessions, and informed the modification of tasks for each individual student.

#### Recruitment of Participants and Context

For Phase III, the students were recruited from the second quarter of the three quarter organic chemistry sequence in spring 2005. Instead of using a background survey to select students, feedback from teaching assistants was solicited and



perspective students were sent information via e-mail. Based on availability and willingness to participate, four students were recruited in spring 2005. Just prior to the first session two students decided, for personal reasons, not to participate. As a result, only two students (Abby and Jack<sup>14</sup>) participated in the Phase III teaching interviews in spring 2005.

In the second summer session of 2005, an additional four students were recruited. Three students (Robert, Erik, and Doug) completed all three teaching sessions. The fourth student decided not to continue due to the time commitment and an unforeseen conflict with his employment schedule.

Therefore, a total of five students participated in all three teaching sessions of Phase III. Each session lasted approximately one hour and a half. The minimum session length was an hour and fifteen minutes, with a few sessions extending to nearly two hours. The sessions in spring 2005 were scheduled after the first midterm but before the second; as a result, these two students were learning the content during the teaching interview sessions. Their lecture material was referred to during the teaching sessions. Each of these sessions was scheduled either before or after lecture with a period of one day between sessions. The three summer session students were scheduled immediately after their first midterm for three consecutive days prior to the topic of aromaticity being taught in lecture.

In addition to supplies of paper and pens, students had access to a periodic table, molecular model kits, and their own work from previous sessions if requested.

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<sup>14</sup> All student names in Phase III of this dissertation are fictional names based on the gender and first letter of the students' actual name. Student names were used in Phase III in order to distinguish between the students in Phase I and Phase III.

### Data Collection

The teaching interviews consisted of three 90-minute sessions in which the concept of aromaticity was the focus. The complete data set for each session included videotaped student work, hard copies of students' work, and the researcher's notes taken before, during, and after the sessions.

Students were given a sequence of six tasks, each containing a set of different problems (see Appendix 5). The complete set of problems for Task 4 and some of the problems used for the interviews in Phase I can be found in Appendix 3. The goal for each task and the associated hypotheses are presented in chapter 6. A set of tasks was not developed specifically for each student; rather, the order and allocation of the problems was modified in each task based on the hypotheses generated for each student during the sessions.

### Data Analysis

The goal of the teaching interviews was to help students develop more desirable ways of understanding aromaticity based on a concept analysis of aromaticity (see Appendix 6). The concept analysis of aromaticity for this study was developed from Herron's (1996) outline of concept analysis. Thus, the key components of a concept analysis would be the critical attributes, defined as, "those features that must be present for an instance to be an example of the concept...An adequate definition of a concept always includes all critical attributes" (Herron 1996, p.122). Variable attributes, on the other hand, refer to "features that ...may be present or absent in examples" (Herron 1996, p.122). Since any concept would have an

infinite number of variable attributes, per this definition, a concept analysis would include only those variable attributes that would help clarify the concept. More desirable ways of understanding were established if students emphasized several critical attributes in their ways of understanding the concept of aromaticity over variable attributes. The critical and variable attributes were assigned based on research discussing the importance and background of the concept of aromaticity (Krygowski, Cyranski et al. 2000; Balaban, Oniciu et al. 2004).

Data analysis for the teaching interviews occurred both during the teaching interview sessions themselves and upon completion of all the teaching interview session.

During the Teaching Interviews: Hypotheses were generated about the students' ways of understanding, which informed the distribution of problems for each task. These hypotheses were formed based on the observed ways of understanding with the focus on interpreting as the mental act. The Duality Principle from Harel's DNR indicated that ways of understanding are influenced by ways of thinking, and vice versa. Even though the expectation of the teaching interview sessions was for students to develop more desirable ways of understanding, a similar expectation of inferring changes in students' ways of thinking was not present because of the short duration of the teaching interview sessions and the focus on a single concept. Therefore, the analyses focused on students' emerging ways of understanding aromaticity as determined by their interactions with the problem tasks. During the hypothesis generation and testing analysis phase of the teaching interviews, only students' ways of understanding were

attended to in order to predict their behavior in certain situations and develop tasks that would bring about cognitive conflict. The resolution of these situations of perturbation would constitute learning from a constructivist perspective.

Upon Completion of the Teaching Interviews: The videotaped data was reviewed for all five students, and the sessions for two students (Robert and Abby) were transcribed for initial analysis. Robert's sessions were transcribed because he demonstrated success in developing the more desired ways of understanding, as well as potential for development of more desirable ways of thinking. Analysis involved an open-coding technique similar to that used for Phase I (Strauss and Corbin, 1998). Initially, Robert's ways of understanding from the first tasks were coded based on categories developed in Phase I. Subsequent analysis identified Robert's emerging ways of understanding aromaticity based on the outcomes of different tasks. The ways of understanding were coded based on the concept analysis of aromaticity, and based on whether Robert had a preferential order in which he attended to different attributes of aromaticity. In general, a specific way of understanding could be characterized at the end of each task. Upon completing the analysis of Robert's ways of understanding, evidence was found revealing that he showed potential for change in his ways of thinking.

Abby's sessions were transcribed because she showed preliminary evidence for success in developing more desirable ways of thinking. The same process of analysis was used. Thus, new characterizations of Abby's ways of understanding aromaticity emerged at the end of each task.

The results from these two students were used as a guide for analyzing the remaining three students. Only supporting segments of these teaching sessions were transcribed to highlight specific areas of interest during those teaching sessions. These last three students did not make the same progress in their development of a desirable way of understanding aromaticity as the first two.

#### Summary of Phase III Methodology

The qualitative data of Phase III was designed to answer the question, “What ways of understanding aromaticity emerge among students as a result of an instructional intervention?” The data was collected from a total of five students participating in the three teaching interview sessions, each lasting approximately one and a half hours. The data was analyzed in two stages; one stage occurred real-time, during and in-between teaching sessions, while the other stage took place after the sessions were transcribed. The data was analyzed with an open-coding technique characterizing the students’ emerging ways of understanding aromaticity.

#### **Summary of Dissertation Methodology**

This dissertation was divided into three phases of data collection corresponding to the three research questions. The two qualitative phases (Phase I and III) had data collected from two different groups of students. Phase II provided a quantitative component focusing on students’ ways of thinking associated with their beliefs about learning in organic chemistry. Table 3-4, following, provides a summary of each phase.

**Table 3-4: Summary of Methodology**

<b>Phase</b>	<b>Participants</b>	<b>Description<sup>15</sup></b>	<b>Analysis</b>
I	11	Recruited SS03 Chem 140B; One-hour semi-structured clinical interviews conducted in F03; Textbook: Ege 4 <sup>th</sup> ed.; Variable achievement levels ranging from TA's to C students	Only the two TA's were included in the analysis of Phase I due to the remaining interviews being of relatively poor quality.
I	10	Recruited W04 Chem 140B; One-hour semi-structured clinical interviews conducted in W04; Textbook: Vollhardt and Schore 3 <sup>rd</sup> ed.; High achieving students (all A students)	Development of several categories of ways of understanding aromaticity and EAS reactions.
II	102	46-item Likert-scale survey administered F03 in Chem 140C	Frequency distribution and principal component analysis of the data.
III	2	Recruited in S05 for three 1½ hr. teaching interviews occurring concurrent with lecture Abby before class and Jack after; Textbook: Vollhardt & Schore 3 <sup>rd</sup> ed.;	Abby full transcription and analysis of emerging ways of understanding to a more desirable ways of understanding aromaticity. Jack summarized.
III	3	Recruited in SS05 for three 1½ hr. teaching interviews occurring on 3 consecutive days prior to topic taught in lecture. Textbook: Vollhardt & Schore 3 <sup>rd</sup> ed.; Robert, Doug and Erik	Robert full transcription and detailed analysis of emerging desirable ways of understanding and potential for change in ways of thinking. Doug and Erik summarized.

<sup>15</sup> Chem 140B and Chem 140C represent the second and third quarters of the three quarter organic chemistry sequence, respectively.

## **CHAPTER 4: RESULTS ON STUDENTS' WAYS OF UNDERSTANDING AROMATICITY AND ELECTROPHILIC AROMATIC SUBSTITUTION REACTIONS**

Chapter 4 describes the results from the interview phase of the research. The interview phase addresses the first research question of this dissertation, “what are students’ ways of understanding aromaticity and electrophilic aromatic substitution (EAS) reactions?” Although not explicitly included in the research question, student ways of thinking are inferred from their ways of understanding and are, therefore, relevant to the analysis of the data (see Duality Principle, chapter 1). As a result, there are three main sections of this chapter, the first addresses students’ ways of understanding aromaticity, the second addresses students’ ways of understanding EAS reactions, and the third addresses students’ ways of thinking that were inferred from the identified ways of understanding.

Two main categories of students’ ways of understanding aromaticity emerged through analysis: 1) students’ ways of understanding the characteristics of aromatic compounds and 2) students’ ways of understanding the identification of aromatic compounds. Students’ ways of understanding EAS reactions were categorized based on their ways of understanding monosubstitution of benzene via the bromination of benzene and their ways of understanding the directing effects of benzene derivatives.

The third section of this chapter discusses the predominant student ways of thinking under three main categories: 1) non-referential symbolic reasoning, 2) non-referential use of terminology and 3) students’ beliefs about learning organic chemistry.

### Students' Ways of Understanding Aromaticity

During the interviews in phase one, several opportunities arose to investigate students' ways of understanding the concept of aromaticity. These opportunities included direct discussion about aromaticity as well as several tasks asking students to identify aromatic compounds from a variety of molecules. The focus of the analysis was not on evaluating correct student responses but on the actions (either verbal or written) that students took to obtain their response when either characterizing or identifying aromatic compounds.

#### Characteristics of Aromatic Compounds

As a result of analysis, this section is divided into three subsections: symbolic characteristics, structural characteristics and Hückel's Rule. This section also presents two basic concepts that proved foundational to students' ways of understanding aromaticity: students' ways of understanding hybridization (in the symbolic characteristic section) and students' ways of understanding resonance (in the structural characteristics section).

When asked about the characteristics of aromatic compounds, 10 of the 12 students analyzed stated that "aromatic" referred to "three things." Thus, these students' ways of understanding the characteristics of aromatic compounds was characterized as *an ordered list of three characteristics favoring Hückel's Rule*. The exact nature of these "three things" varied slightly but generally was categorized by symbolic related characteristics, structural characteristics, and Hückel's Rule<sup>16</sup>.

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<sup>16</sup> Hückel's Rule applies mainly to planar monocyclic systems stating that those systems containing  $(4N+2)$  pi electrons, where N is a whole integer, are aromatic.



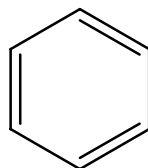
Although Hückel's rule could have been incorporated into either of the other two categories, the students separated Hückel's Rule resulting in the creation of a separate category for discussion.

Two of the students, Students 10B and 6C, did not refer directly to aromaticity as needing the "three things," but did rely on Hückel's Rule as a characteristic of aromatic compounds. Student 6C relied exclusively on Hückel's Rule while Student 10B relied primarily on structural features of the molecule and made Hückel's Rule secondary. A summary table of students' ways of understanding the characteristics of aromatic compounds is included at the end of this section (see Table 4-3).

#### Symbolic Characteristics of Aromatic Compounds

Each of the students recognized benzene as aromatic and associated the term "aromatic" with a compound that was "stable and unreactive." The nature of that stability and the reason for the diminished reactivity, as the students interpreted it, is the focus of this section beginning with the evaluation of students' ways of understanding the symbolic characteristics of aromatic compounds.

Symbolic characteristics include those that can be readily observed by merely looking at the structure of an organic compound. For aromatic compounds, a simple but obvious example would be the requirement that aromatic compounds be cyclic.



**Figure 4-1: Skeletal Structure of Benzene**

As seen in the figure above, benzene is cyclic. One symbolic feature that the students in the study mentioned is that the double bonds in the ring need to be conjugated (alternating single and double bonds). The final symbolic characteristic mentioned by students is that all of the carbon atoms have to be  $sp^2$  hybridized.<sup>17</sup> To instructors, hybridization refers not only to the mixing of atomic orbitals, but it imparts an understanding of the molecular geometry about a central atom. However, students did not employ hybridization in a structural sense but more as a symbolic feature.

#### Students' Ways of Understanding Hybridization:

Nine of the twelve students in this study held a way of understanding hybridization as *counting bonds*. Student 10B had a unique approach on counting bonds by explaining that “carbon is tetravalent minus one is three, so it’s  $sp^2$ .” Student 10B obtained the number “three” by subtracting one from four, the maximum number of bonds carbon can have. Even using a different route, the number three equated to  $sp^2$  hybridization. Six students’ (3B, 6B, 7B, 10B, 12B, 6C, 9C) way of understanding hybridization was designated as *counting bonds*, including Student 10B, even though he had a unique approach to counting.

Five of the twelve students (4B, 5B, 8B, 9B, 11B) originally equated the symbol for the double bonds with  $sp^2$  hybridization. Three of these students’ ways of understanding hybridization was classified as *symbolic reference without counting*.

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<sup>17</sup> Hybridization is a theoretical construct that refers to the mixing of atomic orbitals to form molecular orbitals of equal energy. For carbon, there is one s atomic orbital and three p atomic orbitals in the outer valence shell. An  $sp^2$  hybrid orbital is a combination of one s atomic orbital and two p atomic orbitals. These hybrid orbitals are involved in the sigma bonds, which establish the framework for the molecular geometry. The remaining p orbital is available for pi bonding, a covalent bond between unhybridized p atomic orbitals above and below the plane generated by the sigma bond between carbon and another atom.

Students 4B and 5B, used counting as their justification of assigning  $sp^2$  hybridization, but used other symbolic features to determine hybridization originally. The way of understanding hybridization for these two students was classified as *symbolic reference with counting*. For example, Student 4B stated, “there’s a double bond involved and it’s  $sp^2$ ,” but she justified her hybridization assignment using a similar argument as Student 3B:

“Well, first of all I know it’s  $sp^2$  because that’s one of the requirements<sup>18</sup> for it to be aromatic, and benzene’s aromatic. And the other thing is that um, here, I have an *H* on each one of these so this is 1, 2, 3, so it’s  $sp^2$ , ... I usually count the bonds if this is my carbon and ... I think of hybridization as in this is, um, I just count it like this. 1, 2, 3 there’s three bonds going towards the *C* so it must be  $sp^2$ .” (Student 3B)

For students who exhibited two different ways of understanding, the student was classified based on the dominant held way of understanding exhibited throughout the interview.

**Table 4-1: WoU Hybridization**

WoU Category	Students
<i>Symbolic reference w/o counting</i>	8B, 9B, 11B
<i>Symbolic reference w/counting</i>	4B, 5B
<i>Counting bonds</i>	3B, 6B, 7B, 10B, 12B, 6C, 9C

Table 4-1 provides a summary of the ways of understanding hybridization identified in the Phase I interviews. The symbolic reference groups are designated as such due to their preference for attending to symbolic features (for example, double bonds).

The ways of understanding hybridization as *counting bonds* posed problems for students when non-bonded electrons, lone pairs, were involved in the molecular

<sup>18</sup> This is not true nor was it stated as a requirement by her professor in lecture.

structure. For example, most students did not have a problem viewing the nitrogen in pyrrole (see Figure 4-2) as  $sp^2$  hybridized because of the hydrogen atom drawn next to nitrogen resulting in a count of three bonds to nitrogen, hence,  $sp^2$  hybridized.



**Figure 4-2: Pyrrole and Pyrrol-1-ide**

However, the structure of pyrrole-1-ide posed a myriad of problems for students.

With regard to hybridization, Student 6B applied his way of understanding

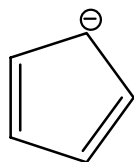
hybridization as *counting bonds* to help him identify pyrrole-1-ide as aromatic:

“The nitrogen here [*refers to pyrrole-1-ide*] is *sp* because it is involved with two bonds. So what’s left over is two *p* orbitals with lone pairs. So if you had the 4 *p* from before and these 2, it’s 6 *p* orbitals and it’s aromatic.” (Student 6B)

Hence, Student 6B correctly identified pyrrole-1-ide as aromatic using reasoning based on an incorrect assignment of hybridization. This assignment of  $sp$  hybridization to the nitrogen atom in the structure to pyrrol-1-ide was unique to Student 6B. In addition, the *counting bonds* way of understanding resulted in Students 3B, 4B and 5B assigning  $sp$  hybridization to structures containing two “bonds” and one or two lone pairs.

Instead of using hybridization, some students used other symbolic characteristics to classify pyrrol-1-ide as aromatic. Five additional students (7B, 8B, 9B, 10B, and 11B) classified pyrrol-1-ide as aromatic. All of these students made an

analogy with the cyclopentadienyl anion (see Figure 4-3) where the negative charge stemmed from one lone pair and one implicit hydrogen atom present on the carbon atom.



**Figure 4-3: Cyclopentadienyl Anion**

As a result, students equated the anion on pyrrol-1-ide as representing one lone pair of electrons, rather than the actual two lone pairs that should be on the negatively charged nitrogen atom of pyrrole-1-ide, and thereby a total of six *pi* electrons.

Making the correct assignment of two lone pairs of electrons on nitrogen resulted in students identifying pyrrol-1-ide as nonaromatic (with the exception of Student 6B). Two of these students (3B and 12B) designated the nitrogen as  $sp^3$  hybridization clarifying their understanding of hybridization to mean *counting bonds or lone pair*. The remaining students who identified pyrrol-1-ide as nonaromatic used Hückel's Rule designating either 4 *pi* electrons (Student 9C) or 8 *pi* electrons (Student 4B).

Most of the students referenced “three things” needed to classify a compound as aromatic, yet, some students did not distribute their interpretation across the three categories of *symbolic*, *structural* and *Hückel's Rule*. Instead they focused on two symbolic characteristics and Hückel's Rule, avoiding any reference to structural features. For example, Student 3B stated, “I think of  $4N + 2$ ...and I also look for other things, like, if it's conjugated and it has to be cyclic, too.” Student 3B was able

to correctly designate eight of thirteen structures as either aromatic or nonaromatic focusing solely on the symbolic characteristics. Most of the molecules were heterocycles<sup>19</sup>, representations that she hadn't seen in class or read about in her textbook. Except for the teaching assistants interviewed, the remaining students had not been exposed to aromaticity in relation to heterocycles.

### Structural Characteristics of Aromatic Compounds

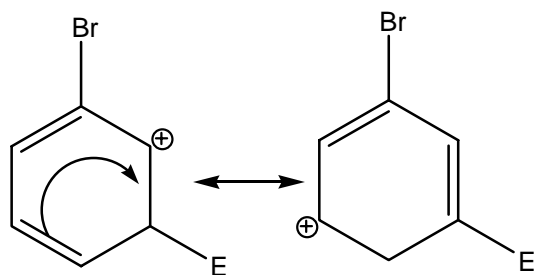
Structural characteristics of aromatic compounds refer to distinctions regarding the structure that are not readily observed using the symbolic structure. These include the presence of implicit hydrogens on the carbon atoms, resonance structures and what students referred to as a “continuum of  $p$  orbitals.” For the majority of students, incorporation of structural features of aromatic compounds did not necessarily imply that they focused on the actual molecular structure, but rather manipulated the symbolic representation in order to account for the structural features. Students referred to the structural requirement for aromaticity as having resonance structures (Students 6B, 7B, 8B, 10B and 11B) or a “continuum of  $p$  orbitals” (Students 4B, 5B, 9B and 12B) depending on the course instructor.

Both groups of students showed indisputable evidence of losing track of the presence of the implicit hydrogen atoms. Thus, students' ways of understanding the implicit hydrogens atoms would be as secondary structural features that were ignored. Bodner and Domin documented students' views of symbolic representations as merely “*letters and numbers and lines*, which have no physical meaning to [the

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<sup>19</sup> *Heterocycles* in this dissertation refers to cyclic compounds in which either nitrogen, oxygen, sulfur or boron are part of the cycle.

student]”(p.25). Students’ ways of understanding symbolic representations as *lines and letters*<sup>20</sup> could result in their losing track of the implicit hydrogen atoms. The hydrogen atoms that are not explicitly drawn out in the symbolic representation would often be forgotten with students who had the *lines and letters* ways of understanding. A common consequence of this *lines and letters* ways of understanding is the presentation of pentavalent carbon atoms in non sequitur resonance structures as seen in the example below from Student 4B.



**Figure 4-4: Student 4B Non Sequitur Resonance Structures**

The carbon attached to the electrophile, *E*, also has an implicit hydrogen atom attached, resulting in that carbon having five bonds, rather than the four allowed in the representation on the right of Figure 4-4. Although the anomaly in this student’s electron movement (skipping a carbon atom) was atypical, the drawing of a pentavalent carbon was not, with many students ignoring the implicit hydrogen atoms at a reaction site.

Student 3B was one of five students in the organic chemistry course who included “continuum of *p* orbitals” as a requirement for aromaticity. All of the

<sup>20</sup> The majority of symbolic representations in organic chemistry include mainly lines and letters. Therefore, the way of understanding is referred to as *lines and letters* rather than *lines, letters and numbers*. This, however, does not imply that the numbers hold any more significance for students than the lines and letters.

students in this group (3B, 4B, 5B, 9B and 12B) held a correct way of understanding the continuum of  $p$  orbitals as having a  $p$  orbital in each atom in the ring. All of the students held a way of understanding the continuum of  $p$  orbitals related directly to hybridization. Each of these students held a way of understanding hybridization as *counting bonds*. Consequently, students assigned one complete pair of electrons to  $p$  orbitals since they were not counted as a bond.

Additionally, Student 5B had a need for visual confirmation of the continuum of  $p$  orbitals. As a result, she drew all  $p$  orbitals in order to better “see the ring of  $p$  orbitals” when determining aromaticity. She did not, however, draw the  $p$  orbitals on her resonance structures when explaining directing effects. She did not view the continuum of  $p$  orbitals as equivalent to drawing resonance structures. Similarly, students from the organic chemistry course that required resonance structures as a characteristic of aromatic compounds did not consider the dispersion of electrons throughout a  $p$  orbital continuum. Thus, the students’ ways of understanding resonance became an important consideration for analysis.

#### Students’ Ways of Understanding Resonance Structures<sup>21</sup>:

Students’ ways of understanding resonance structures fell into two main categories: one related to the mechanics of drawing resonance structures, and the other related to the underlying structural meaning of the combined resonance structures. Not all students’ ways of understanding could be identified due to insufficient

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<sup>21</sup> Resonance structures are different Lewis Structure (see Table 4-7) representations that, combined represent the overall hybrid structure of a molecule.



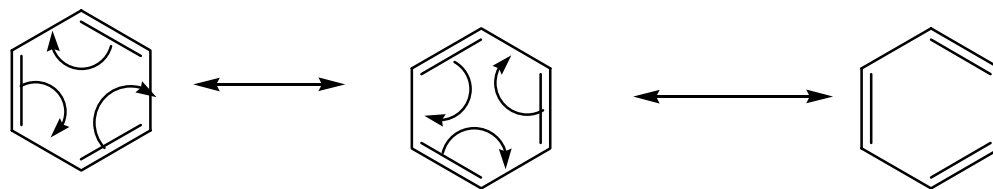
evidence. For example, Student 11B could not draw the resonance structures of benzene and provided the following claims regarding resonance structures:

“Double bonds exist all around the ring and makes the bonds that much stronger.” And later, “Resonance is delocalized throughout the ring and don’t exists.” (Student 11B)

The first quotation could be interpreted to mean that the electrons in the double bonds are distributed around the ring, or that there are three double bonds around the ring.

The second quote referred to delocalization but did not elaborate on *what* was delocalized. As a result, the analysis of Student 11B’s way of understanding resonance proved inconclusive.

Students’ ways of understanding resonance, with regard to the mechanics of drawing resonance structures, comprised two main components: namely, moving the double bonds and/or lone pairs of electrons by “pushing electrons” with or without producing the sufficient number of resonance structures. The sufficient number related to a memorized number (Students 4B, 6B, 7B, 8B, 9B and 10B). This way of understanding was designated *moving symbols to produce quantity*. Another way of understanding the mechanics of drawing resonance structures was designated *moving symbols to produce quality*. For these students (Student 5B and 12B) as well as for chemists, the goal when drawing resonance structures was to draw a sufficient number so that each structure corresponded to a unique symbolic representation of the molecule.



**Figure 4-5: Resonance Structures of Benzene**

Figure 4-5 demonstrates that benzene has two unique contributing resonance structures. The structure on the far right is the same as the structure on the far left and is, therefore, not a unique structure. Students with the way of understanding *moving symbols to produce quality* paid close attention to each of the contributing resonance structures as unique representations.

The resonance structures in Figure 4-4 from Student 4B provided part of the evidence that her way of understanding resonance was *moving symbols to produce quantity* even if the structures didn't make sense. She did not like writing resonance structures and avoided them when she could because she felt that she did not have skill in drawing the resonance representations.

Students' ways of understanding the structural meaning of the resonance structures fell into two main categories. One category of ways of understanding, *separate oscillating entities*, revealed that students believed resonance structures were separate entities that the molecule oscillates very quickly between (Students 3B, 4B, 7B and 10B). As a result, two students (3B and 10B) with the *separate oscillating entities* way of understanding associated the ability to form resonance with time. For example, Student 3B explained that she did not have to draw resonance structures for the intermediate of the bromination of benzene (see Figure 4-13) because "this here

gets deprotonated so fast that it [drawing resonance structures] shouldn't be important." Student 10B stated that "Both resonance forms are, well, both are happening but neither are happening at the same time kind of thing."

Another way of understanding the structural meaning of resonance structures was that of a *hybrid structure of all the resonance forms*<sup>22</sup> (Students 5B, 6B and 9B). Student 9B stated that resonance structures showed that "the electrons are now resonating throughout the system equivalently." Student 9B explained her use of the term "resonating" to mean that the electrons "travel all the way around" the ring. Student 6B referred to each structure in the bromination of benzene as "contributing to the overall structure." Student 5B stated that a resonance structure is a representation of "where the electrons could be" but that "the electrons actually spread themselves throughout the ...ring."

**Table 4-2: WoU Resonance**

	<b>WoU Category</b>	<b>Students</b>
Mechanics of Resonance	<i>Moving symbols to produce quantity</i>	4B, 6B, 7B, 8B, 9B, 10B
	<i>Moving symbols to produce quality</i>	5B, 12B
Interpretation of Resonance	<i>Separate oscillating entities</i>	3B, 4B, 7B, 8B, 10B
	<i>Hybrid structure of all resonance forms</i>	5B, 6B, 9B

<sup>22</sup> While this way of understanding is more correct than the *separate oscillating entities*, chemists also consider the stability of each individual resonance structure when accounting for the contribution towards the overall structure. In other words, each individual resonance structure may not contribute equally to the actual resonance hybrid structure.

Table 4-2 summarizes the various ways of understanding associated with the concept of resonance. Students were only associated with a given category if sufficient evidence was found to support their inclusion.

Students from both organic chemistry courses<sup>23</sup> mainly used the reference to these structural features as a characteristic of aromatic compounds included in the “three things” required for aromaticity. Table 4-3 provides a summary of students’ ways of understanding the characteristics of aromatic compounds.

**Table 4-3: WoU Characteristics of Aromatic Compounds**

<i>Ordered list of three characteristics favoring Hückel’s Rule</i>				
<b>1. Hückel’s’ Rule</b>	<b>2. Symbolic Characteristics</b>	<b>3. Structural Characteristics</b>		
6C-exclusively	Cyclic	3B, 9C		
10B-only two characteristics	Conjugated double bonds	3B, 6B, 7B, 8B, 11B, 9C	Resonance	6B, 7B, 8B, 10B, 11B
All other students	Sp <sup>2</sup> hybridized	4B, 5B, 9B, 12B	Continuum of p orbitals	4B, 5B, 9B, 12B

Student 6C and 10B could not be considered as having a way of understanding consistent with an *ordered list of three characteristics favoring Hückel’s Rule*. They are included in the table in order to provide a full account of each student’s ways of understanding the characteristics of aromatic compounds. Students 3B and 9C held a way of understanding that incorporated two symbolic characteristics as part of the “three things” rather than the typical one from each category.

The students in this study did not always apply their ways of understanding the characteristics of aromatic compounds to the task of identifying aromatic compounds.

<sup>23</sup> Recall that students in the second group of interviews were recruited from two different instructors teaching the same second quarter organic chemistry course content.

They would use the drawing of either all the  $p$  orbitals or resonance structures, or identifying hybridization of atoms in the ring as a heuristic to aide in their identification of aromatic compounds. As a result, students would ignore most of their three characteristics of aromatic compounds in favor of the heuristic approach.

### Identifying Aromatic Compounds

This section presents results on students' ways of understanding the identification of aromatic compounds and consists of three subsections addressing 1) students' identification of aromatic compounds considering structural characteristics, 2) identification by analogy of recognized compounds from past experience, and 3) the universal application of Hückel's Rule. It is important to note that these subsections are not mutually exclusive, however, the categorization of students' ways of understanding is a result of observed student preferences with some overlap between categories depending on the structure before the student.

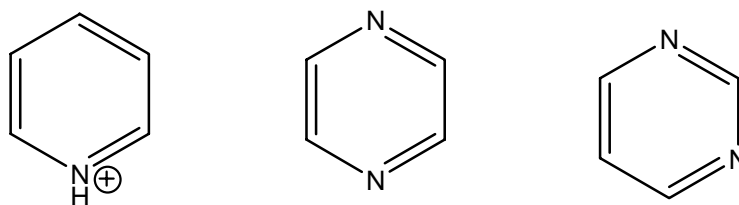
Students' ways of understanding relative to the identification of aromatic compounds was segregated into three categories: recognition of the structure as aromatic by recall or analogy, identification based on structural considerations, and the universal application of Hückel's Rule. As part of the interview, all of the students had to identify the aromatic compounds from a selection of 13 different compounds. Based on evidence from earlier interviews, students 8B, 9B, 10B and 11B were given an additional five compounds to identify as aromatic or not. The categories in this section emerged from an analysis of students' justifications for their assignment of aromaticity that were not consistent with their ways of understanding the

characteristics of aromatic compounds. Consequently, a second set of categories, based on what students did and said during the identification portion of the interview, was created.

#### Recognition of Structure by Recall or Analogy

Four students (4B, 6B, 10B and 6C) used recognition or analogy to identify aromatic compounds. This was the least prevalent category for the interviewees due to the fact that most of the students were not familiar with a majority of the structures presented. The graduate teaching assistant, Student 6C, had the necessary background to identify most of the structures by recognition. As a result, this was his prevailing method of identification.

Rather than focus on the method of identification, this category originated from the desire to address the students' way of understanding aromaticity by *analogous structures*. The remaining three students did not identify structures as aromatic based mainly on recognition but by viewing certain structures as analogous to benzene.



**Figure 4-6: Aromatic Structures from Interview Sheet 5b**

Students 4B, 6B and 10B viewed the structures in Figure 4-6 as analogous to benzene and identified them correctly as aromatic. In addition to the way of understanding

aromaticity by analogy, Students 6B and 10B also attended to structural considerations for the identification of aromatic.

#### Identification Based on Structural Considerations

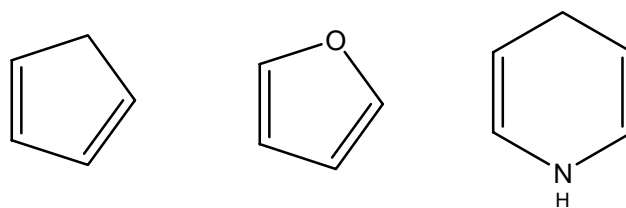
Although structural considerations were an integral part of the “three things” that characterize a compound as aromatic, only four students (5B, 6B, 8B and 10B), concerned themselves with structural features when identifying aromatic compounds. The two structural characteristics of aromatic compounds that students relied on to identify the aromatic compounds were (a) the generation of resonance structures (Students 8B and 10B) and (b) hybridization with the goal of determining the presence of a continuum of pi electrons (Students 5B and 6B). It is worth noting that Student 6B used hybridization and *p* orbital distribution, even though he was enrolled in the course that emphasized resonance structures, not the “continuum of *p* orbitals.”

There were a total of seven aromatic compounds among the thirteen structures given. Student 5B used hybridization exclusively, drawing the *p* orbitals on each atom of the ring. Student 10B used resonance twice (see Appendix 3, Structures 4a-5 and 4c-3) to aid in identification of aromatic compounds, while Student 6B used hybridization once (see Appendix 3, Structure 4a-5). In each of these instances, the student relied solely on the structural features to identify the aromatic compound.

Student 8B used resonance and Hückel’s rule to identify three aromatic structures (see Appendix 3, Structures 4a-5, 4c-2 and 4c-3). Structure 4c-2 (see Appendix 3 or Figure 4-20) was cyclopentadienyl cation, a structure that is not aromatic, having only four *pi* electrons. Student 8B designated Structure 4c-2 as

aromatic because she could draw resonance structures “distributing the charge throughout the ring.” The structure common to the above students was structure 4a-5 which was pyrrol-1-ide (see Figure 4-2).

Even though most students did not attend to structural features to identify aromatic compounds, eight of the twelve students (4B, 5B, 6B, 7B, 8B, 9B, 10B, and 6C) used structural features to justify why a structure was *not* aromatic. In these cases, the students used mainly hybridization for the determination of the structures in Figure 4-7 as non-aromatic.



**Figure 4-7: Student Designated Non-Aromatic Compounds**

All eight students observed that the top carbon of the first structure was  $sp^3$  hybridized and, therefore, not aromatic. Only four of these eight (4B, 5B, 7B, and 9B) designated the last structures as not aromatic based on hybridization. The other four students (6B, 8B, 10B and 6C) focused on an inability to draw resonance structures. For the middle structure, only four students (6B, 7B, 9B and 10B) designated that the oxygen in furan as  $sp^3$  hybridized and, therefore not aromatic. Three of the remaining four students (4B, 5B, and 8B) used Hückel’s Rule. Student 6C recognized furan as aromatic. Only Students 7B and 9B consistently used hybridization as their justification for these compounds being non-aromatic.



Students' interpretation of these structures having  $sp^3$  hybridized atoms often led the students to choose to use structural characteristics to justify their determination of these compounds as non-aromatic. For students who consistently evaluated structural features (5B, 6B, 7B, 8B, 9B and 10B), the way of understanding the identification of aromatic compounds was characterized as attending to *structural considerations*. The designation of the way of understanding referring to structural features does not imply that students were attending to the actual molecular structure. These students used hybridization or resonance in their designation of aromaticity. As stated in the discussions of both of these concepts, students' ways of understanding hybridization and resonance were not consistent with the students attending to the molecular structure; they were manipulating symbols.

The above two categories, identification based on recognition or using structural considerations, represent the less frequently used methods of determination of aromatic compounds. Instead, most students used Hückel's Rule both to identify aromatic compounds, as well as to justify why a compound was not aromatic, even if Hückel's Rule did not apply or was not necessary.

#### Universal Application of Hückel's Rule

All students interviewed for this study used Hückel's Rule at some point during the interview. Students' ways of understanding Hückel's Rule,  $(4N + 2)$ , was related directly to a counting act involving the counting of  $\pi$  electrons. Some students (4B, 5B, 11B and 9C) counted any electrons designated as being in  $p$  orbitals as part of the  $\pi$  electrons. The designation relied on the students' ways of understanding

hybridization. As a result, pyrrol-1-ide was identified as not aromatic by Student 4B because it had eight  $\pi$  electrons resulting from the designation of nitrogen as  $sp$  hybridized (counting only the two bonds). Student 9C designated pyrrol-1-ide as not aromatic because it has four  $\pi$  electrons resulting from the designation of nitrogen as  $sp^3$  hybridized.

One student (6B) chose to count  $p$  orbitals in a self-made algorithm to determine the number of  $\pi$  electrons. His algorithm consisted of counting the number of atoms in the conjugated ring system, after which he added one if an anion was present, or subtracted one if a cation was present. This algorithm was applicable for five ring systems of carbon atoms from which it was devised. Applying this algorithm to five-membered rings with one nitrogen atom present provided correct identification for two of three structures.

The *universal application of Hückel's Rule* way of understanding was confirmed when half of the students presented with Interview Sheet 4d (Appendix 3) designated cyclodecapentaene, (see Appendix 3, Structure 4d-1) with ten  $\pi$  electrons, as aromatic. In the two dimensional representation of cyclodecapentaene, the structure appears planar even though it is not and is, therefore, not aromatic. Students also designated pyrene, a clearly benzenoid structure of five fused benzene rings, (see Appendix 3, Structures 4d-3 and 4d-4) and pentalene (see Appendix 3, Structure 4d-5), two fused cyclopentadiene rings, as not aromatic even though they are because they did not fit Hückel's Rule.

The *universal application of Hückel's Rule* indicated a way of understanding the identification of aromatic compounds as a *counting act* with the structure having the “right number of electrons” (those being typically 2 and 6 *pi* electrons) being identified as aromatic. For most students, Hückel's Rule is the only measure of aromaticity ignoring symbolic characteristics.

The *universal application of Hückel's Rule* resulted in students' ways of understanding aromaticity, in general, as belonging to cyclic molecules with double bonds that have the correct number of *pi* electrons. The stability of aromatic compounds and structural characteristics became secondary factors in students' ways of understanding aromaticity.

**Table 4-4: WoU Identification of Aromatic Compounds**

<b>Category</b>	<b>Students</b>
<i>Analogous Structures</i>	4B, 6B, 10B, 6C
<i>Structural Considerations</i>	5B, 6B, 7B, 8B, 9B, 10B
<i>Universal Application of Hückel's Rule</i>	All students with the exception of 10B

The categories in Table 4-4 are ways of understanding based on categories that emerged from the data. Students were designated into each category based on their behavior during the interviews. It was not the intent of the analysis to categorize individual students' ways of understanding aromaticity based on an overall analysis of the interview as a whole unit. The ways of understanding in Table 4-4 are products of the mental act of interpreting when students were engaged in the task of identifying aromatic compounds. If the student recognized the compound as aromatic, no further action was considered either by the student or the researcher.

In order to study the application of the concept of aromaticity in relation to students' ways of understanding aromaticity, half of the interview questions involved problem solving for electrophilic aromatic substitution reactions.

### **Students' Ways of Understanding Electrophilic Aromatic Substitution Reactions**

During the student interviews in Phase I, there were several opportunities to observe students' ways of understanding electrophilic aromatic substitution (EAS) reactions. The results of these observations fall into two main categories—bromination of benzene, and directing effects for subsequent EAS reactions. The bromination of benzene provided problems with which to probe students' ways of understanding a single EAS reaction of benzene, and their ability to apply their understanding of aromaticity in organic reactions. Students' ways of understanding the need for a catalyst, other students' variant bromination methods, and the interpretation of the bromination reaction method, are presented in this section.

The second section for EAS reactions focuses on students' ways of understanding directing effects of subsequent EAS reactions. In other words, it will focus on students' ways of understanding the directing effect<sup>24</sup> of the substituent on a mono-substituted benzene ring when it undergoes further substitution. Students' ways of understanding the directing effects are associated with their understanding of whether the benzene ring is activated or deactivated as a result of the substituent on the ring. Students either ignored activating and deactivating effects, memorized the

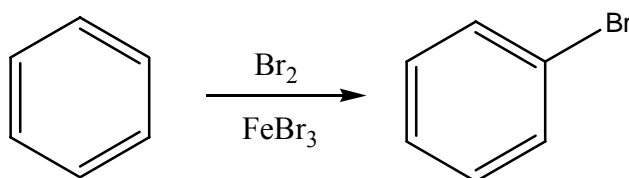
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<sup>24</sup> The directing effects of a substituent of the benzene ring determine not only where on the ring a new substituent may react, but also how susceptible the ring is to further reaction. For example, benzene rings that have activating groups, like aniline, tend to be very reactive towards EAS and result in poly-substitution products.

activating and deactivating effects, or created some meaning associated either with symbolic manipulations or probability of reaction.

### Bromination of Benzene

Bromination of benzene provides the starting point from which students had the opportunity to apply their understanding of aromaticity, as well as directing effects. Students were asked to give the reactants, to show the reaction mechanism, and to justify their responses. In the interview question asking students to show the reaction for the bromination of benzene, all the students interviewed understood that they would begin with benzene as one of the reactants and end with bromobenzene as the product. Most of the interviewed students employed the use of a catalyst (either  $\text{FeBr}_3$  or  $\text{AlBr}_3$ ) for the bromination of benzene (see Figure 4-8).

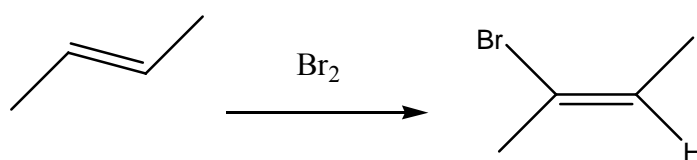


**Figure 4-8: Bromination of Benzene**

Two students (Students 6C and 4B) used heat and/or light with bromine and benzene while one student (Student 12B) used benzene and  $\text{HBr}$  only. Although each student's way of understanding is based on his or her specific background, the results will provide an amalgamated presentation of their ways of understanding for specific sets of circumstances. The first set of circumstances occurred with students who used heat, light or other reagents rather than a catalyst in the bromination of benzene.

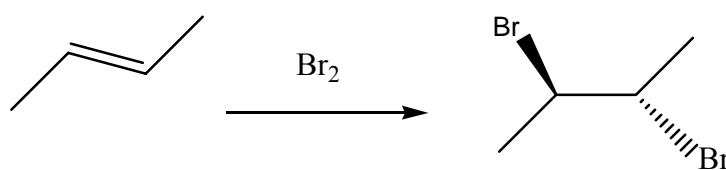
Students' Ways of Understanding the Use of Heat, Light or Other Reagents

Of the three students who *did not* use a catalyst, one was a graduate teaching assistant (TA), Student 6C, who was currently teaching discussion sections in the third quarter in an organic chemistry sequence. This TA exhibited evidence that he did not understand the structural stability of benzene. For example, after writing the reagents ( $\text{Br}_2$  and heat) for the bromination of benzene, he was asked what the bromination of a simple alkene would look like. The first product that he showed for the bromination of *trans*-2-butene was an implausible substitution product where one of the hydrogen atoms on the double bond was replaced by bromine to form *trans*-2-bromo-2-butene.



**Figure 4-9: Electrophilic substitution of *trans*-2-butene**

Upon further questioning, he also wrote the correct product of an addition of bromine across the double bond to form *meso*-2,3-dibromobutane.



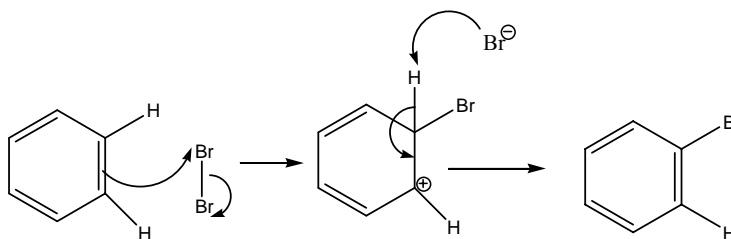
**Figure 4-10: Nucleophilic addition of *trans*-2-butene**

After consideration, he chose the nucleophilic addition product as the major product stating, “if it can happen, it will happen. It’s just a matter of proportion in organic chemistry.” Referring back to bromination of benzene, Student 6C noted that removing a hydrogen rather than adding another bromine on benzene resulted in a

restoration of aromaticity that to him meant having six *pi* electrons in a ring.

Therefore, Student 6C correctly noted that the only product for bromination of benzene would be the mono-substituted bromobenzene.

When comparing the bromination of benzene with the bromination of the alkene, Student 6C commented that “it’s harder to add Br to benzene because you have an intermediate that doesn’t have aromaticity.” It is important to note the term “add” as used by this subject, since many students view EAS reactions as an *addition* of a substituent onto the benzene ring, rather than a *substitution*. Only three out of the twelve students explicitly stated that the reaction was a substitution reaction where bromine substituted for a hydrogen atom. Two students explicitly stated that the reaction was electrophilic addition because of the addition of bromine onto the benzene ring. Most of the remaining students referred to the reaction either as “catalyzed” or merely as “bromination” when asked about the class of reaction. This is another indication that students lose track of the implicit hydrogens<sup>25</sup>. This is apparent in the reaction mechanism for the bromination of benzene proposed by Student 6C.



**Figure 4-11: Student 6C Bromination of Benzene Mechanism**

To show the mechanism, Student 6C drew out the two hydrogens in the immediate area of reaction on benzene. Typically, only the hydrogen being

<sup>25</sup> Refer to Table 4-7 for examples of symbolic representations in organic chemistry.

substituted in benzene would be explicitly indicated in the intermediate resonance-stabilized structures of the mechanism. In Student 6C's intermediate, bromide removed one of the hydrogens, resulting in the bromobenzene product with only one hydrogen drawn on the final product. Student 6C did not mention resonance stabilization of the intermediate cation, nor the fact that his product did not exactly match his original representation of bromobenzene with all hydrogens implicit. He also ignored heat in his mechanism. According to Student 6C, heat was needed because "benzene is stable and doesn't want to give up its aromaticity" which it did in the intermediate step.

One of the students (3B) who did use a catalyst suggested that the reaction could also occur if "you add a lot of heat or something like that...but at normal temperature I'm assuming you need to use the  $\text{FeBr}_3$ ." This *use of heat* as an alternative to a catalyst suggests that the student views addition of heat as a method to increase the likelihood of reaction in an otherwise unreactive system. Student 3B exhibited a way of understanding the characteristics of aromaticity as being "very stable and ...very unreactive" without exhibiting evidence that she knew why.

Likewise, Student 6C did not exhibit evidence that he understood the delocalized electrons as grounds for aromatic stability. He did hold the way of understanding associated with Hückel's Rule indicating that six *pi* electrons in a ring meant that the ring was aromatic. He also recognized benzene as the "quintessential aromatic structure."



Another student (4B) used *heat or light* with bromine “to impose a radical reaction.” Her reason for why bromine alone would not work was “because benzene is so stable because of the resonance forms that it won’t react at all.” As a result, she understood that something needed to be added with bromine to get a reaction. She had a strong preference for drawing benzene with the circle in the center of the ring rather than showing the double bonds. Nearly all of her representations were drawn this way. When rationalizing the directing effects, she drew two resonance forms showing two double bonds in the ring, but did not relate these back to her original proposal of a free radical mechanism. She could not draw the free radical reaction mechanism nor complete the resonance representations of the directing effects of bromine. Student 4B lost track of the implicit hydrogens and referred to the reaction as adding bromine to the benzene ring. Even in the resonance forms that she drew, she did not include any hydrogen atoms (see Figure 4-4)

The student using HBr (Student 12B) did not address any special reaction conditions as a result of benzene’s aromatic character. He chose not to use Br<sub>2</sub> because he “only want[ed] to add one bromine to the ring.” He could not, however, show the mechanism. Student 12B was the only student of the 12 interviews analyzed in this study who did not address the aromatic character of benzene. This disregard for the aromatic character of the ring was typical of the first group of interviewees with only two students, 3C and 8C, using iron (III) bromide with bromine. In addition, one student remembered that something more needed to be added with bromine for the reaction to proceed, but could not remember the reagent. This idea that something

more than bromine must be added to get bromination of benzene was also present in those students who chose to use a catalyst with bromine.

### Students' Ways of Understanding the Need for a Catalyst

Students who remembered that iron (III) bromide or aluminum bromide were involved in bromination of benzene had various interpretations of why they were used. Of the 12 interviews, 9 students used one of the two catalysts, with preferences dependent on the course instructor and the material presented during lecture.

One of the nine students, Student 9C, an undergraduate teaching assistant, stated that  $\text{FeBr}_3$  stabilized the transition state to prevent addition of both bromine atoms to the ring; yet, he could not draw the reaction mechanism.

Student 11B gave the following reason for the use of aluminum tribromide, but did not mention that it acted as a catalyst:

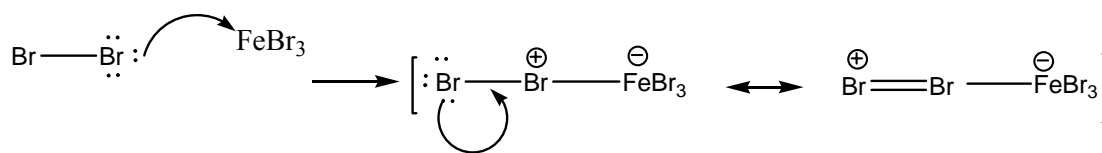
The benzene ring is stable enough so it won't react. The aluminum tribromide activates the bromine, this actually becomes a negative charge [*refers to Al attached to bromine*] and it [*bromine*] becomes electrophilic. The *pi* electrons can add, can nucleophilic attack the electrophilic bromine. (Student 11B)

This student's way of understanding  $\text{AlBr}_3$  was solely as an activator of bromine to make it more susceptible to attack from the *pi* electrons in benzene. He did indicate that the aluminum atom became negatively charged when it interacted with bromine, but did not indicate appropriate formal charges on either bromine atom, even though his explanation referred to bromine as electrophilic.

The remaining seven students, who used  $\text{FeBr}_3$  or  $\text{AlBr}_3$ , did explicitly say that it functioned as some sort of catalyst. Two of those seven, Students 3B and 7B, merely

stated that a catalyst was needed but could not explain why beyond the *memorized fact* that benzene, as an aromatic compound, was stable and unreactive. Both of these students were able to draw the reaction mechanism in what would be considered a relatively correct fashion.

The five students who used a catalyst (Students 5B, 6B, 8B, 9B and 10B), mentioned that the catalyst was needed to “activate”, “polarize” or create a “positive charge” on bromine. When asked if the reaction would work without the catalyst, one student, Student 8B, said, “I’m not sure if it would work without  $\text{AlBr}_3$  but it speeds it up.” This comment indicated that the student understood a catalyst as increasing the *rate of reaction* rather than increasing the *likelihood* of the reaction. All five of these students focused on the need to *create a more positive bromine* atom without focusing on the reason behind that need. Their responses, explaining why the catalyst was needed, focused on the creation of a bromine entity with varying degrees of positive character. Students 9B showed the full positive charge on the reactive bromine as one of two resonance structures (see Figure 4-12) for the catalyst complex, while most indicated that the outer reactive bromine had partial positive character due to the catalyst.



**Figure 4-12: Student 9B Activation of Bromine**

The majority of students temporarily ignored the aromatic character of benzene as the main reason for needing a catalyst. Thus, their way of understanding the need for the catalyst was as a generator of positive character on the outer bromine atom in the  $\text{Br}_2$  molecule after it coordinated to the catalyst. Student 10B was an exception, as he related the partial positive character as making “bromine more electron deficient and more susceptible to attack from the electron rich benzene ring.”

Only two other students (3B and 7B) who had *memorized* the need for a catalyst, and not the function of the catalyst, referred specifically to the aromatic character of benzene to explain why. This reference was based on a superficial understanding of aromaticity.

Focusing on generating positive, electrophilic character on bromine for some students became the main characteristic of the reaction mechanism. In those cases, the students continued to manipulate the symbols with primarily the bromobenzene product in mind.

#### Students' Ways of Understanding the Bromination of Benzene Reaction Mechanism

The eight students who used a catalyst produced what was deemed as four classes of reaction mechanisms for the bromination of benzene. Based on whether the students drew the resonance structures of the reaction intermediate or whether they showed the regeneration of the catalyst. The four classes are: 1) showing resonance intermediate with regeneration of the catalyst; 2) showing resonance intermediate without regeneration of the catalyst; 3) not showing resonance intermediate with

regeneration of the catalyst; and 4) not showing resonance intermediate without regeneration of the catalyst.

Showing Resonance Intermediate with Regeneration of the Catalyst:

Three of the eight students (6B, 7B, 10B) using a catalyst included all three of the resonance structures of the intermediate as well as the regenerated catalyst. Two of these students, (6B and 7B) identified the reaction specifically as an electrophilic aromatic substitution reaction where hydrogen was exchanged for bromine on the benzene ring. Although both of these students could state the *name* of the reaction, their way of understanding EAS reactions primarily focused on the activated bromine, giving it the role of attacking the benzene. The following excerpt from Student 6B is an example of the reasoning that both of these students demonstrated in the interviews:

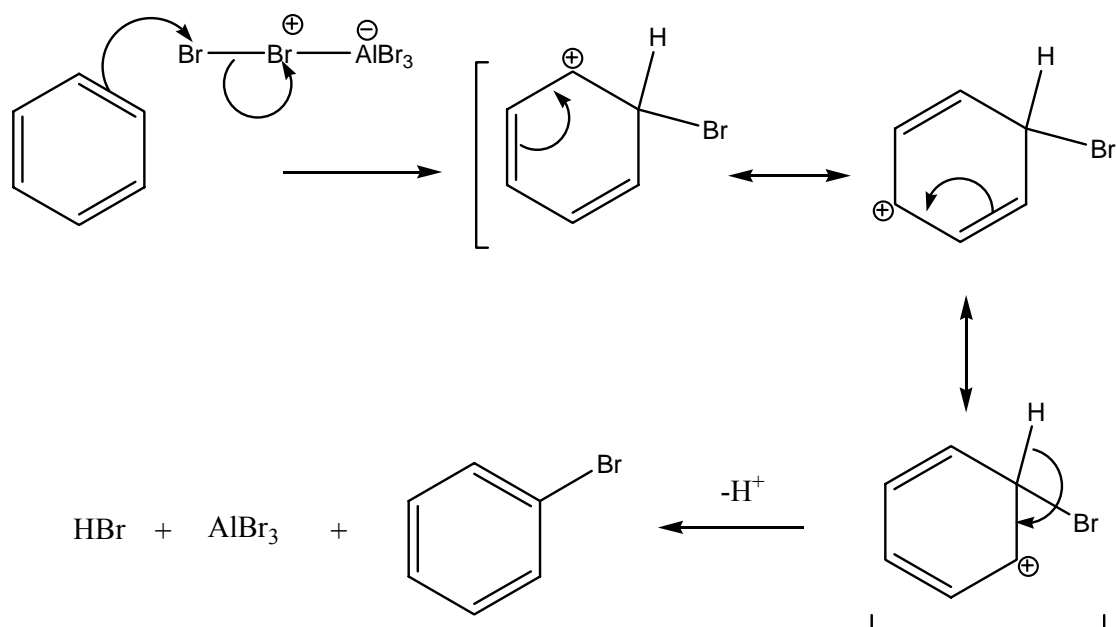
Electrophilic aromatic substitution. Meaning you want an electrophile to attack which means you want this [refers to benzene] to have nucleophilic properties.(Student 6B)

The more appropriate designation in organic chemistry would be to refer to the entity with the greater electron density, in this case benzene, as attacking the entity that is electron deficient. However, the textbook these students used (Vollhardt and Schore, 1999) did designate the electrophile as the attacking entity. This inconsistency from the typical designations in organic chemistry was a source of frustration for Student 10B.

Student 10B did not specify the name of the reaction but did indicate that bromine replaced one of the hydrogens on the benzene ring. He explained that naming reactions was not important to him, but rather he focused on understanding why the

reaction proceeded the way it did by looking at the direction of electron flow from electron rich environments to electron deficient environments. This was his overall way of understanding organic chemistry reactions.

Figure 4-13 shows a general representation of the reaction mechanism given by these students. The products of the reaction are correct, even if the reaction mechanism is not completely correct from a chemist's perspective.



**Figure 4-13: Bromination of Benzene Reaction Mechanism**

Individual student variation of the mechanism shown in Figure 4-13 included Student 6B showing  $\text{H}^+$  leaving by itself to regain the aromatic character of the ring with subsequent splitting of  $\text{AlBr}_4$  to form  $\text{HBr}$  and  $\text{AlBr}_3$ . Student 7B wrote incorrectly the positive charge on aluminum and a negative charge on bromine in the first step. Student 10B did not draw the hydrogen atom on the carbon with bromine, but rather

he drew the intermediate cation in that position, resulting in the generation of three incorrect resonance structures.

While Student 10B demonstrated the result of losing track of the implicit hydrogens, all three of these students exhibited this difficulty at some point during the interview. Student 7B created a resonance structure with two pentavalent carbons on pyrene (See Appendix 3, Interview Sheet 4d, Structures 4d-3 and 4b-4) while Student 6B could not determine whether the anionic carbon in cyclopentadienyl anion had one or two hydrogens (See Appendix 3, Interview Sheet 4c, Structure 4c-3).

Despite the fact that Student 10B lost track of the implicit hydrogens, he exhibited a strong understanding of the need for the catalyst, in relation to the aromatic character of benzene (see page 112). Student 10B justified the need to regenerate the catalyst as a characteristic of catalysts. His way of understanding the resonance intermediate was that of a hybrid structure of the three resonance structures.

Student 6B and Student 7B exhibited the same way of understanding the need to regenerate the catalyst, but their way of understanding the intermediate resonance structures was not that of a hybrid structure. Student 6B specifically referred to the intermediate as an allylic system that “transferred electrons toward the positive charge.” This reference coincided with his showing the arrow from a double bond in the intermediate towards the cation. Student 7B indicated that the electrons were “resonating throughout” the intermediate, showing a movement from one resonance structure to another in a motion indicating movement of the electrons towards the positive charge in each of the resonance structures. This indicated that Student 7B held

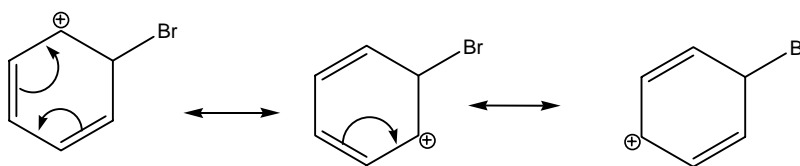
a way of understanding resonance as oscillating between structures rather than representing a hybrid structure. The *oscillating* way of understanding resonance was also present for students who did not regenerate the catalyst but did draw the intermediate resonance structures.

Showing Resonance Intermediates without Regenerating the Catalyst:

Two Students (8B and 9B) showed the resonance structures for the intermediate but did not show a regeneration of the catalyst. Both of these students held the *oscillating* way of understanding resonance. Student 8B did not finish the reaction mechanism because she had trouble drawing all of the resonance structures. She became frustrated because she knew that there were three structures that she “had to draw” but could not come up with what she felt was an appropriate third structure. She did draw all three structures designated in the example of the reaction mechanism in Figure 4-13 but crossed out the structure with the cation opposite the bromine stating, “I’m trying to get the positive charge to move around the ring but I’m doing something wrong so it’s not working.”

The structure that Student 8B created appeared out of order to her because she moved two double bonds in the first resonance structure. The result being that she crossed out the third structure (see Figure 4-14). Not only did Student 8B hold the *separate oscillating entities* way of understanding resonance, but she also showed clear expectations on exact order and identity of the resonance structures indicating that she also held the *moving symbols to produce quantity* way of understanding the mechanics of resonance.





**Figure 4-14: Student 8B Bromination Resonance Intermediates**

As seen in Figure 4-14, Student 8B also did not draw the hydrogen attached to the carbon with bromine, resulting in designating the reaction as “electrophilic addition because you’re adding bromine to the ring.” Because she struggled to draw the resonance structures in what she viewed was the correct order, she did not finish the mechanism and did not show the bromination product.

Student 9B also did not regenerate the catalyst, but did draw out the resonance structures indicating a way of understanding resonance consistent with the oscillating electrons, rather than a hybrid structure. Like Student 10B, she recognized the substitution of one of the hydrogen atoms on benzene for bromine, but did not remember the EAS name. Student 9B’s focus remained on the aromatic ring and the goal to re-establish aromaticity by removing the hydrogen as the final step in the reaction. Analysis of Student 9B’s data revealed that when the student’s goal was focused on the products, representing all of the intermediate resonance structures was ancillary.

Regenerating the Catalyst without Showing the Intermediate Resonance:

Only one student (3B) drew a reaction mechanism that focused on the regeneration of the catalyst over the representation of the full mechanism, including all intermediate resonance structures. Aromaticity was a concept that had little meaning for her.

Because this [*refers to benzene*] is a very very stable compound and it's not going to want to, um, give up its aromaticity, or its whatever, its, uh, like this configuration.

As a result of her way of understanding aromaticity based on a recognizable symbolic structure, Student 3B focused on regenerating the catalyst in her mechanism rather than the driving force of the reaction in re-establishing the aromatic character of the benzene ring. To further support the effect of her weak understanding of aromaticity, as noted in the section on interpreting the catalyst (see page 110), Student 3B incorrectly believed mentioned that adding heat would result in bromination if a catalyst wasn't available.

It is not only the effect of a student's way of understanding aromaticity that influences a student's representation of a reaction mechanism, but understanding from other segments of organic chemistry as well.

Neither Regenerating the Catalyst nor Showing Intermediate Resonance:

Two students (5B and 11B) represented the reaction mechanism for bromination of benzene with neither intermediate resonance structures nor regeneration of the catalyst. Student 11B incorrectly stated that the reaction was an electrophilic addition reaction because bromine was added to the ring, but otherwise he did not engage in further discussion of the mechanism.

Student 5B recognized the reaction as a substitution of one hydrogen for bromine but confused the mechanism with an  $S_N1$  reaction. The generation of a carbocation in a reaction that had two steps prompted a way of understanding the reaction mechanism as  $S_N1$ . Student 5B reconciled the nucleophilic component of the

$S_N1$  with benzene acting as a nucleophile in the bromination reaction. Further questioning regarding her reaction mechanism resulted in the following interaction.

**Student:**  $S_N1$  is single step nucleophilic substitution. It's not single step. It's a single nucleophile. There's one thing that reacts with it. ...For this? How is it nucleophilic substitution?...I was so bad at this...I didn't understand it. I just did it.

**Interviewer:** Did you do well?

**S:** I got an A. (laughs)...The point of a nucleophilic substitution is to replace. So something needs to come in and replace it.”

The above interaction led to a discussion on the need for iron (III) bromide.

**Student:** You need  $FeBr_3$  to break  $Br_2$  apart. The only other way to do that is with light to form a radical. Benzene, I guess, under crazy situations would form a radical. But why would it want to?

The *breaking apart and reassembling* way of understanding substitution reactions was consistent with what most students observed when learning  $S_N1$  reactions. In  $S_N1$  reactions, the first step could be viewed as breaking apart a molecule, while the second step resulted in a reassembly to a different molecule. Student 5B viewed the re-establishing of aromatic character analogous to reassembling the two parts in an  $S_N1$  reaction. The breaking apart of bromine was analogous to the first step of an  $S_N1$  reaction.

Although Student 5B did not show the resonance structures for the intermediate, her reaction mechanism appeared consistent with that represented earlier in this chapter (see Figure 4-13). Her rationalization of the reaction being nucleophilic substitution rather than electrophilic aromatic substitution would not have been discovered in a “normal” testing situation. This provides a clear example of a student's

ability to obtain a correct response based on undesirable ways of understanding. As a result these rationalization patterns, Student 5B was able to excel in the course in spite of her weak understanding of the material.

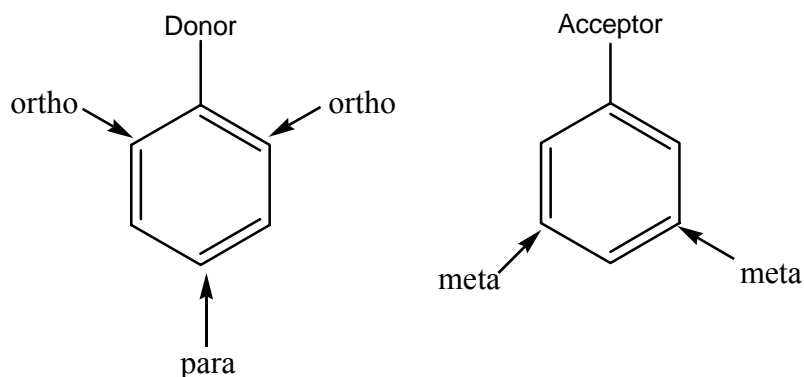
**Table 4-5: Students' WoU Bromination of Benzene**

Category	Students	Student WoU
Use of heat, light, or other reagent	3B, 4B, 6C, 12B	<i>No catalyst but heat (6C)</i> <i>Yes catalyst or heat (3B)</i> <i>Heat to Impose a radical rxn (4B)</i> <i>HBr without catalyst (12B)</i>
Need for a catalyst	3B, 5B, 6B, 7B, 8B, 9B, 10B, 11B, 9C	<i>Generator of a positive charge (5B, 6B, 8B, 9B, 9C, 11B)</i> <i>Electron deficient (10B)</i> <i>Memorized fact (3B, 7B)</i>
Bromination of Benzene reaction mechanism	3B, 5B, 6B, 7B, 8B, 9B, 10B, 11B	<i>Using a catalyst (6B, 7B, 10B)</i> <i>No regeneration of the catalyst (8B, 9B)</i> <i>Regeneration with no intermediate (3B)</i> <i>No regeneration and no intermediate (5B, 11B)</i>

#### Directing Effects of Benzene Derivatives

The ability to rationalize patterns became apparent when students were required to discuss reasoning behind the results of substitution reactions on benzene derivatives.<sup>26</sup> Directing effects of mono-substituted benzene derivatives refers to the preferred positions on the ring during subsequent EAS reactions. The directing substituents can either activate the benzene ring (make it more susceptible to reaction than unsubstituted benzene) or deactivate the benzene ring. The following schematic represents the directing positions of two generic substituents:

<sup>26</sup> A benzene derivative is a benzene ring that already has some degree of substitution. Bromobenzene is an example of a benzene derivative.



**Figure 4-15: Benzene Derivative Directing Positions**

As seen in the Figure 4-15, above, substituents that can donate an electron pair direct to the ortho and para positions, while substituents that can accept an electron pair direct to the meta positions. The relationship between the electron donating or accepting ability of a substituent, and the placement on the ring of another substituent, are due to the electronic characteristics of the intermediates. Typically substituents that direct to the ortho and para positions are ring activating while substituents that direct to the meta positions are ring deactivating. The noted exception is the halides that direct to the ortho and para positions but are ring deactivating.

Students in organic chemistry are often asked to predict the major products of EAS reaction on benzene derivative. Most instructors of organic chemistry courses require students to predict a pathway and product distribution of di-substituted benzene derivatives. Although the main emphasis of the interview questions in this study focused on di-substitution, at the end of the interview students were also asked to devise a pathway for the formation of one tri-substituted product. Through analysis of the various questions in the interview, students were nearly evenly distributed into

three main categories. One category consisted of students who ignored the activating and deactivating effects and focused only on the directing effects of a substituent. Another category consisted of students who recalled the activating and deactivating effects from memory as closely associated to the directing effects. The final category consisted of students who had more scientific meaning for the directing and activating/deactivating effects beyond a memorized table.

This section presents the results of each category for 11 of the 12 students' ways of understanding the effects of a substituent on benzene during further EAS. The remaining student (Student 11B) is not discussed beyond the fact that he had memorized the directing effects of bromine (or halides in general) as meta directors, and since any subsequent problems posed could not be readily solved by this student, further discussion of EAS directing effects with Student 11B did not take place.

#### No Consideration of Activating/Deactivating Effects

Five students (5B, 7B, 10B, 6C and 9C), including both teaching assistants, were classified as *not considering activating/deactivating effects*. These students ignored the activating or deactivating effects of the substituent on the benzene ring and instead focused the results of their problem solving on the directing effects.

Student 9C, the undergraduate TA, noted that he had memorized that ortho and para directors had lone pairs on the substituent that could donate into the ring, while meta directors were electron withdrawing, and addressed activating and deactivating effects only with this comment:

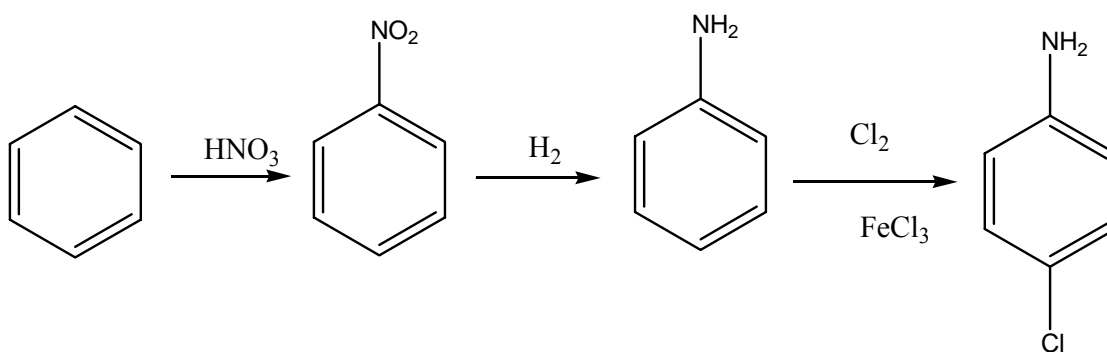
There are activating and deactivating groups for both ortho, para and meta directors...I have to look at the table in the book to know.... I memorized a table in the book for an exam.(Student 9C)

Activating/deactivating effects were not considered in Student 9C's problem solving.

Thus, the student exhibited a way of understanding directing effects emphasizing where the new substituent *will* go and not the likelihood of the reaction occurring.

This way of understanding was observed when students focused only on directing effects.

Even though Student 9C took into account directing effects, when asked to synthesize para-bromobenzoic acid from bromobenzene, he did not consider the possibility of the formation of the ortho product. Ignoring activating and deactivating effects resulted in the following reaction pathway for the synthesis of para-chloroaniline that would prove unsuccessful:



**Figure 4-16: Student 9C Synthesis of *para*-chloroaniline**

Disregarding the fact that the reagents for the first two reactions are not correct, Student 9C suggested a pathway that would generate a polychlorinated product due to the intense activating effect of the amino (NH<sub>2</sub>) group on benzene.

Each of the students who ignored the activating and deactivating effects produced a similar reaction pathway for the synthesis of *para*-chloroaniline.

Student 6C, the graduate TA, was the only one of the four who could not remember the EAS reagents and skipped the nitration step. Although Student 6C ignored the activating and deactivating effects, he accounted for the directing effects beyond the sole reliance of memory. He reasoned through the explanation of why electron-donating substituents direct to the ortho and para positions, but could not produce an explanation for why electron-accepting substituents direct to the meta position.

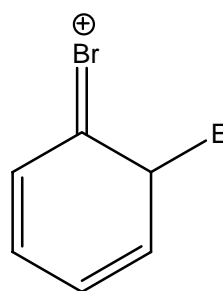
I always think of it in terms of ortho and para not meta...in terms of arrow pushing and that makes sense. But why is it meta? (Student 6C)

Because of the ease of “arrow pushing” with the lone pair of electrons on the ortho and para directing substituent, he was able to justify the directing effects. He could not produce the same reasoning with the meta directing substituents. Student 6C admitted that thinking of directing in terms of lone pair donating resulted in his needing to memorize that the methyl group was ortho and para directing because it does not have lone pair. He also resorted to memorization when discussing the directing effects of the halides.

As with Student 9C, Student 7B also resorted to memorization of the directing effects, but not based on a table in a book. Student 7B recognized the same trends for the ortho and para directors as Student 6C and memorized the rest. However, she also memorized the resonance intermediates that were used to explain the ortho and para



directing character of halides despite their deactivating, electron withdrawing nature. She specifically highlighted the following resonance contributor saying, “The resonance structure offers more stabilization than the electron withdrawing destabilizes it, so the ortho-para wins out.”

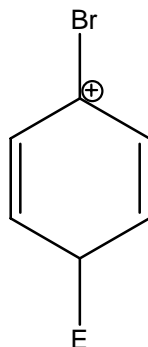


**Figure 4-17: Student 7B Major Resonance Contributor for EAS with Bromobenzene**

Further investigation of Student 7B’s ways of understanding the directing effects of bromine resulted in her reference to her textbook that had the resonance form in Figure 4-17 highlighted as a major contributor, and the reason that the halides are ortho and para directing. She also mentioned that ortho and para directors are activating while meta directors are deactivating, with the exception of the halides. Student 7B did not, however, apply the activating and deactivating nature of the substituents in any of her synthetic pathways, emphasizing instead the directing effects.

Student 5B also had a key resonance structure that she used to explain the directing effects of bromine for EAS reactions. She drew three resonance structures for substitution at each of the three positions, and highlighted the structures with the

cation at the carbon containing the bromine as the major contributing structure (see Figure 4-18).



**Figure 4-18: Student 5B Major Resonance Contributor for EAS of Bromobenzene**

Student 5B did not include the hydrogen atom on the carbon associated with bromine in any of her resonance structures, even though she included it in her reaction mechanism that she drew earlier. Referencing Figure 4-18 as a tertiary carbocation:

**Student:** Even though it's bromine, it's more stable somehow. Because here [*refers to resonance structures with E in the meta position*] it's never in a position of a tertiary bond.

**Interviewer:** So are you calling this tertiary?

**S:** Yeah. I don't know if it's the interaction between the bromine and the positive charge that stabilizes it or if it's the fact that there is some bond here, some bond here and some bond here and that's why it becomes a tertiary bond, a tertiary carbocation.

Student 5B later explained that she mainly relied on her memory for directing effects, but would produce the resonance structures mentioned only if she were asked to do so on a test. Before the above discussion, Student 5B mentioned that bromine was a deactivator, and ortho and para directing, but did not mention activating and

deactivating effects for the remainder of the interview. She did not take activation or deactivation of the benzene ring into account when proposing her synthetic pathways, but focused on the directing effects instead. At one point, she confused the amino,  $\text{NH}_2$ , group with a nitro,  $\text{NO}_2$ , group as a meta director because it contained nitrogen, but remembered later that it was ortho and para directing.

Student 5B did not attribute real meaning to the proposed synthetic pathway; her emphasis was putting pieces together. Based on her recalling the amino group as a meta director, Student 5B proposed a pathway for the synthesis of 1,2-dichloro-4-nitrobenzene that began by substitution of chlorine, followed by substitution of the amino group to the para position with the final substitution of chlorine to the number 2 position. After remembering that the amino group directed ortho and para, she inserted a step converting the amino group to a nitro group. When questioned about the change, she stated that inserting the additional step was equivalent to starting over and writing the synthetic pathway without the amino group substitution. “You still get the same product,” she affirmed.

For a synthetic chemist, adding an additional step implies a lower yield of the final product, or the collection of less of the final product. In addition, the substitution in the final step would occur on a highly deactivated benzene ring resulting in very little product, if any. However, Student 5B's proposals were not related to the attainment of a *quantity* of the product or *quality* of product (by ignoring completing reactions). This disregard for the *real meaning* of the synthetic pathway was present in all but two students (6B and 9B).

Rather than refer to a memorized table or facts, Student 10B provided clear evidence that he reasoned through the directing effects based on the resonance structures of ortho and para directors, as well as the meta directors. Student 10B focused on the quantity rather than the quality of resonance structures drawn for EAS with bromobenzene, indicating an extra resonance structure existed “because the electrons have more places to go.” With regard to activating and deactivating, Student 10B gave the following explanation:

**Interviewer:** And did you say anything about activating and deactivating?

**Student:** I didn't use those terms. No. I don't know if they're exactly synonymous. I kind of use it as they're kind of tied into the same general principles with directing and that kind of stuff. Well, if you have something that's meta directing it's ortho and para deactivating. If you have something that's ortho and para, it's activating ortho and para and it's not necessarily deactivating meta. Like I said, the meta one is stable but just ortho and para are just more stable because of the extra resonance structure.

**I:** Ok. So bromine is activating ortho and para and deactivating meta?

**S:** Yeah. That's what they say in the book but I don't think about it that way and I don't like necessarily saying that even. I don't know if this is right or wrong. It doesn't necessarily deactivate the meta, it just activates the ortho para more substantially.

Student 10B mentioned activating and deactivating relative to the directing effects, rather than the likelihood of reaction, but only after the interviewer brought up the terms. Thus, the activating effects were relative to positions on the ring and not relative to the reactivity of benzene.

The four students who focused on directing effects over the activation of the benzene derivative held a way of understanding directing effects as the location that

the substituent *will* go on the ring. These students could not provide a reasonable synthetic pathway for para-chloroaniline. The students who mentioned activating and deactivating effects as memorized facts also exhibited the same difficulty with the synthesis of para-chloroaniline.

#### Activating and Deactivating as Memorized

Three students (3B, 8B and 12B) incorporated a discussion of the activating and deactivating effects of the benzene derivative. The discussion, however, was limited to revealing how they had memorized the traits of specific classes of substituents.

Student 12B's memorization techniques extended into the directing effects as well. For him, any substituent with nitrogen directly attached to the benzene ring was a meta director and, therefore, deactivating. A substituent with oxygen attached to the ring was an ortho and para director and, therefore, activating. Halides were a memorized exception. Alkyl groups were not mentioned. This generalization regarding nitrogen groups posed a problem for the synthesis of 4-chloro-2-nitroaniline. Student 12B could not propose a pathway that met his criteria due to the fact that one of the nitrogen groups would have to direct ortho to the other. After a few moments, he gave up. Even though he had memorized the trend with regard to activating and deactivating, these features were taken into consideration during proposals of synthetic pathways for EAS reactions, as was the case with Students 8B and 3B.

Student 8B continued having trouble with drawing the resonance structures for EAS reaction with benzene derivatives. She did know how many she should write,

but when asked to show why bromine is ortho and para directing, she produced the same intermediate structure as given as an example from Student 7B (see Figure 4-17). After struggling with drawing resonance structures for the methylation of bromobenzene and the bromination of toluene, she resorted to the following explanation of directing effects to justify her understanding:

**Student:** NO<sub>2</sub> is strongly deactivating because you can draw resonance of the NO<sub>2</sub> group. Bromine is weakly deactivating because it can donate to the ring instead of take away. Activators are all strong and direct ortho para. Strong deactivators direct meta and weak deactivators direct ortho para. CH<sub>3</sub> is a strong activator and adds three Br's to the ring if you brominate toluene. But I don't remember how many will attack whether it's one two or three. It's probably one.

**Interviewer:** What is it activating?

**S:** Ok, I don't know why I am running into the same problem [*refers to problem with drawing resonance*]. I know there should be an extra resonance structure....So what is it activating? Uh. [*pause*] For some activating it can donate electrons, but for CH<sub>3</sub> I don't know how to answer that.

**I:** Bromine, when you drew the mechanism on the other page, donating electrons into the ring.

**S:** Yeah....So, why is it deactivating? [*pause*] OCH<sub>3</sub> isn't as strong an activator as CH<sub>3</sub>.

**I:** So CH<sub>3</sub> is stronger?

**S:** Right. It's more strongly activating because it can't donate into the ring but this [*refers to methoxy attached to benzene*] can so it is more like bromine but instead of deactivating it's only strongly activating compared to CH<sub>3</sub> which is very strongly activating.

**I:** How do you know that?

**S:** I just memorized it. That's the case for most of this stuff. I just memorize just where it falls in ortho, para or meta.

Student 8B subsequently provided another example of a meta directing group (a peptide-like structure) and showed how it had a resonance structure resulting only from the substituent attached to the benzene ring. Thus, the ability to have resonance without involving the *pi* electrons in the benzene ring indicated, for Student 8B, a strong deactivator, while donating electrons into the ring indicated ortho and para directing but varying degrees of activation, from deactivating in halides to strongly activating in the *methoxy* substituent. The methyl group, however, was very strongly activating because it could not donate electrons into the aromatic ring. Thus, Student 8B ignored the activating and deactivating effects when proposing synthetic pathways.

Student 3B ignored these effects when proposing synthetic pathways as well; however, she may have done so as a result of confusion that arose for her during the original discussion of directing effects. Initially, Student 3B indicated a way of understanding that activators have lone pairs that they can donate into the ring, with halides being a memorized exception as exemplified in the segment below:

**Interviewer:** Ok. So what does that mean, it's a deactivator?

**Student:** Um, it is electron withdrawing, which means that it deactivates the molecule and, um, I guess deactivation doesn't cause a reaction to happen as fast, so if you had a deactivator and an activator the activator would take precedence over the deactivator.

**I:** Ok. How do you know that it's ortho para directing?

**S:** Because there's this wonderful little table in my book that we had to memorize.

**I:** You had to memorize for the exam?

**S:** We didn't have to memorize it, but know what general like  $\text{NH}_2$  and  $\text{NR}_2$  would be.

This discussion revealed that her way of understanding deactivation was related to the rate of reaction rather than the likelihood of reaction. For Student 3B, the absence of the lone pair indicated that the substituent was deactivating, with the exception of the methyl group. During further discussion, she observed that the nitro group also had lone pairs (referring to those located on the oxygen atoms of the nitro group) and then began to question her own understanding. After drawing out a generic EAS reaction mechanism using nitrobenzene as the starting material, she realized that the lone pair on oxygen may be located too far away to stabilize the cation of the intermediate, yet she was not convinced and later admitted that “I don’t have the slightest clue” and relied on the table in the book.

#### Activating and Deactivating with Meaning

The final category of students relied more heavily on creating meaningful explanations and did not account for the direct effects merely by memorization. As a result, their synthesis proposals were more scientifically accurate.

Four students (4B, 5B, 6B and 9B) provided evidence that activating and deactivating had real meaning for them, relative to benzene and in relation to the synthetic pathways in subsequent EAS reactions. Three of these students had *scientifically accurate meaning* when proposing the synthetic pathways while one student, Student 4B, *relied on more symbolic clues* than the other three students revealed.

Student 4B, as noted on page 111, used heat and light and could not draw the mechanism which she referred to as a free radical mechanism. In subsequent EAS



reactions and while explaining directing effects, she resorted to the cationic intermediate and certain resonance structures thereof. When rationalizing the directing effects, Student 4B did not highlight the same structure as Student 7B (see Figure 4-17). Instead, Student 4B described the resonance structure, similar to the structure in Figure 4-18, as having a highly substituted carbocation because “a carbocation is most stable when it’s most substituted.”

The resonance structure in Figure 4-18 did not represent the hydrogen atom on the carbon with bromine, and this was one of two resonance structures that Student 4B drew to explain why bromine directed ortho and para. For Student 4B, completing all the resonance structures was not necessary after she had drawn the structure in Figure 4-18. Student 4B also drew two resonance structures for attack at the meta position to show that the cation did not end up in the more substituted position as above.

With regard to activating and deactivating, Student 4B did not rely on memory but focused on symbolic clues:

**Student:** The way that we talked about it was that whenever there’s a substituent that can donate any electrons into the ring, that’s going to make it more reactive to another substituent. Whereas with bromide, because it’s electronegative it’s not necessarily destabilizing the resonance but it has the ability to pull electrons from that carbon and so its going to deactivate it just in terms of making it a little bit less susceptible to further.

**Interviewer:** Now is it more reactive than benzene?

**S:** Yes. Much more reactive than benzene.

**I:** Ok, so if you had to put it in order of reactivity, benzene, bromobenzene, and aniline. Or?

**S:** Yes.

Thus, Student 4B focused on the ability of an atom to donate electrons. Specifically, she looked for atoms with lone pair of electrons, her symbolic clue. With respect to the deactivating effect of bromine, she referenced the electronegativity of bromine as the major factor; however, Student 4B's way of understanding deactivating was not relative to the reactivity of benzene, which she said was less reactive than bromobenzene. Her way of understanding deactivating referred to the order in which substituents needed to be added to the ring. In her proposal for the synthetic pathway of para-bromoaniline, she first suggested adding bromine to the benzene ring and then the amino group. Then Student 4B changed her mind because she remembered that bromine was deactivating, and so she added the amino group first, followed by bromine. For Student 4B, the ring activator should be added first and then the ring deactivator. She later explained her reasoning by stating that "the stronger group wins" in relation to adding deactivating groups to the benzene ring in 1,2-dichloro-4-nitrobenzene. She initially added chlorine that subsequently directed the nitro group to the para (or number 4) position.

So once you get those two down, then the nitro group is a strong deactivator and it directs meta, so you know that the next group will add in at one of these positions [*referring to meta positions relative to the nitro group*] (Student 4B)

For Student 4B, directing effects related to the presence of a lone pair on the substituent, while activating and deactivating referred to the order in which one should conduct the EAS reactions in a synthetic pathway.

For Students 6B and 9B, *directing* related to the stability of the resonance intermediate, while *activating* and *deactivating* effects referred to the ability of the substituted ring to undergo EAS and to what degree. Both of these students proposed synthetic pathways with scientifically accurate meaning relative to the ability to attain the desired product.

Both Students 6B and 9B drew four resonance structures for substitution in the ortho (6B) or para (9B) positions. Student 6B highlighted the same structure as presented for Student 7B (see Figure 4-17) as the major contributor, as well as the number of resonance structures, as the reason why bromine directs to the ortho and para positions. Regarding the deactivating effect of bromine, Student 6B stated, “we’ve taken away some of it’s electron density so it will be less likely to react.” Student 9B used the same reasoning for the directing effects of bromine. With regard to the deactivating effect of bromine, Student 9B made the following comments:

That whole deactivating thing means it doesn’t like having the positive charges in the first place because it can stabilize that positive charge much less than this [*refers to methyl group*] or this [*refers to hydroxy group*] could. Bromine is not like methyl and oxygens because it is so electronegative but it does have lone pairs that can be donated if it needs to. (Student 9B)

Student 9B related bromine to the other ortho and para directors, explaining why bromine behaved different from all other ortho, para directors.

Both students 6B and 9B used their way of understanding of directing effects and ring activation when proposing synthetic pathways for polysubstituted benzene derivatives. For the synthesis of para-chloroaniline, they were the only two students

who suggested a pathway in order to avoid polychlorination of aniline. As a result, they both proposed that chlorination of benzene should occur first, followed by nitration to the para position, and finally reduction of the nitro group to form the amino group.

For the synthesis of 1,2-dichloroaniline, both students discussed the plausibility of such a product, due to the fact that the second step (nitration) would result in a strongly deactivated ring. Both proposed the final step as a chlorination of the benzene derivative, but expressed doubt about whether it would occur and how much product would result. As with all other students (with the exception of the TAs), neither of these students had an organic chemistry laboratory experience and based their conclusions based on their understanding of structure and reactivity. As a result of their reasoning, two additional EAS questions were posed, resulting in equally reasonable proposals for the reaction pathways from each student.

Student 9B admitted that she searched for the underlying meaning behind organic chemistry reactions, and relied on an understanding of the reaction mechanism rather than memorization if possible, and she pointed out that, “there are just some reaction that are never explained like the reduction of the nitro group to the amino group. You just have to memorize the reagents that make that work.”

Student 6B admitted to relying on reaction mechanisms, but in an entirely different way:

I try to remember what happens and not just memorize. If I see the mechanism it is a lot easier to memorize the reaction because I can see what happens.

Student 6B focused on what happened in the reaction mechanism rather than why it happened, as expressed by Student 9B. Student 6B explained that writing out the reaction mechanism while studying made performance on the exams easier because most of the questions did not ask for the mechanism, just the reagents. Student 6B believed that memorizing the reaction mechanisms aided in preventing him from making foolish mistakes on an exam.

**Table 4-6: Students' WoU Directing Effects of Benzene Derivatives**

<b>Way of understanding</b>	<b>Students</b>	<b>Student WoU examples</b>
<i>Ignored activating and deactivating effects</i>	5B, 7B, 10B, 6C, 9C	Focused on directing effects (5B, 7B, 10B, 6C, 9C)
<i>Memorized activating and deactivating effects</i>	3B, 8B, 12B	No application while proposing synthetic pathways (3B, 8B, 12B)
<i>Activating and deactivating with meaning</i>	4B, 5B, 6B, 9B	Symbolic (4B) Probability of reaction (5B, 6B, 9B)

### **Students' Ways of Thinking About Aromatic and Electrophilic Aromatic Substitution**

The Duality Principle describes ways of understanding and ways of thinking as developmentally interdependent. As a result, a discussion of students' ways of understanding is incomplete without also including a discussion of the students' ways of thinking that are associated with their ways of understanding. The ways of thinking presented in this section are based on the categories of ways of understanding described in the previous sections. With the mental act of interpreting as the lense through which the data was analyzed, three main classes of students' ways of thinking were observed.

The first way of thinking classification is non-referential symbolic (NRS) reasoning (Harel in press [b]). NRS is a term used in mathematics education to describe students' ability to manipulate mathematical symbols without a corresponding understanding of the mathematical construct.

The second classification is similar to the first, but rather than students' non-referential symbolic reasoning, this class distinguishes students' ways of thinking as non-referential use of terminology. For this way of thinking, the students' language references are not scientifically or structurally based.

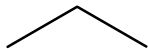
The third classification involves students' ways of thinking associated with their beliefs about organic chemistry. During the interviews, students provided candid, unsolicited references to their beliefs about organic chemistry.

#### Non-Referential Symbolic Reasoning

Chemistry employs the use of symbolic representations as a foundational component by which chemists communicate. In organic chemistry, there are a variety of symbolic representations used for molecular structures. Three of the most commonly used representations are: the Lewis structure, the condensed structural formula, and the line-angle formula (commonly referred to as the skeletal structure). Lewis structures include all the atomic symbols connected by lines presenting covalent bonds and showing nonbonding electrons as pairs of dots associated with a specific atom. These structural representations are the least preferred representation in organic chemistry since they are cumbersome for large molecules. The condensed structural formulas are written without showing the individual bonds or lone pairs of electrons.

The atomic sequence is generally written in actual bonding order of the central atoms with multiple bonds and other substituents bonded to the central atom clearly distinguished. The line-angle formula or skeletal structure is most often used because of its economical factor of omitting all carbons and hydrogens. Thus, each terminus of a line represents a methyl group while each apex represents a carbon atom with enough hydrogen atoms to produce a tetravalent carbon. The following examples in Table 4-7 are of the three variations of structural representations for propane,  $C_3H_8$ .

**Table 4-7: Symbolic Representations of Propane**

Lewis Structure	Condense Formula	Skeletal Structure
$  \begin{array}{ccccccc}  & & H & & H & & H \\  & &   & &   & &   \\  H & - & C & - & C & - & C & - & H \\  & &   & &   & &   \\  & & H & & H & & H  \end{array}  $	$CH_3CH_2CH_3$	

Organic chemists are known to use combinations of each of these representations for a single molecule. As a result, it is important for students to be familiar with the features and limitations of each type of representation, and to be able to move among them. In order to designate stereochemistry about a central atom, organic chemists employ another representational feature in the dashed or wedged line notation. In these representations, the atomic symbol of the central atom is explicitly written out with a dashed line representing a bond below the plane of the page, while a wedged line represents a bond above the plane of the page, and a normal line represents a bond in the plane of the page.

In addition to the structural representations, organic chemists also employ a number of additional representations used to denote the flow of electrons in the course of a chemical reaction. The most common of these representations is the use of curved arrows in reaction mechanisms showing the flow from an area of rich electron density (typically a nucleophilic site) to an area of less electron density (an electrophilic site). Thus, the symbolic representational system in organic chemistry incorporates a variety of representations that are used interchangeably and simultaneously depending on the context.

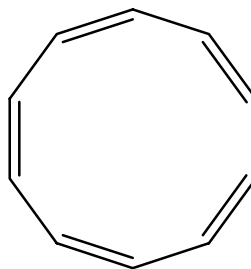
Bodner and Domin (2000), in their study on the roles of representations in problem-solving in chemistry, found that students do not readily interpret the symbols as representing a physical reality. Instead, “They tend to handle chemical formulas and equations that involve these formulas in terms of letters and lines and numbers (p. 25).” Bodner and Domin, therefore, did not refer to students’ using symbols because they “cannot correctly be called symbols because they do not represent or symbolize anything that has physical reality (p.25).”

NRS reasoning is compatible with the findings of Bodner and Domin, with the distinction that student *do* make use of the symbols. The students use the symbols in their reasoning and rationalization patterns and, therefore, in opposition to the suggestion from Bodner and Domin, they should be referred to as symbols even though they may not represent a physical reality.



### Heuristics Associated with Aromaticity

Nearly all students in this study explained that aromaticity meant that “three things” had to be present. Of these three things, the students overwhelmingly favored Hückel’s Rule when identifying aromatic compounds. The universal application of Hückel’s Rule resulted in the way of understanding aromaticity as cyclic structures with double bonds that obey the requirement of having  $(4N + 2)$  *pi* electrons, with *N* limited to a positive whole number.



**Figure 4-19: 1,3,5,7,9-cyclodecapentaene**

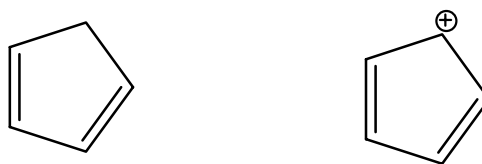
A clear example of this is the identification of the structure in Figure 4-19, 1,3,5,7,9-cyclodecapentaene<sup>27</sup>, as aromatic because “it fits the  $4N + 2$  rule and you can push the electrons all around (Student 8B).” Student 8B exhibited two heuristics in this comment: the use of Hückel’s Rule and the view of resonance as “pushing electrons around.” The universal application of Hückel’s Rule implied NRS reasoning, as students neglected the actual structural characteristics of the given molecule. Focusing on “pushing electrons” when drawing resonance structures in many cases meant moving double bonds or lone pairs of electrons with the use of curved arrows.

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<sup>27</sup> This structure is not aromatic because it is not planar. As a result, the p orbitals do not align to create the opportunity for the electrons to delocalize throughout the ring.

Student 4B did not have skill in drawing resonance structures (see Figure 4-4). Her example of a resonance structure with a pentavalent carbon was representative of students who focus on the “pushing electron” heuristic and lose track of the actual structure.

Yet, even those students with skill in drawing resonance structures would often propose non-sequitur resonance structures. For cyclopentadiene (see Figure 4-20, below), Student 11B correctly designated it as non-aromatic because it had only four pi electrons. However, he claimed that it was like the cyclopentadienyl cation in that he could still draw resonance structures to displace the electrons around the ring. His focus on moving double bonds prevented him from realizing that one carbon was  $sp^3$  hybridization containing two hydrogen atoms and no available  $p$  orbital for delocalization of electrons.



**Figure 4-20: Cyclopentadiene and Cyclopentadienyl Cation**

The use of hybridization by some students also became a heuristic for classifying aromatic compounds. For example, Student 3B classified the cyclopentadienyl cation as aromatic because all of the carbons are  $sp^2$  hybridized.

#### Interpretation of Symbolic Clues

Students also exhibited non-referential symbolic reasoning through their interpretation of a variety of symbolic clues. Most of the symbolic clues that students

discussed during the interview were a result of their search for symbolic patterns in learning organic chemistry. The search for symbolic patterns could be employed to minimize the cognitive effort on the part of the students; consequently, students tended to over-generalize the pattern, resulting in unscientific structural implications. The symbolic clues took precedence over structural integrity based on foundational chemical concepts. In other words, the symbolic clues existed for the students in a separate realm that did not require the understanding of the actual molecular structure. For instance, several students' (4B, 7B, 8B, 9B, 10B and 11B) ways of understanding an anion associated with an organic molecule as representing one lone pair used this symbolic clue to identify pyrrol-1-ide as aromatic with six  $\pi$  electrons.

Another example of the existence of NRS reasoning could be seen in the two students (6B and 9B) whose ways of understanding resonance stability was directly associated with the quantity of structures rather than the quality of the individual structures, *moving symbols to produce quantity*. Even though these students understood that resonance structures represented the overall hybrid structure, they emphasized the quantity of resonance structures during their explanations of directing effects, rather than the quality of any individual structure as being a major contributor to the overall structure. Giving each resonance structure equal contribution to the overall hybrid structure represented a case where students did not observe the symbolic representations as representing a physical reality. For Students 6B and 9B, the relative stability of each resonance structure was ignored because they justified the

directing effects based on the *number* of resonance structures produced rather than the *character* of one particular resonance form being especially stable.

These examples show students using symbolic clues to provide justification that was not merited on the actual physical reality of the molecular structure. The students in this study also developed patterns from symbolic clues that did not necessarily imply a structure unfounded by the physical reality. These students used the symbolic clues with memorization of exceptions, without reference to any structural reasoning. For example, Students 3B, 6C and 12B held a way of understanding activating substituents as atoms with lone pairs of electrons with the exceptions (*methyl* groups and halides) memorized, but not necessarily justified. These students used the presence or absence of lone pairs on the benzene substituent as their indication of where to direct the subsequent EAS reaction.

Interpreting the symbolic representations in organic chemistry in terms of lines, letters, numbers, arrows and dots resulted in a disconnected view of the symbols representing anything with real physical meaning as per Bodner and Domin (p.142). However, students' disjunction between the symbolic representation and the physical structural implication was not only based on their NRS reasoning, but was also based on the verbal or linguistic representational system referred to as "use of terminology."

#### Non-Referential Use of Terminology

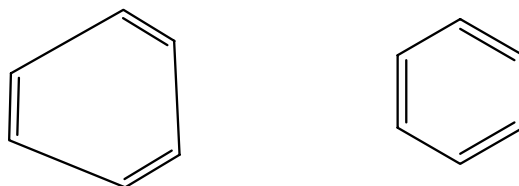
In organic chemistry, instructors require students to communicate ideas through not only the symbolic representations but also through the use of terminology. This dissertation uses "terminology" to reference specific chemical terms in addition

to vocabulary recognized from everyday language with a scientific meaning. Students' misuse or misunderstanding of specific chemical terms, or their use of vocabulary either non-scientifically or inconsistent with the chemical definitions, denoted the presence of a non-referential use of terminology (NRT) way of thinking.

#### Students' Ways of Understanding 1,3,5-cyclohexatriene

Chemical nomenclature<sup>28</sup> is the most common use of chemical terminology yet students have very little experience naming chemical compounds outside of chemistry. The name of a molecule represents a physical entity. In organic chemistry, the name of a molecule refers to a specific symbolic representation that in turn references the actual physical structure of the molecule.

In the interviews for this dissertation, students were asked to draw the structure of 1,3,5-cyclohexatriene followed by an inquiry about whether this molecule actually exists. Students predominantly drew the two structures in Figure 4-21.



**Figure 4-21: Student Representations of 1,3,5-Cyclohexatriene**

Three students (4B, 5B and 9B) drew a structure similar to the one on the left of Figure 4-21, indicating alternating single bonds having a longer bond length, and double bonds having shorter bond lengths. This is the most correct representation of the 1,3,5-cyclohexatriene. Students 4B and 9B stated that the structure did not exist

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<sup>28</sup> Chemical nomenclature refers to naming chemical compounds.

because it would require localization of the *pi* electrons in the double bond. Since the *pi* electrons in benzene are delocalized, they explained that the structure did not represent benzene and, therefore, did not exist.

Student 5B drew the same symbolic representation but did not draw the same conclusions. She claimed that the molecule did exist but was not stable:

**Student:** It's not happy because of the bond angles. They're compressed. Sure it exists because this is your typical length single bond and your typical double bond.

**Interviewer:** How does it relate to benzene?

**S:** It has a higher heat of hydrogenation. And it's not as stable. This guy probably wants to react, break a bond, to release ring strain.

In Figure 4-21, the majority of students drew the structure on the right. Even though they drew benzene, Students 7B, 10B and 11B claimed that 1,3,5-cyclohexatriene would not exist because the *pi* electrons were localized in the double bonds.

Students 6B, 8B, 12B and 9C drew the benzene structure and claimed that the molecule did exist because it was benzene. They claimed that the name benzene was the common name for 1,3,5-cyclohexatriene. As a result, they associated the actual meaning of the name, 1,3,5-cyclohexatriene, to the symbolic structure that they drew, rather than the actual meaning of the name designating three localized double bonds providing evidence for NRT.

More commonly, students interpreted vocabulary used in organic chemistry in a non-scientific and structurally inconsistent manner. These interpretations were

inferred based on several uses during the course of the interviews and they provide additional evidence for the presence of NRT.

### Students' Interpretation of Vocabulary

The analysis of the students' interviews in this study provided several instances in which inappropriate references appeared in their use of terminology. The examples provided below, however, are based on several interviews with follow-up questioning to clarify students' understanding. Other instances in which the students' interpretations were questionable, but not substantiated by further evidence or questioning, are not included here as evidence of NRT.

Student 3B proclaimed early in the interview that she was “not very good with terminology.” The analysis of the interview provided several opportunities to support her claim and provide evidence for NRT. She often used “everyday interpretations” of the vocabulary as justifications for her reasoning. For example, Student 3B claimed that aromatic compounds were special because “they give off odors, which is a unique thing.” When asked if anything else “gives off odors”, she replied, “no.” Student 3B held an unscientific way of understanding the *term* aromaticity with her interpretation based on everyday language rather than the scientific meaning. Aromatic compounds do not all have fragrance and are not the only compounds that have fragrance.

Student 4B interpreted the use of “strongly” deactivating as meaning that it gave preference for directing the substituent over something “weakly” deactivating, claiming that “the stronger group always wins.” Many other students had interpretations of activating or deactivating inconsistent with the actual chemical

interpretation. Student 3B claimed that having a deactivator slowed down the rate of reaction but did not effect the probability of reaction. Student 8B claimed that activators were all strong, and held the same way of understanding as Student 4B, that “the stronger group always wins.” For the majority of situations, Student 8B’s reasoning would not pose a problem, however, she also held the way of understanding that activators have lone pairs of electrons adjacent to the ring. The methyl group did not have a lone pair and, therefore, by her reasoning, was not an activator. Instead, it was an even stronger activator than the groups with a lone pair because of the tertiary carbocation in the intermediate resonance forms.

Her interpretation of “strong” related to the structure’s ability to undergo EAS at a higher rate of reaction than benzene. She did not consider “strength” resulting in more than one substitution product as evidenced by her preference to add the amino to the benzene ring before the chloro group in her proposed synthesis of para-chloroaniline. She claimed that “adding  $\text{NH}_2$  first is better because I will get the product faster.”

Three students (4B, 7B and 9B) used the phrase “resonating throughout” to describe resonance structures. Students 4B and 7B interpreted resonance to mean the oscillation between structures. Student 9B used the phrase despite her clearly communicated claim that she understood resonance as hybrid structures. Her use of the term “resonating throughout” referred, instead, to the movement of electrons throughout the  $p$  orbitals. Each of the above examples provided the basis for the inference of the NRT way of thinking.



### Students' Beliefs about Organic Chemistry

This final section on students' ways of thinking focuses on the beliefs students have about organic chemistry. These beliefs are associated with learning organic chemistry and include students' views on the characteristics of organic chemistry. During the interviews, students often spontaneously commented on their beliefs about learning organic chemistry or their views about the characteristics of organic chemistry, with the latter predominant.

The most prevalent belief about learning organic chemistry was the perception that students had to memorize all the organic reactions. All of the students experienced varying degrees of frustration during the EAS portion of the interview when they could not *remember* the appropriate reagents for a given reaction. With the exception of the bromination reaction, the students all agreed that knowing all of the reaction mechanisms was not necessary or productive. In general, most of these students recognized that a similar mechanism occurred for the EAS reactions. They did not bother with the details of why each set of reagents worked. As a result, most students could write a mechanism for the bromination reaction showing the activation of bromine because it was "part of what we needed to know for the test." These same students could not write the mechanism for nitration and the generation of the nitro electrophile in situ, a mechanism that would not be part of their exam.

Student 6B claimed that he memorized the reaction mechanisms rather than just reagents and added, "I try to remember what happens and not just memorize. If I

see the mechanism it is a lot easier to memorize the reaction because I can see what happens.”

Student 9C agreed that knowing the reaction mechanism was the key strategy for learning organic chemistry. He referred to “knowing” as having written out the reaction mechanism and then memorizing it. As a teaching assistant, he recommended to his students writing the reaction mechanisms, as well as all the structures, claiming, “you don’t learn it until you have seen it on paper and preferably drawn it yourself.”

Student 9C made several statements about learning organic chemistry. He claimed that lectures were useless and that “real learning only occurs in section and in small groups.” He explained that participating in a small study group as an undergraduate student benefited his learning greatly. He also revealed that he did not value molecular modeling kits because “everything on a test is on paper anyway and kits take so much time.”

The reference to material that would be on an exam was common for the students interviewed. Students focused their learning on what they expected to be on an exam. As a result, many students found that memorizing organic reactions proved successful. Student 5B provided the following information:

**Student:** I was so bad at this last quarter. I didn't understand it. I just did it.

**Interviewer:** (*laughs*) Did you do well in it at least?

**S:** I got an A. I don't know how honestly.

Student 5B later explained that she would like to have developed a better understanding of organic chemistry but did not have the time. She felt that it was too late for her to go back and understand the concepts from the past. She also stated that she was still getting top grades so she did not have a real incentive to “stop memorizing and start understanding.”

Beyond the reaction mechanisms, some students (5B, 8B, and 6C) believed that organic chemistry was “all about pushing electrons around (Student 5B).” Student 5B claimed that she just memorized the electron pushing and did not really know why electrons moved the way that they did. Student 8B viewed electron pushing as “just the way it is in organic chemistry” adding, “I just memorized it. That’s the case for most of this stuff.”

For most of the students, organic chemistry fulfilled a requirement for their entry into a health-related field. They wanted to achieve a high grade with as little effort as possible. These students did not view organic chemistry as relevant to their future career except for their grades in the course and the need to take a professional school entrance exam, part of which tested students’ ability in organic chemistry.

## **CHAPTER 5: STUDENTS' WAYS OF THINKING: BELIEFS ABOUT LEARNING ORGANIC CHEMISTRY**

Beliefs comprise one of the categories of ways of thinking in Harel's DNR-based instruction. A written survey was developed and administered in order to quantitatively assess the prevalence of certain beliefs of the organic chemistry students in this study. The focus of this chapter is on the analysis of the 46-item Likert-scale survey administered to just over 100 organic chemistry students enrolled in the final quarter of the three quarter organic chemistry sequence during fall quarter of 2003. This chapter includes an analysis section as well as a discussion section.

The analysis portion of the chapter includes three sections. The first section presents the results of a descriptive analysis of the data, based on the responses given by students on the survey. The next section presents the results of a principal components analysis of the data. This section defines the seven principal components identified by Varimax (orthogonal) rotated factor analysis. The final section of the analysis discusses the correlation data relative to the principal components and demographic variables.

The discussion portion of the chapter presents the significance of the results and interprets their meaning relative to the purpose of the survey and within the context of the overall dissertation.

### **Analysis of the Written Survey**

#### **Descriptive Analysis**

The results of the frequency distribution for each item in the Likert-scale survey can be found in Appendix 7. The survey employed in this study contained 40

questions directly related to students' epistemological beliefs in the organic chemistry course. In addition, there were six demographic questions. The Likert-scale survey was coded with the value "1" assigned to the "strongly agree" response; "2" to the "agree" response; "3" to "neither"; "4" to "disagree"; and "5" to "strongly disagree". Items with mean response values between 2.25 and 3.25 are referred to as neutral items due to the fact that students were evenly distributed and had no preference towards "agree" or "disagree".

The population that completed this survey was equally distributed across gender lines. They were predominantly biology majors between the ages of 19-20. Most of the respondents expected to receive a grade of A or B as their final course grade. The group was distributed evenly in their response to the exams being representative of their organic chemistry knowledge. The majority of respondents (32%) agreed that the course was one of the most difficult in their college experience

In the 40 items probing students' ways of thinking associated with beliefs in organic chemistry, students' answers were evenly distributed (they neither favored agree or disagree with these items) across eight items in the survey. These included items probing their beliefs related to their grade as their course goal (Item 7), their reliance on familiarity of content of insight and creativity (Item 9), their reliance of pKa<sup>29</sup> values (Item 11), their relating to previous science courses (Item 14), their learning occurring predominantly before exams (Item 19), their understanding as

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<sup>29</sup> pKa is a measure of the relative acidity of a compound. Acid-base processes can provide models for the reactivity of polar organic molecules.

recalling information (Item 21), their understanding resulting in being better informed on current events (Item 30) and their working in study groups (Item 34).

The students held a slight preference for the “agree” option for six items related to remembering reactions (Item 3), viewing organic chemistry as many pieces of knowledge (Item 8), relating organic chemistry to the real world (Item 17), referring to the main skill learned as “solving organic synthesis problems” (Item 18), “memorizing new vocabulary” (Item 20), and “being able to memorize all required information” (Item 24).

Another item relating to the need to memorize reactions in organic chemistry (Item 3) reflected a slight majority of students in agreement with this probe resulting in 44% of respondents agreeing and 9% strongly agreeing. An additional memory probe (Item 15) resulted in 79% of students agreeing that memorizing reagents was “crucial to success” in organic synthesis problems. While another memory-related item (Item 4) resulted in nearly the opposite response with 48% disagreeing that learning equated to “memorizing reaction” with another 8% strongly disagreeing. One explanation for this contradiction would be related to the very direct wording of Item 4, versus the more subtle phrasing of Items 3 and 15, regarding beliefs about memory. Item 4 stated that “the best way to learn reactions was to memorize them” while Items 3 and 15 did not use the word “memorize” but rather referred to students’ learning associated with “remembering the right reagents.”

The majority of respondents favored agreement over disagreement for most of the item probes. Item 32 related to a student’s reliance on having a competent

teaching assistant received 61% agreement, while Item 31 revealed students' preference for a decent instructor, with 84% in agreement. In addition, 84% of students also agreed that they relied on "being familiar with the instructor's expectations in the course" (Item 38).

Students generally agreed with items related to their beliefs about learning as an active process. Item 1 had the strongest response with 51% "strongly agreeing" and 42% "agreeing" that reading the text, working problems and paying close attention were valued behaviors. They also showed favor towards the idea of being an active participant in their learning by their responses to three additional items (25, 26, and 28). Item 25 related "reasoning logically" as a skill learned in organic chemistry resulting in 77% of respondents replying "strongly agree" or "agree". Item 26 probed students' use of their mistakes as a learning tool, with 83% of students agreeing. Finally, Item 28 explicitly questioned whether students learn by rethinking, restructuring and reorganizing information, with which 66% agreed.

Items 2, 5, 29, 37, and 40, which probed students' levels of effort in learning organic chemistry also resulted in a majority of positive responses. Seventy-six percent responded that they "use their carefully prepared class notes while studying for an exam" (Item 2), and 80% agreed that lecture attendance was "important". Eighty-six percent of students agreed that they value electron pushing to aide in their understanding of organic chemistry (Item 37).

Items 5 and 40 both probed students' use of time. Item 5 referred specifically to spending a great deal of time to understand reaction mechanisms, while Item 40

merely stated that learning in organic chemistry required a large time commitment. These items each had an agreement response rate of 86%.

Two probes (10 and 39) resulting in overwhelming positive responses presented statements about students' beliefs regarding the concepts of organic chemistry. Item 10 had 91% of respondents in agreement with 21% of those strongly agreeing that "learning in organic chemistry was directly related to molecule structure, reactivity and organic synthesis". Item 39 presented a statement regarding organic chemistry concepts building upon each other, resulting in 80% agreement.

The final probe that revealed a majority of positive responses focused on learning organic chemistry by solving many problems over analyzing a few in detail (Item 6). Forty-one percent of students agreed with this probe, while 26% strongly agreed; only 8% disagreed.

There were several probes that revealed a majority of students in disagreement; for example, Items 35 and 36—related to the use of molecular modeling kits and computer molecular modeling software—resulted in 24% of students "strongly disagreeing" with each item, and 40% and 42%, respectively, "disagreeing".

Another item that resulted in strong disagreement was a probe stating that the student had a strategy of skipping what they did not understand, and hoping it would not be on an exam. Twenty-three percent of students strongly disagreed while 48% disagreed with that statement.

With regard to learning, statements about students' need to focus learning on spectroscopy (Item 13) resulted in 66% of student disagreeing, while a focus on



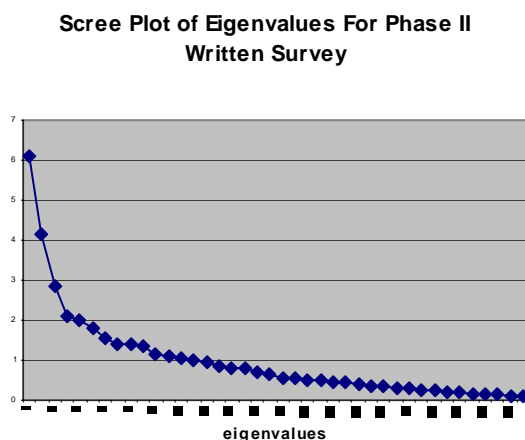
learning new vocabulary (Item 22) resulted in 62% of students disagreeing. Students also disagreed with Item 12 that “only few people were capable of really understanding organic chemistry” (59%).

Regarding learning strategies, students slightly disagreed (53%) that “spending too much time on one problem” was a “waste of time” (Item 23). Fifty-nine percent disagreed that they had “no legitimate recourse” during an exam if they could not remember a specific reaction mechanism (Item 16). The final item of dissent probed students’ beliefs that a student could pass the class “without an understanding of organic chemistry” (Item 27) 44% of students disagreed with this statement, while 8% strongly disagreed.

The descriptive results provide a hopeful view of students’ learning in organic chemistry, with students responding relatively favorably to most probes. However, in the following section of this chapter, principal component analysis revealed several factors in which students’ responses were consistently unfavorable.

#### Principal Component Analysis of Correlation Matrix

Principal component analysis (PCA) was used to reduce the number of variables and to detect structure in the relationships between variables (Anderson 1984). PCA produced 13 principal components in which the eigenvalues were greater than one, a requirement of the Kaiser criterion (Kaiser 1958).



**Figure 5-1: Scree Plot**

A scree plot indicated that there were approximately 4-8 components worth further inspection. The structure of the various components was explored using Varimax (orthogonal) rotation, studying the magnitudes of the various loadings (the degree of association) for each survey item with each component. The number of factors extracted by rotation varied from 3-13 factors where the patterns of loadings on each component were compared manually. Loadings were only considered associated with a given principal component if the magnitude of the rotated loading was greater than 0.5. A consistent pattern of the loadings emerged after rotating seven factors resulting in further classification of the first seven principal components. The loadings of the probes were examined to determine the meaning of the dimensions of the principal components analysis.

These seven principal components accounted for 51% of the total variance. The interpretation of each of these seven components is discussed below, based on the loadings of the individual items. For simplicity, the components are referred to as PCA1, PCA2, PCA3....PCA7. Table 5-1 summarizes the results of the rotated

principal components analysis, as well as the demographic correlations with each principal component.

**Table 5-1: PCA Summary Table**

<b>Principal Component</b>	<b>Interpretation</b>	<b>Rotated Factor Pattern</b>	<b>Demographic Correlations</b>
PCA1 (15%)	Memorize-oriented belief that does not value intellectual and practical benefits of organic chemistry	10: +0.74 15: +0.51 17: +0.72 21: +0.59	Pos: Grade Neg: Exams representative
PCA2 (10%)	Independent learners with desire for a coherence	1: +0.64 5: +0.67 11: +0.56 20: +0.66 25: +0.59 26: +0.66 39: +0.57 33: -0.60	Neg: Difficulty
PCA3 (7%)	Non-Users of Molecular Modeling Media	35: -0.89 36: -0.86	None
PCA4 (5%)	Independent learners with value of practical benefits of organic chemistry	19: -0.73 30: +0.56	Pos: Representative
PCA5 (5%)	Independent learners who spend little time in learning organic chemistry	31: -0.66 32: -0.75 38: -0.60 40: -0.62	Pos: Difficulty
PCA6 (5%)	Independent analytical learners	6: -0.61 34: -0.76	Pos: Gender (favoring Female)
PCA7 (4%)	Memorize-oriented learners	12: -0.57 27: +0.61	Pos: Representative

The distribution of the survey probes into the three different categories of beliefs was used to aid in the interpretation of these seven principal components (see Table 3-3).

### Characteristics of PCA1

PCA1 accounted for 15 % of the variability in the data set. During the rotated factor analysis, the pattern of loadings for PCA1 revealed that items 10, 15, 17 and 21 consistently had a high degree of association with this first principal component. In addition, items 4, 7, 16 and 23 had relatively high eigenvector values in the 40 x 40 cross-correlation matrix (see Appendix 8). Item 10 associated learning in organic chemistry with acquiring knowledge related to molecular structure, reactivity and organic synthesis. This item was labeled as a desirable response for the coherence category (see Table 3-3). In the context of the other items favoring memorization, I concluded that these students may have responded highly to Item 10 due to the fact that they recalled these three terms; molecular structure, reactivity and organic synthesis. An interesting contradiction would appear if students did indeed value these features of organic chemistry that were highlighted as “important” in both their text and lecture. Support for the claim that they did not value the items listed in Item 10 and may merely have recalled them as important was detected in the loading of Item 20 in the 40 x 40 correlation matrix (see Appendix 8). Item 20 also refers to students valuing molecular structure. The loading for this item in PCA1 was relatively high and negative (-0.19) indicating that PCA1 did *not* encode the value of molecular structure during problem solving in organic chemistry. Using these survey items, PCA1 was interpreted as encoding for a memorize-oriented belief about learning organic chemistry that did not value the intellectual or practical benefit of organic chemistry.

### Characteristics of PCA2

The pattern of loadings from the rotated factor analysis for PCA2 revealed a consistently strong positive association with Items 1, 5, 11, 20, 25, 26 and 39 while consistently displaying a strong negative association with Item 33 (“skip and hope” probe). The interpretation of PCA2 was consistent with independent learners with a desire to construct a coherent structure in order to build the conceptual framework of organic chemistry. PCA2 accounted for 10% of the variability in the data.

### Characteristics of PCA3

The loading pattern of PCA3 from the rotated factor analysis revealed a strong negative association with Items 35 and 36. These items related to use of molecular modeling kits and computer modeling software, respectively. PCA3 accounted for 7% of the variability. The distribution data reflected a similar pattern. PCA3 revealed a strong association between student responses on Items 35 and 36. In other words, students responding negatively to Item 35 would also tend to respond negatively to Item 36. PCA3 encoded for the non-users of molecular modeling media.

### Characteristics of PCA4

The rotated factor analysis loading patterns of PCA4 revealed a strong positive association with Item 30 (*understanding current events*) and a strong negative association with Item 19 (*all learning occurs before an exam*). PCA4 seems to, therefore, encode for independent learners who acknowledged the practical benefit of learning organic chemistry. PCA4 accounted for 5% of the variance.

### Characteristics of PCA5

PCA5 demonstrated a rotated factor analysis loading pattern with strong negative associations with Items 31, 32, 38 and 40. Items 31, 32 and 38 related to students' reliance on having a good instructor (Item 31), a good teaching assistant (Item 32) and knowing the instructor's expectations (Item 38). Item 40 probed students' associations with the time commitment involved in learning organic chemistry. As a result, PCA5 was interpreted as encoding for strong independent learners, who did not consider the time commitment significant in their learning of organic chemistry. PCA5 accounted for 5% of the variability.

### Characteristics of PCA6

The loading pattern for the rotated factor analysis revealed that PCA6 had strong negative associations with Item 6 (*solves many problems over analyzing a few*) and Item 34 (*uses study groups*). In addition, the 40 x 40 correlation matrix (see Appendix 8) showed relatively strong positive loadings for items 10, 11, 14 and 27. Strong positive associations with Items 10, 11 and 14 indicated a type of student who viewed organic chemistry as having a coherent structure, while Item 27 probed students' beliefs that one could pass the course without understanding organic chemistry. PCA6 was interpreted as encoding for independent analytical learners. "Analytical learners" preferred to solve fewer problems and analyze them in depth. PCA6 accounted for 5% of the variance in the data set.

### Characteristics of PCA7

The rotated factor analysis loading pattern for PCA7 revealed strong positive association with Item 27 (*pass without understanding*) and strong negative association with Item 12 (*only few are really capable of understanding*). In order to interpret the loading pattern of this group, two strong loadings in the 40 x 40 correlation matrix were also considered (see Appendix 8), Items 3 and 21. Both of these items showed a strong preference for memorizing, with Item 21 indicating that “understanding directly referred to recalling” information. As a result, PCA7 seems to encode for learners who focused on memorizing rather than understanding, because understanding for them was associated with recall. Consequently, Item 21 indicated that these PCA7 encoded for learners who did not believe that only few people were capable of understanding organic chemistry, perhaps because they associated understanding with the ability to memorize. PCA7 accounted for 4% of the variance in the data.

These seven components could be combined to form five by viewing PCA1 and PCA7 as similar, based on students’ memorize-oriented way of thinking. These two components combined would be interpreted as the “memorize-oriented” learners, thus accounting for 19% of the variability. PCA2 and PCA6 could also be combined, indicating independent, analytical learners, and accounting for 15% of the variability. However, there were no statistically significant correlations between any pairs of principal components. As a result, correlations on demographic information were conducted on the separate principal components over any combination of the principal components.

### Correlations with Demographic Information

The demographic information included probes on gender, age, major, expected course grade, whether the exams were representative of their knowledge, and the students' perceived difficulty of the organic chemistry course. The correlation between each of these and each principal component was evaluated with only statistically significant correlations ( $p < 0.5$ ) being reported.

PCA1 encoded for memorize-oriented learners who did not value intellectual or practical benefits of organic chemistry. These students had a significant positive correlation with the expected grade probe ( $p < 0.0001$ ) and a significant negative correlation with the exams representative of their knowledge probe ( $p = 0.0004$ ). This indicated that this group expected a high grade but did not view their exam scores as representative of their knowledge.

PCA2 encoded for independent learners exhibiting a desire for a coherent structure in their learning of organic chemistry. PCA2 had a significant negative correlation with the difficulty probe ( $p = 0.0005$ ). This indicated that these students did not believe that the course was relatively difficult.

PCA3 encoded the molecular modeling probes and had no significant correlations with the demographic items.

PCA4 encoded for independent learners with value of practical benefits of organic chemistry. PCA4 had a slightly statistically significant positive correlation with the representative probe ( $p = 0.450$ ), indicating that learners in PCA4 believed that their exams were reflective of their knowledge in organic chemistry.



PCA5 encoded for independent learners who spent little time in learning organic chemistry. The PCA5 group had a slightly significant positive correlation to the difficulty probe ( $p = 0.0455$ ). This displayed a belief that the course represented one of the most difficult in their experience.

PCA6 encoded for independent analytical learners who displayed a statistically significant correlation with the gender probe ( $p = 0.0212$ ). Thus, female students were more likely than male students to fall into this category.

PCA7 encoded for memorize-oriented learners. PCA7 had a significant positive correlation with the representative probe ( $p = 0.0208$ ) indicating that this group also believed their exams were representative of their knowledge.

The above sections presented the results of the analysis of the statistical data from the written survey probing students' beliefs in organic chemistry. The remainder of the chapter will comprise a discussion of the results.

### **Discussion of Written Survey Results**

This discussion focuses on an examination of the findings, the limitations of the survey data, and recommendations for further research with regard to the written survey.

#### Examination of the Findings of the Survey Data

This section presents the discussion of the distribution analysis, the principal component analysis, and the correlation with demographic data.

Discussion of Distribution Analysis:

As stated earlier, students responded favorably for most of the probes in the written survey. Table 5-2 represents a summary of the results. *SA* in this table refers to students responding with “strong agreement”. *A* refers to an item with a majority of students responding in “agreement”. *D* refers to students responding predominantly in “disagreement”. *N* refers to “no clear preference” in student response.

**Table 5-2: Distribution Analysis Summary**

Category	Desirable											
<b>Independence</b>	<b>1</b>	<b>2</b>	<b>5</b>	<b>13</b>	<b>26</b>	<b>28</b>	<b>29</b>	<b>34</b>	<b>35</b>	<b>36</b>	<b>40</b>	
	SA	A	SA	D	A	A	SA	A	D	D	SA	
<b>Coherence</b>	<b>10</b>		<b>11</b>		<b>14</b>		<b>20</b>		<b>37</b>		<b>39</b>	
	A		N		N		A		SA		SA	
<b>Concepts</b>	<b>25</b>						<b>30</b>					
	A						N					
Category	Undesirable											
<b>Independence</b>	<b>4</b>	<b>6</b>	<b>16</b>	<b>19</b>	<b>23</b>	<b>31</b>	<b>32</b>	<b>33</b>	<b>38</b>			
	D	A	D	N	D	A	A	D	A			
<b>Coherence</b>	<b>8</b>		<b>9</b>		<b>18</b>		<b>22</b>					
	A		N		A		D					
<b>Concepts</b>	<b>3</b>	<b>7</b>	<b>12</b>	<b>15</b>	<b>17</b>	<b>21</b>	<b>24</b>	<b>27</b>				
	A	N	D	A	A	N	A	D				

Ideally, respondents would predominantly agree with the desirable beliefs and predominantly disagree with probes that indicate undesirable beliefs. As seen in Table 5-2, this was not the case.

Students did not value spectroscopy, or molecular modeling media, as indicated by the predominant disagreement with Items 13, 35 and 36 for the desirable beliefs of the independent category. This could be explained by an absence of

laboratory experience<sup>30</sup> and the lack of need to account for the reactivity of molecules as a result of three-dimensional molecular structure. Spectroscopy, as a major component of analysis in organic chemistry laboratory, could be viewed as more valuable if students had more practical experience of the theoretical experience included in lecture.

The lack of need to account for reactivity from a molecular structure perspective could be a direct result of students' reliance on the instructor as the purveyor of information. The results exhibited this in the students' agreement with the undesirable beliefs related to students' reliance on a "good instructor" for their learning of organic chemistry (Items 31, 32 and 38). The textbook, as authority, did not require students to account for reactivity from a molecular structure perspective on most problems, despite their encouragement in the forewords of the texts (see chapter 1). In addition to the problems in the text, the problems on exams did not require the students to account for reactivity from the perspective of molecular structure. This resulted in the students' choosing not to use molecular modeling media.

Students' agreement with Items 8 and 18 indicated the possible presence of the belief that organic chemistry lacked a coherent structure. However, students strongly agreed with Item 38 (*concepts build upon each other*), which would contradict the *pieces belief* indicated by responses to Item 8, in particular. Therefore, the distribution data did not reveal a consistent pattern regarding students' beliefs about the coherence of organic chemistry.

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<sup>30</sup> Students at the university where this study took place were not required to enroll in the organic chemistry laboratory course concurrently with the lecture.

This contradiction of ideal responses was also present in the concept category. However, with only two items denoted as desirable, and only one (Item, 25) with a majority of responses in agreement, the distribution of student responses revealed only the possible presence of students with the memorize-oriented way of thinking (by their agreement with Items 3, 15, and 24). The pattern of student responses in the principal components analysis also supported the possible presence of the memorize-oriented way of thinking (discussed in the following section).

#### Discussion of Principal Components Analysis:

The results of the survey data show that seven principal components accounted for 51% of the variance in the data. Table 5-1 summarizes the results of the interpretation of the seven principal components as well as the correlations with the demographic item probes.

The results of the Phase II survey indicate that most of the students classified in one of the seven principal components could be classified as independent learners, as observed by the classifications of PCA2, PCA4, PCA5 and PCA6 accounting for 25% of the variance. The second largest contingent held beliefs strongly associated with a memorize-oriented way of thinking (PCA1 and PCA7) accounting for 19% of the total variance.

Although PCA2, PCA4, PCA5 and PCA6 were interpreted as independent learners, only PCA4 could be interpreted as encoding for non-memorize-oriented belief about learning organic chemistry as indicated by the relatively strong negative loadings of Items 3 (-0.24) and 4 (-0.26) in the 40 x 40 cross-correlation matrix (see

Appendix 8). The presence or absence of a memorize-oriented belief for PCA2, PCA5 and PCA6 could not be established due to the inconsistent variations and relatively small associations for Items 3 and 4 (and other memory probes) in all three of these principal components. As a result, only 19% of the variance could account for the memorize-oriented belief about learning organic chemistry. PCA4, the only significant non-memorize-oriented component, accounted for a mere 5% of the variance in the data set. In summary, the results quantitatively identify a memorize-oriented belief about learning organic chemistry accounting for 19% of the total variance.

Analysis of the data did not warrant further combinations of principal components beyond those with the memorize-oriented belief and those interpreted as independent learners. In fact, even these combinations showed inconsistent behavior as indicated by the correlation analysis with the demographic data.

#### Discussion of the Demographic Correlation Analysis:

The discussion of the demographic correlation focuses on two cases where closely related groups correlated with the same demographic variable in very different manners.

Overall, independent learners who had a desire for coherence (PCA2) did not view the course as especially difficult, while independent learners who spent little time in their studies (PCA5) did view the course as difficult. This was not surprising; the students who focused on building a coherent structure of organic chemistry would be expected to have a better foundation on which to build their knowledge.

Memorize-oriented learners who did *not* value the intellectual or practical benefits of organic chemistry (PCA1) had a positive correlation with the expected grade and a negative correlation with the exams representative of knowledge probe. This is in contrast to the other memorize-oriented group (PCA7) who showed a positive correlation with the exams being representative of their knowledge. One interpretation of the correlations for PCA1 could be that students who displayed a lack of appreciation for the intellectual or practical benefits of organic chemistry either were high achievers (based on high grades) who disagreed that the exams accurately reflected their knowledge. Another interpretation could be that they were students who desire to be high achievers (expect a high grade but may not receive it) but did not perform to that standard on exams.

The correlation with the demographic variables did not provide compelling evidence linking any one group of responders with specific demographic indicators. One unexpected result was the correlation of females with the independent analytic learners group. This was unexpected due only to the fact that no gender correlations were expected, as none have been reported in the literature in performance in organic chemistry.

Further revision of the survey may result in fewer principal components accounting for a greater percentage of the variance in the survey responses. This is a consideration of the limitations of the survey data, as well as recommendations for further research using the survey.

### Limitations of the Survey Data

The findings of the survey data revealed a total of 13 principal components having eigenvalues greater than one. The components were narrowed to seven principal components by analysis of a scree plot and patterns of rotated factor analysis. The high number of principal components to be considered created a much broader group of variables than originally expected. Modification of the survey may narrow the number of principal components while still accounting for a high percent of the variability of the data. A smaller number of principal components accounting for a greater percentage of the variability would result in data that described a greater portion of the students.

Although validity was examined during the development phase of the survey via student interviews and consultation with organic chemistry instructors, redesign of the survey before administration for this dissertation could have resulted in possible validity issues. For example, most of the learning tool items were added based on instructor recommendations to the survey. Although inclusion of these items reflected the value of the experts regarding how new knowledge in organic chemistry is created, the students did not value most of these learning tools in their own learning. This was particularly evident in PCA3, which was directly associated with two of these tools, molecular modeling kits and computer modeling, and accounted for 7% of the variance.

The reliability coefficient values (as measured by Cronbach  $\alpha$ ) were above 0.7 for all items. For measuring affective domains, values above 0.7 indicated strong reliability (Gabel 1986).

All of the survey data was collected at one university. As a result, the generalizability of the results could not be considered beyond this particular institution. The results were, however, consistent between the unchanged probes in the initial administration during spring quarter of 2003. Spring quarter generally has the highest enrollment in the third quarter of the year-long organic chemistry sequence at this university due to the fact that most students begin their three quarter sequence in fall and end it in spring. Pilot data was collected in two discussion sections (N=45) during spring 2003 with very similar frequency distribution results on unchanged probes. This would indicate that the survey results were most likely generalizable across the student sample at this particular university. An additional administration at the same institution with an increase in the number of respondents would help confirm this conjecture. Generalizability across institutions would be an area of future research.

#### Recommendations for Future Research Using the Written Survey

As indicated earlier, administering the written survey at different institutions would provide information relative to the generalizability of the results across a broader demographic domain. As a result, a revised survey could be made available for administration by chemistry educators at various institutions.



In addition, as with the MPEX (Redish, Saul et al. 1998) survey, the Phase II survey could be administered to various levels of students and experts to evaluate differences in their responses. Redish also used the MPEX survey at the beginning of the course and at the end of the course to measure change in expectations. This survey could also be used to measure change in students' beliefs in organic chemistry by administering it at the beginning of the year-long sequence and at the end.

Further revision of the survey would be required to decrease the number of principal components while increasing their account on the variance of the data. Therefore, before any extended distribution, the survey should be revised and refined to better account for students' ways of thinking associated with their beliefs in organic chemistry. This could include removing some or all of the items from the learning tools group, as well as refining items that provided inconsistent data. For example, Item 10 probed students' beliefs about learning, relative to knowledge of molecular structure, reactivity and organic synthesis. This probe was intended to indicate a favorable inclination toward the students' understanding of underlying concepts versus memorizing reactions. However, the loadings for Item 10 were strongest in PCA1 encoding for a memorize-oriented belief about learning organic chemistry.

One goal of this survey was to evaluate quantitatively the students' ways of thinking associated with beliefs in organic chemistry that would influence their ways of understanding in organic chemistry. Although the data indicated that further revision of the survey would be warranted, the results of this administration of the survey did provide insight into the predominate beliefs confirming the presence of the

memorize-oriented way of thinking in organic chemistry. The impact of these beliefs will become apparent in the presentation of the results of the DNR-based teaching interviews of Phase III.

## CHAPTER 6: RESULTS ON WAYS OF UNDERSTANDING THE CONCEPT OF AROMATICITY AS A RESULT OF DNR-BASED INSTRUCTION

One of the goals of incorporating the Phase III teaching interviews in this research was to explicate the potential for developing desirable ways of understanding as a result of an instructional intervention where the design was informed by the constructivist ideas of what constitutes student learning (von Glasersfeld 1995). Based on the results of the Phase I interview data, it was postulated that students in this study would exhibit non-referential symbolic (NRS) reasoning at the outset of the teaching interviews. As a result, helping students develop referential symbolic reasoning became the cognitive objective during the design of problem tasks. Referential symbolic reasoning, as the cognitive objective, provided the impetus for the design of the learning tasks to guide students in their development of more desirable ways of understanding the concept of aromaticity. Yet, due to the short duration of the teaching interviews, students' referential symbolic reasoning was not expected to be robust.

The teaching interviews, conducted individually with five students over three sessions, each lasted approximately ninety minutes. During each session the students solved several tasks, each designed to lead them to develop and/or refine their ways of understanding aromaticity. The tasks were typically comprised of several different problems leading to one particular learning objective. (It is important to remain cognizant of the fact that the development of students' ways of understanding as a result of each learning task does not imply that students developed *desirable* ways of understanding from any one task.) The design of each task was intended to guide students in their development of a way of understanding based on a hypothetical

learning trajectory, discussed more fully later in this chapter. After students completed a set of problems from one task, subsequent tasks were designed to account for a hypothesis generated by the researcher on their current way of understanding, and to create cognitive conflict. The culmination of the entire set of tasks was designed to help students develop a more desirable way of understanding the concept of aromaticity than the traditional lecture approach.

The first section in this chapter highlights the hypotheses about the development of students' way of understanding, based on each of the six tasks comprising the core of the teaching interview sessions. The sequence and exact nature of the tasks were slightly modified for each individual student, based on their results from the previous teaching interview sessions.

After the hypothetical learning trajectory, this chapter presents the results of the analysis of the teaching interviews for two students, Robert and Abby<sup>31</sup>. I present a detailed analysis of Robert's way of understanding, and then use the results from Abby as supporting evidence for the potential of developing more desirable ways of understanding as a result of an instructional intervention. Robert's analysis was chosen to provide an example of a student who developed more desirable ways of understanding aromaticity, as well as to display evidence of the potential for change in one's ways of thinking. Abby, on the other hand, did not exhibit any evidence of a change in her ways of thinking, but she did display evidence of developing more desirable ways of understanding aromaticity. More desirable ways of understanding

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<sup>31</sup> These are fictitious names, maintaining only the students' gender and first letter of their real names. (Student names were assigned in this chapter to more readily differentiate Phase III of the study from Phase I, where students were assigned a number.)

were established when students emphasized the critical attributes of aromaticity over the variable attributes (see Appendix 6 for concept analysis of aromaticity).

In addition, this chapter includes a discussion of the overall results of the analysis for the remaining three students, two of whom did *not* develop desirable ways of understanding aromaticity, which is partially a result of their ways of thinking associated with their beliefs about organic chemistry.

### **Pre-Teaching Interview Hypotheses**

The sequence of tasks for the teaching interviews was based on the development of a hypothetical learning trajectory constructed for developing the concept of aromaticity, where subsequent tasks were designed specifically to perturb students' existing ways of understanding. Only tasks associated with the development of the concept of aromaticity are presented below, however, most of the students required additional intervention regarding the concepts of hybridization and resonance.

#### Teaching Interview Session 1

The goal for the first teaching interview session was not only to introduce the concept of aromaticity through problem solving, but also to evaluate each student's initial ways of understanding aromaticity, and to confirm the presence of non-referential symbolic reasoning.

#### Task 1: Establishing Characteristic Features of Benzene

The first task presented to the students was a historically-based (Krygowski, Cyranski et al. 2000) situation in which aromatic compounds differ substantially from

what would be expected, based on trends in heats of hydrogenation for cyclohexene, cyclohexadiene, and cyclohexatriene compounds. This first task included a discussion of the molecular structure of the six-membered rings, in order to evaluate the student's ways of understanding the symbolic representations, and infer NRS. The overall purpose of the first task was for the student to recognize the culmination of the set of solutions, resulting in the student's way of understanding benzene as having specific characteristics due to its unique stability. The hypothesis was that students would focus on superficial symbolic features, for example the cyclic ring with conjugated double bonds, over the actual molecular structure of benzene.

### Task 2: Distinguishing Between Aromatic, Anti-Aromatic and Nonaromatic Compounds

The purpose of Task 1 was for students to identify characteristic features of benzene in order to account for its increased stability. Even if students addressed supposed structural features (for example, hybridization of the carbon atoms), Task 2 was designed to perturb these superficial symbolically-based characteristics and introduce molecular orbital (MO) theory<sup>32</sup> as a tool for distinguishing between aromatic and anti-aromatic compounds using cyclobutadiene. Task 2 concluded with the student distinguishing between aromatic, non-aromatic and anti-aromatic cyclopentadiene and its corresponding ionic compounds. The hypothesis for the final

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<sup>32</sup> Molecular Orbital (MO) theory here refers to the linear combination of atomic orbitals to form molecular orbitals with varying energy-levels. During the teaching interviews, the students' way of understanding MO theory was not evaluated in-depth. MO theory was used as a tool to distinguish between the stabilization of aromatic compounds and the destabilization of anti-aromatic compounds. MO theory was also used as a tool for students to generate Hückel's Rule for generalizing a trend in MO patterns of various aromatic compounds.

problems of Task 2 was that students would ignore molecular structure features, for example that cyclopentadiene is non-planar, and focus on molecular orbital theory to justify their responses.

### Task 3: Deriving Hückel's Rule and Refining Characteristics of Aromatic Compounds

The final task for the first teaching interview session was intended to exploit the new presumed preference for MO theory. The student would extend their ways of understanding the characteristics of aromatic compounds by deriving Hückel's Rule through pattern recognition from the MO diagrams of benzene and various polycyclic aromatic compounds.

### Teaching Interview Session 2

The goal for the second session was two-fold: 1) to assess students' current ways of understanding by asking them to identify aromatic compounds, and 2) to extend the concept of aromaticity to heterocycles. The exact nature of the compounds to be identified and the sequencing of these tasks varied slightly per student. In addition, Session 2 typically incorporated an instructional intervention based on results from the first session. Typically, this included revisiting the concepts of hybridization and resonance.

### Task 4: Application of Aromaticity: Identifying Aromatic Compounds

Problems in Task 4 asked students to identify aromatic compounds from a variety of options and to justify their identifications. Students were also asked to identify compounds as either anti-aromatic or non-aromatic. The purpose of this set of problems was to provide the researcher with feedback on students' developing ways of

understanding the concept of aromaticity throughout the last two teaching sessions. (The problems in this task extend into the third teaching interview session but are presented as Task 4 because the first of these problems occurred prior to Task 5.)

#### Task 5: Extending Aromaticity to Heterocycles<sup>33</sup>

Task 5 typically occurred as the final task of Session 2. Students were presented with experimental data that revealed that each heterocycle (furan, pyrrole and thiophene) was aromatic with varying degrees of stability. The intent of these problems was to establish aromatic stabilization as a driving force for structural considerations. These tasks were purposely sequenced following the students' development of Hückel's Rule in order to redirect them to the molecular structural aspects associated with aromaticity. Upon discussion of heterocycles, the final problem in Task 5 asked students to identify the aromatic compounds from three possible structures. The hypothesis was that students would focus on features of the molecular structure with less superficiality than at the beginning of Session 1.

#### Teaching Interview Session 3

The goal of Session 3 was for students to apply their way of understanding aromaticity to problem solving in organic synthesis via electrophilic aromatic substitution reactions.

#### Task 6: Application of Aromaticity: Bromination of Aromatic Compounds

The mechanism of bromination of benzene was presented to students while explaining that the aromatic stability required the activation of bromine with a Lewis

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<sup>33</sup> Aromatic heterocycles, in this dissertation, are aromatic rings containing oxygen, nitrogen and/or sulfur. There are many more examples of aromatic heterocycles containing a variety of different atoms. For a complete review of these compounds see Balaban et al. (2004).



acid catalyst. Students were subsequently asked to approximate the rates of the two-step bromination reaction. The second problem in this task asked students to identify the preferred location of substitution on naphthalene, and to justify their response. The purpose of Task 6 was to evaluate students' applications of their ways of understanding aromaticity in electrophilic aromatic substitution reactions. In addition to naphthalene, some students were also asked to identify the preferred location of bromination for anthracene and phenanthrene (see Appendix 5).

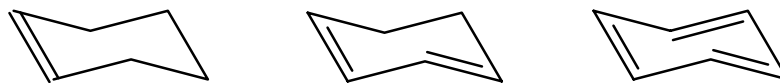
### **Results of Teaching Interview Sessions: Robert**

The results of the teaching interview sessions with Robert are presented according to the ways of understanding generated by each task. In addition, Robert's way of thinking was inferred from the initial ways of understanding portrayed in the first tasks and in the last tasks, in order to evaluate any changes in his ways of thinking. There was no expectation that a student's ways of thinking would change in this short-term teaching interview intervention.

#### Robert Task 1: Initial Ways of Understanding

During the sequence of problems for Task 1, Robert exhibited clear evidence of non-referential symbolic reasoning. This section presents the initial ways of understanding resulting in the inference of NRS reasoning through Robert's three-dimensional representation of benzene and his way of understanding hybridization.

For both cyclohexene and cyclohexadiene, Robert drew three-dimensional structures analogous to the "chair formation" of cyclohexane. He continued the use of the chair conformation even when drawing his initial representation of benzene.



**Figure 6-1: Robert's Chair Conformational Structures**

Although a molecular modeling kit was available, Robert did not attempt to build a model of either of these structures. The drawing of chair-like structures indicated a strong association between six-membered carbon rings and the chair conformation.

After Robert drew benzene in a chair conformation, he was asked about the hybridization of each carbon in benzene. He replied, "I'm kind of guessing that this is  $sp^2$ ...No. Is it  $sp^3$  or  $sp^2$ ?  $Sp^3$  or  $sp^2$ ? 'Cause there-yeah." Further discussion revealed that his confusion was associated with carbon having both a single bond on one side and a double bond on the other. In addition, Robert's way of understanding hybridization can be categorized as *symbolic reference without counting*. Thus, Robert equated a single bond with  $sp^3$  hybridization and a double bond with  $sp^2$  hybridization. For benzene, Robert viewed each carbon as having both a single bond and double bond resulting in confusion over which type of bond to attend to for assigning hybridization. After Robert reviewed hybridization, including assigning bond angle values for each of  $sp^3$ ,  $sp^2$  and  $sp$ , he paused and finally proclaimed, "I got 'em!" and assigned  $sp^2$  to each carbon. He did not, however, immediately change his chair structure conformation.

Because the purpose of Task 1 was for students to generate initial characteristics of aromatic compounds from benzene, it was important to address the inaccuracy of Robert's three-dimensional structure. I did this by asking Robert how he accounted for the  $sp^2$  hybridization in his three-dimensional structure. He replied,

“Um, so all the hydrogen, they should be planar, too.” And drew two hydrogens point down on the chair conformation. He paused for over thirty seconds and proclaimed, “It’s not right.” After nearly two additional minutes, Robert realized his mistake:

**Robert:** Shouldn’t they be flat? Yeah. So actually [*he redraws the structure correctly (see Figure 4-1)*] Something like this. Yeah. Yeah, basically it should be flat.

**Interviewer:** Ok. So what made you change your mind from the chair structure to the planar structure?

**Robert:** Well, I realized that it’s just  $sp^2$ . It’s just planar and if you look at this [*refers to chair*] then, you know. If you look at this structure, it’s tetrahedral. If you look at each carbon.

In the above transcript excerpt, Robert realized that carbon atoms in the chair conformation are tetrahedral. It appeared that he was not relating his explanation to the actual molecular structure of cyclohexane, but instead he recalled that each carbon in the chair conformation of cyclohexane had single bonds, was  $sp^3$  hybridized, and thus, tetrahedral.

Given benzene’s planar structure and contributing resonance structures, Robert distinguished the main characteristics of benzene resulting in aromaticity. In the following excerpt from the end of Task 1, it is interesting to note that Robert uses non-scientific language to explain the distinguishing characteristics, preferring to write down the scientific terminology on paper.

**Robert:** It’s lower reactivity. That’s one thing. It’s stable so it doesn’t really, you know, it doesn’t go on reaction fast. I think having this aromatic molecule here [*points to symbolic representation of benzene*], or whatever, is gonna make the entire molecule stable.

**Interviewer:** So there are some structural characteristics of benzene that you can use to help you determine if other molecules are aromatic? It's cyclic?

**R:** Yeah. It's a ring [*writes the word "ring"*]. It's flat [*writes the word "planar"*]. And all the electrons can be shared throughout all the carbons. [*pauses*] I don't really--

**I:** So you have delocalization of the *pi* electrons?

**R:** Yeah. [*writes the words "delocalized pi electrons"*]

Roberts' initial way of understanding aromaticity was characterized as an *unordered list of four critical attributes*. One important point is that Robert attended to the reactivity of benzene before he mentioned structural features. Historically (Krygowski, Cyranski et al. 2000), the stability of benzene resulted in a desire by chemists to identify its structure (which was unknown until Professor F. August Kekulé reportedly had a dream of a snake biting its tail, in order to account for the unpredicted stability). The entire class of aromatic molecules was initially characterized by the unusual stability that they exhibited. The fact that Robert began his characterization with the stability of benzene revealed that he had not forgotten the context of the problem, despite the veering of the discussion towards the molecular structure. Stability, however, became a contradictory factor relative to aromaticity during Task 2, and, perhaps as a result of the conflicting ideas Robert encountered in Task 2, was not mentioned again by Robert as one of the characteristics of aromatic compounds.

#### Robert Task 2: Stability and Aromaticity Became Independent Factors

As expected, Robert predicted that cyclobutadiene would be aromatic because of the structural features (he wrote, "ring, planar, delocalization of *pi* electrons")

neglecting reactivity. He later claimed that the molecule was aromatic but unstable because of ring strain, ignoring the MO diagrams of benzene and cyclobutadiene. During Task 2, Robert explicitly stated that aromaticity and stability were independent, despite his initial characteristic of aromatic compounds as stable (at the end of Task 1).

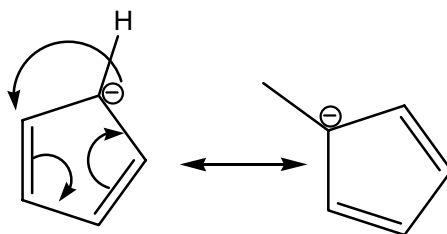
Task 2 also involved distinguishing between aromatic, anti-aromatic and non-aromatic compounds using cyclopentadiene and its ionic counterparts (see Appendix 5). Robert drew the MO diagrams for these compounds and correctly distributed the electrons. He immediately stated that the cyclopentadienyl anion was aromatic because the MO diagram was similar to benzene, but he was not sure if it was planar because one carbon is  $sp^3$  hybridized. After Robert drew resonance structures for all three compounds, he reconciled the issue of planarity in the following way.

**Robert:** Ah. In fact, I can draw it. So this is 120 and 109.5. So there are four  $sp^2$  and one  $sp^3$ . Um. So it can be, like, not. Wait. 120. [*writes "117.9"*] So an angle between like, you know, the three. These like carbon, carbon, hydrogen. It can be like this degree. It's not like flat flat but it's kind of flat with a little, like, tetrahedral shape.

Robert rationalized planarity for the anion by stating that the bond angle changes to accommodate the delocalization of the electrons. He did not, however, apply the same reasoning to the delocalization of electrons in cyclopentadiene. Immediately after explaining that cyclopentadiene was not aromatic because it was not planar, due to the  $sp^3$  hybridized carbon, Robert drew two resonance structures for cyclopentadiene (indicating that there would also be a third structure). Thus, his way of understanding the symbolic representation of molecules was consistent with *lines*

and letters<sup>34</sup> by ignoring the implicit hydrogen atoms and drawing resonance for cyclopentadiene. His way of understanding hybridization as *symbolic reference without counting* (attending to the single bonds only) resulted in a correct assignment of  $sp^3$  hybridization, without accounting for the implicit hydrogens.

Robert's way of understanding resonance was characterized as *moving symbols to produce quantity* as displayed by the following example.



**Figure 6-2: Robert's Cyclopentadienyl Anion Resonance**

In the above symbolic representations, Robert moves the negative charge to a separate carbon rather than distributing the lone pair. Robert explicitly defined resonance as “two different structures can...contribute to the overall structure.” He later explained that there would be five structures for both the anion and the cation to delocalize the charges across each carbon. Despite his acknowledgement of several structures, Robert generally drew only two structures each time he drew resonance. Both of these ways of understanding, *lines and letters* and *moving symbols to produce quantity*, supported the presence of non-referential symbolic reasoning.

At this point in Task 2, Robert had drawn resonance structures for all of the molecules. He had explained that the cyclopentadienyl anion was aromatic because of

<sup>34</sup> The *lines and letters* way of understanding symbolic representations denotes that the student does not attend to the actual physical meaning of the symbolic representation, but views the symbols as merely lines and letters (see chapter 4 for a more detailed discussion).

a MO diagram that resembled the MO diagram of benzene, reconciling the planarity of the molecule as not *completely* planar, but *close to* planar. Cyclopentadiene was not aromatic because it was not planar, even though he drew resonance structures. The remaining cyclopentadienyl cation was considered aromatic but unstable, based on the MO diagram being similar to the MO diagram of cyclobutadiene. At this point, Robert had a way of understanding aromaticity that did not account for the added stability that he mentioned in Task 1.

Robert was able to utilize the MO diagrams without comprehending their meaning. Further instruction on the meaning of the MO diagrams resulted in Robert designating cyclobutadiene and cyclopentadienyl cation as anti-aromatic compounds. Reconciliation of the planarity of cyclopentadienyl anion also occurred through direct instruction. The student was asked to relate the relative stability of  $sp^3$  hybridization with the net gain in stability for an aromatic molecule upon restructuring the geometry to  $sp^2$  hybridization. The resulting change in hybridization would allow for delocalization of the lone pair throughout the ring. There was no attempt to directly address Robert's undesirable ways of understanding structure and resonance.

### Robert Task 3: Refining Aromatic Characteristics

Task 3 involved deriving Hückel's Rule through recognition of a pattern in the MO diagrams of benzene and several polycyclic aromatic compounds, and refining the characteristics of aromatic compounds given Hückel's Rule. Robert accomplished both in a relatively short time frame. He derived Hückel's Rule ( $4N+2$ ), accounting for  $N$  being a whole number greater than or equal to zero as

“molecular orbital levels.” The refined characteristics of aromatic compounds comprise four components that Robert described as “four rules: it has a ring, it has to be planar, you have to be able to delocalize the *pi* electrons, and it has to fit this rule, this  $(4N+2)$  rule.” Revisiting all previous molecules confirmed the credibility of Hückel’s Rule for Robert. Thus, Robert’s way of understanding aromaticity after Task 3 was associated with four rules: ring, planar, delocalization of pi electrons, and must fit  $(4N+2)$ . This way of understanding for Robert was characterized as *a list of four characteristics*.

#### Robert Task 4: Identifying Aromatic Compounds

The discussion in this section focuses on Robert’s identification of aromatic, anti-aromatic and non-aromatic compounds during Session 2. The first problems for Task 4 (see Appendix 3, Interview Sheets 4a and 4b) were presented before Task 5, while the remaining problems in Task 4 (see Appendix 3, Interview Sheets 4d and 4e) were presented to Robert after Task 5 since these contained molecules with heteroatoms, the topic of Task 5.

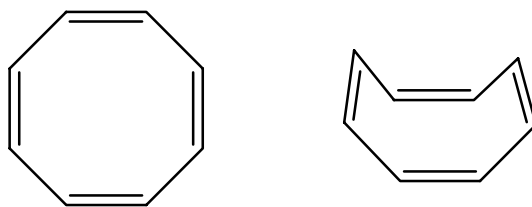
Robert identified all but one of the structures for the molecules (on Interview Sheet 4e) correctly. He identified cyclopentadiene as anti-aromatic rather than non-aromatic. Cyclopentadiene was a structure that Robert had reviewed (per his request) just prior. Without explaining which structure was incorrect, Robert was asked to assess his responses, given that one was incorrect. It took nearly four minutes for Robert to discover his mistake. He justified his revised answer by stating, “it [*cyclopentadiene*] doesn’t have *pi* delocalization.” In Task 2, Robert had explained



that cyclopentadiene was not aromatic because it was not planar, given the  $sp^3$  hybridized carbon (recall, however, that he did draw resonance structures). Later during Task 2, Robert designated cyclopentadiene as anti-aromatic on the basis of the MO diagram.

In Task 4, Robert's initial assignment of anti-aromatic was again founded on the MO diagram, and the presence of only four  $\pi$  electrons. Upon reevaluation, Robert's reassignment of cyclopentadiene as non-aromatic was not referenced as resulting from the non-planarity of cyclopentadiene, but the inability to delocalize the  $\pi$  electrons throughout the cyclic structure. For Robert, this meant the inability to draw valid resonance structures.

Recall that Robert's way of understanding resonance was *moving symbols to produce quantity*. Introduction of Hückel's Rule resulted in a reinforcement of NRS reasoning, due to his reliance on resonance. As a result, Robert continually assessed cyclooctatetraene as anti-aromatic rather than non-aromatic. Figure 6-3 shows the typical representation of cyclooctatetraene on the right, while the left representation is more consistent with the actual three-dimensional tub shaped structure.



**Figure 6-3: Cyclooctatetraene Representations**

Robert's way of understanding resonance as *moving symbols to produce quantity* would not reveal the non-planar nature of cyclooctatetraene. Students would only

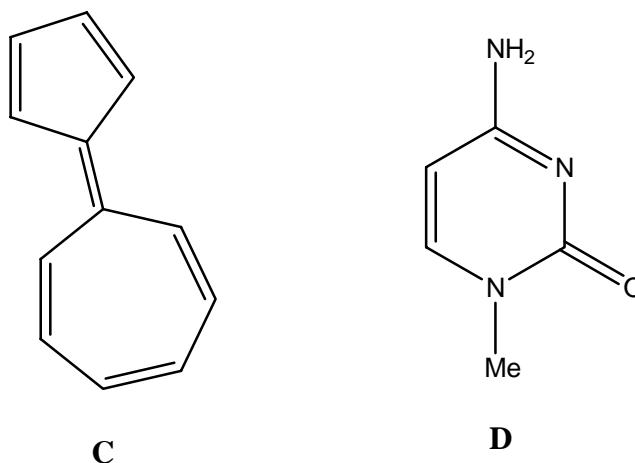
know this through building a model of the structure, or through interpretation of either IR or NMR spectra. During the teaching interviews, Robert could not be persuaded to build models of the structures because he felt confident in his ability to draw the structures on paper.

Identifying aromatic compounds for the heterocycle portion of Task 4 revealed that Robert's understanding of hybridization had changed from *symbolic reference without counting* to *symbolic reference with global structural considerations*. In other words, Robert still associated  $sp^3$  hybridization with atoms connected by single bonds, but he now accounted for the structural feasibility of changing hybridization in order to create a more stable aromatic compound. As a result, Robert identified all of the heterocycles on Task 4 (Interview Sheets 4a and 4b, part of the interviews in Phase 1) correctly. Robert's way of understanding aromaticity expanded to account for transformation of hybridization in favor of aromaticity.

For Robert, Task 4 concluded with Interview Sheet 4e, which included a list of compounds that appeared on an exam written by Robert's organic chemistry instructor in a previous term. Robert explained his assignments of aromaticity and anti-aromaticity to each compound solely on the basis of Hückel's Rule. Later discussion revealed that he had attended to other features, but had only mentioned the deciding feature,  $(4N+2)$ , because all of the molecules on Interview Sheet 4e (see Appendix 3) were deemed cyclic, planar, with  $sp^2$  hybridized atoms throughout the ring. He had developed a heuristic that he explained as follows:

Like first I'm gonna look at if it's planar. That's the first thing I'm gonna look at, you know, like is everything  $sp^2$ ? Then you can check if every atom has  $\pi$  orbitals and then after that I would count the  $\pi$  electrons and apply the *four N plus two*.

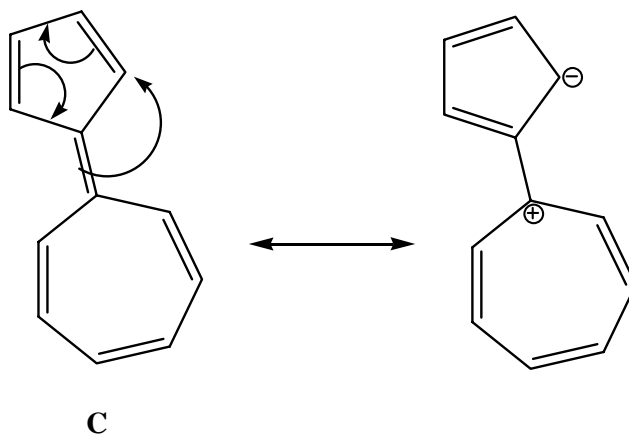
Structure C and D were the only two structures that posed a problem for Robert (see Figure 6-4).



**Figure 6-4: Interview Sheet 5e Structures C and D**

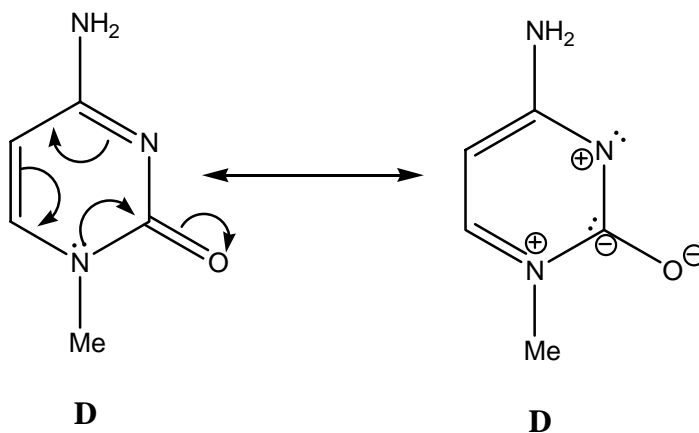
Robert claimed that the double bond between the two rings in structure C, and the double bond between carbon and oxygen in structure D, could not move because “it is stuck between the two and can not, you know, delocalize. That  $p$  orbital is full and can not, you know, help move the electrons around the ring.” Further probing revealed that for both situations Robert believed that the occupied  $p$  orbitals blocked the ability to draw resonance similar to an  $sp^3$  hybridized carbon and, as a result, he designated these molecules as non-aromatic. He confirmed this by stating that they did not have resonance structures. When I informed him that these two structures were aromatic and asked him to account for this, he accounted for it through

resonance with one resonance structure for C (see Figure 6-5) and drew an analogous resonance structure with structure D (see Figure 6-6).



**Figure 6-5: Robert's Resonance For Structure C on Interview Sheet 5e**

Figure 6-5 demonstrates Robert's way of understanding resonance as *moving symbols to produce quantity*. He moved the central double bond to an adjacent carbon, and only drew two resonance structures. This confirmed that Robert maintained NRS reasoning. Figure 6-6 provides further evidence for Robert's NRS reasoning.



**Figure 6-6: Robert's Resonance For Structure D on Interview Sheet 5e**

The flow of arrows in the left structure in Figure 6-6 shows that Robert moved the lone pair of electrons on nitrogen completely off of nitrogen and onto the adjacent carbon atom to the right. The resulting resonance for the structure on the right did not pose problems for Robert, despite the multiple occurrences of charge separation. Recall that “quantity” of resonance, for Robert, was two structures. For Structure D, Robert had two resonance forms and, therefore, he was satisfied with the structure he drew (as illustrated on the right of Figure 6-6). This structure would not be considered a viable option for any chemist.

#### Robert Task 5: Accounting for Heterocycle Aromaticity

In Task 5, students were presented with data revealing that certain heterocycles were aromatic, and asked to account for this using resonance theory. Robert immediately drew several pairs of resonance structures, resulting in several pairs representing the same structure. He then drew the MO diagram for furan (see Appendix 5) accounting for eight  $\pi$  electrons, resulting in two unpaired electrons occupying a higher, anti-bonding molecular orbital level. After performing the above actions, Robert paused for just over six minutes, after which the following interaction occurred:

**Robert:** This is aromatic structure?

**Interviewer:** It's aromatic?

**R:** Yeah. Is it?

**I:** It is aromatic. Explain the aromaticity. [*points to problem*]

**R:** Mmm. Well, uh, there are two extra electrons here. [*points to MO diagram*]

I: Oh, Ok.

R: So, there should not be eight, I mean, electrons available for  $\pi$  bonding. Or  $\pi$  orbitals. So these are filled up but should be one for each anti-bonding orbitals and that makes it...you know. [*pause 30 seconds*] I just don't know what—like, what does it mean by, like, large resonance energy? Is it like saying less stable?

I: It's saying more stable.

R: More stable? Ok. Well. I think it has to do something with these two electrons in anti-bonding orbitals but I don't know why.

I: What is the hybridization of the oxygen?

R: It's  $sp^3$ .

I: Ok. And if it's  $sp^3$ , can either one, either pair of those electrons, delocalize in the ring?

R: Yeah. I think so.

I: So, you're saying that both pair are delocalized in the ring? But when we saw something where the electrons, when we had lone electrons, there was destabilization.

R: Right.

I: So if it's aromatic, how could that happen?

R: There's one extra pair of electrons? Like. Ok. You have to get--if--can you just make it like  $sp^2$  orbital and in that way, then these two electrons can just be over here? [*refers to an area outside the ring*]

I: Ok.

R: And you can use the extra two electrons to just, uh, delocalize  $\pi$  electrons. Yeah. So can you do that with like other, with like nitrogen or something like, instead of oxygen?

In the above interaction, Robert recognized the similarity with the hybridization of the cyclopentadienyl anion, and realized that only one lone pair need contribute to the delocalization of the *pi* electrons. When he referred to the other pair “being out there,” Robert drew an orbital outside of the ring attached to oxygen. He anticipated the next problem by asking whether this occurred with nitrogen.

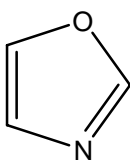
Robert accounted for the aromaticity predominantly through the use of the MO diagram to address the issue of extra electrons (when considering eight). As a result, his way of understanding aromaticity included paired electrons in bonding molecular orbital levels. He also associated aromaticity with the number of electrons, but what bothered him most were the extra electrons in the anti-bonding orbitals.

The transcript excerpt above also reveals NRS reasoning because he originally included both lone pairs of electrons in his MO diagram, even though he referred to the hybridization of oxygen as  $sp^3$  hybridized. If Robert visualized the placement of the lone pair in  $sp^3$  hybrid orbitals, he would not have included either one of them in his MO diagram.

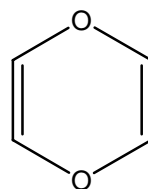
For pyrrole and thiophene, Robert did not draw out resonance structures, but accounted for the aromaticity by stating that nitrogen and sulfur would be  $sp^2$  hybridized, contributing only one pair of electrons to delocalization. Robert accounted for the difference in stabilization by explaining that furan “has a higher electronegativity so it tries to retain the electron. That’s why it’s hard to give up the electron”.

Through the interactions in Task 5, Robert added a new requirement to his characteristics for aromaticity, “it has to be  $sp^2$ .” Although being planar was already part of his characteristics, it appeared to be important for Robert to add the hybridization factor as one of the characteristics for aromaticity. Robert expressed the refined characteristics, as “it’s a ring, planar,  $sp^2$ , delocalized  $\pi$  electrons and all the lower bonding orbitals are filled up.” He did mention the  $(4N+2)$  Rule, stating, “you have to do this [*refers to the characteristics above*] first, and then you can apply  $4N$  plus 2.” Robert’s way of understanding aromaticity increased the number of characteristics, as well as required a distinct order in which these characteristics should be evaluated. This way of understanding aromaticity was labeled as an *ordered list of six characteristics favoring critical attributes*. Four of these six characteristics (ring, planar,  $sp^2$  and delocalized  $\pi$  electrons) constitute critical attributes in the concept analysis of aromaticity (see Appendix 6) while the remaining two ( $[4N+2]$  and lower bonding orbitals filled) constituted variable attributes.

Applying this way of understanding resulted in Robert’s assignment of aromatic and anti-aromatic to the following two structures, respectively.



oxazole



1,4-dioxine

**Figure 6-7: Two Heterocycles with More Than One Heteroatom**

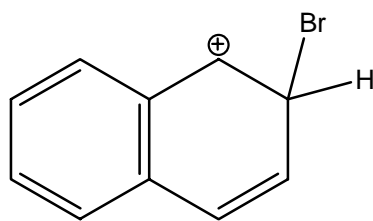


Robert expressed conflict about his designation of anti-aromatic to 1,4-dioxine. “For this one, I thought like, you know, it can, like, won’t oxygen like give up two electrons for  $\pi$  orbital, but what about the other oxygen? Does it have to? I’m kind of wondering if it should be anti- or aromatic?” Further discussion about the driving force for rearranging the molecular geometry about the heteroatom towards  $sp^2$  hybridization did not resolve this conflict. Robert explained that he could visualize the delocalization of electrons around the ring with each oxygen atom alternating between  $sp^3$  and  $sp^2$  hybridization “depending on where the electrons were at the time.” This revealed that Robert held a way of understanding resonance as *separate oscillating entities*, resulting in each entity representing a different state of the molecule.

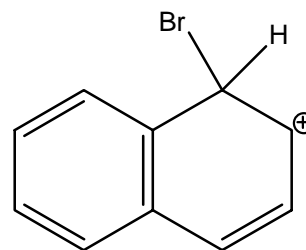
#### Robert Task 6: Bromination of Naphthalene

Application of the concept of aromaticity for organic synthesis problems was evaluated using the bromination of naphthalene. After instruction on bromination of benzene in teaching interview Session 3, Robert was asked to predict which position on naphthalene would result in the brominated substitution product.

Initially Robert chose substitution at the C2 position because, “these should be the same because of the secondary cation [*refers to C2 structure*] and a secondary cation [*refers to C1 structure*]. I think this one [*refers to C2 structure*] would be the major product because it is less crowded. That’s all I can think of.” (See Figure 6-8)



Substitution at C2



Substitution at C1

**Figure 6-8: Robert's Initial Resonance of EAS on Naphthalene**

Robert's way of understanding resonance as *moving symbols to produce quantity* also resulted in his limiting to just two the number of resonance structures drawn. After his initial explanation about steric hindrance (referred to as crowding by Robert) as the only factor influencing the preferred substitution, the following interaction occurred.

**Interviewer:** But what happens if you draw all of the resonance structures?

**Robert:** Um. [*takes a new sheet of paper and begins to draw resonance*]

{3 minutes pass}

**R:** Are there like more than two?

**I:** Yeah.

**R:** Oh. [*takes a new sheet of paper and attempts again*]

{An additional 7 minutes pass}

**I:** I see what you're struggling with. You don't want to break up the aromaticity of the second ring.

**R:** Yeah. I don't think I can do that. I think now this one [*refers to substitution at C1*] is more stable.

**I:** And why?

**R:** Because there are more resonance structures. With this one [*C2 product*] I can only draw one, but with this one [*C1 product*] I can draw two.

Although the number of resonance structures that Robert drew was not correct, his reluctance to break the aromaticity of the second ring revealed that he still incorporated a way of understanding aromaticity as *compounds that are very stable* resulting in his final way of understanding aromaticity at the end of the teaching interview sessions as *an ordered list of seven characteristics favoring critical attribute*.

#### Summary of Robert's Ways of Understanding and Ways of Thinking

Robert developed a more desirable way of understanding aromaticity as a result of an instructional intervention where the tasks were designed to perturb the student's existing ways of understanding. After Task 1, Robert's initial way of understanding aromaticity was *a list of four critical attributes*, emphasizing the stable, cyclic, planar molecule with delocalized  $\pi$  electrons. After completing the final problems of Task 4, Robert had modified his list to include the way of understanding aromaticity *accounting for transformations in hybridization*. This way of understanding required incorporating his previous way of understanding, as well as assessing the compound for a tendency to modify its geometry about one atom (from  $sp^3$  hybridization to  $sp^2$  hybridization), in order to gain aromatic stability.

Task 5 resulted in further refinement of Robert's ways of understanding to an *ordered list of six characteristics favoring critical attributes*. These six characteristics included five critical attributes, "ring, planar,  $sp^2$  hybridized, delocalized  $\pi$  electrons and lower bonding orbitals filled up," and one variable attribute,  $4N+2$ . The ordered

list favored evaluation of the presence of the critical attributes before applying Hückel's Rule. Comparing these five critical attributes to the four mentioned after Task 1 resulted in an acknowledgement that Robert had not merely added another critical attribute to his list. Instead, after Task 1, Robert added two critical attributes ( $sp^2$  hybridization and filled bonding orbitals) and omitted one (stability).

Task 6 addressed the discrepancy of Robert's apparent omission of stability through the application of aromaticity during the electrophilic aromatic substitution reaction of bromination of benzene. Robert's explanations for this task revealed that he did account for the stability of aromatic compounds. As a result, Robert's final way of understanding aromaticity could be characterized as *an ordered list of seven characteristics favoring critical attributes*.

Despite Robert's more desirable ways of understanding aromaticity, this does not imply the development of more desirable ways of understanding hybridization or resonance. Robert's way of understanding resonance as *moving symbols to produce quantity* appeared to be present even during Task 6, when he only drew two resonance structures for the intermediate of the bromination of naphthalene.

There was no evidence that Robert's *ways of thinking* associated with NRS reasoning changed during the teaching interviews, which was expected based on the short duration of the teaching interactions. There was, however, evidence of the *potential* for change in his ways of thinking toward referential symbolic reasoning. This potential was observed during Task 4 with Robert's change in his way of understanding hybridization. Robert's way of understanding hybridization changed

from *symbolic reference without counting* to *symbolic reference with structural considerations*. Although Robert still determined hybridization based on the symbolic features of single bond, double bond, or triple bond, he began to account for structural consequences, a gain in aromatic stability, from a change in hybridization. Accounting for structural consequences only provided evidence for a potential change in his ways of thinking, due to the fact that he did not exhibit more evidence of referential symbolic reasoning. Nevertheless, Robert's persistent way of understanding resonance as *moving symbols to produce quantity* (with the quantity, for Robert, being limited to two structures) revealed the continued presence of NRS reasoning.

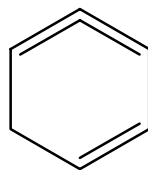
### **Teaching Interview Sessions with Abby**

This section presents the results of Abby's teaching interviews. Rather than highlight developments and changes as a result of each task, this section presents results on the evolution of her ways of understanding aromaticity from each of the three teaching sessions.

#### Abby Teaching Session 1

For Abby, teaching interview Session 1 incorporated Tasks 1 and 2 with an introduction to Task 3. Abby's way of understanding symbolic representations of molecules revealed a way of understanding consistent with *lines and letters* as evidenced by her drawing resonance for cyclopentadiene in Task 2. She did not pay attention to the implicit hydrogens resulting in her non sequitur resonance structure for benzene in Task 1 (see Figure 6-9). Ignoring implicit hydrogens extended to her model building, where she neglected to add hydrogen atoms to her molecular model. As a

result, she had no problem showing the validity of the resonance structure in Figure 6-9 when the model lacked hydrogen atoms. When she was asked to add the hydrogen atoms to the model, she merely moved a hydrogen atom to generate the model for the structure represented in Figure 6-9. Removing the hydrogen atom in the model revealed that Abby did not attend to the actual molecular structure, and did not comprehend the physical meaning of resonance.



**Figure 6-9: Abby's Resonance Structure for Benzene**

Abby's way of understanding resonance was characterized as *moving symbols to produce quantity*, where quantity, for Abby, was an arbitrary number that was not consistent (as in Robert's case) of preferring to draw two structures. Abby's way of understanding was designated as *to produce quantity*, because she explained, "I stop drawing when I think I have drawn enough." "Enough" did not refer to each structure being a unique representation, which would indicate a characterization of *moving symbols to produce quality*. Rather "enough" referred to an internal feeling that she had drawn enough. For interview Session 1, this number of drawings appeared to be when Abby had drawn two additional structures to the original structure.

Abby's way of understanding hybridization could not initially be assessed because she said that she did not remember hybridization, and did not think about it in organic chemistry. After a short review of hybridization, Abby acknowledged that she remembered hybridization but was unclear about the term, stating, "I know it's, I just

count the bonds.” As a result, her way of understanding hybridization was designated as *counting bonds*. As a result of the above-mentioned ways of understanding, it was confirmed that Abby employed NRS reasoning.

Abby’s initial way of understanding aromaticity from teaching Session 1 (Task 1 and 2) was based on her understanding of benzene as cyclic, planar, and stabilized by resonance. Her initial way of understanding was categorized as *list of three critical attributes*. Although MO diagrams were discussed in Task 2, Abby did not incorporate this information into her initial characterization of aromatic compounds.

### Abby Teaching Session 2

Teaching Session 2 incorporated a review of Task 2, Task 3, the first problems of Task 4, and finished with Task 5. Session 2 began with a review of Task 2, followed by instruction on the mechanics of resonance, by drawing  $p$  orbitals as explicit components of the symbolic representation. Abby was very uncomfortable with her resonance structures in Session 1, therefore, drawing  $p$  orbitals on structures was introduced as a heuristic. Providing this heuristic served the dual purpose of setting her more at ease and improving her ability to draw resonance structures.

For each of the cyclopentadiene structures in Task 2, Abby drew the resonance structures and the corresponding MO diagram. For Task 3, Abby drew resonance structures for the polycyclic aromatic compounds to confirm aromaticity. Task 3 was originally conducted near the end of Session 1; however, Abby refused to draw resonance for the polycyclic aromatics because of their size. With the  $p$  orbital heuristic, Abby not only drew resonance structures, but also spontaneously drew a

number consistent with having each structure as a unique representation. Abby continued to draw resonance structures focusing on building unique representations consistent with a change in her way of understanding to *moving symbols to produce unique representations*.

Using MO diagrams in Task 3, Abby derived Hückel's Rule as  $4N+2$ . This generated a way of understanding aromaticity consistent with a *universal application of Hückel's Rule*. On Task 4 (Interview Sheet 5d; see Appendix 3) Abby demonstrated her preference, in which she based her response solely on Hückel's Rule. This change in her way of understanding aromaticity resulted in her focusing on the variable attribute,  $4N+2$ , over the critical attributes that comprised her initial way of understanding aromaticity. In other words, Abby's ways of understanding aromaticity appeared to deteriorate.

Task 5, which involved data from heterocycles, attempted to address this apparent decline in Abby's ways of understanding. Abby designated furan as "not aromatic" due to its having eight *pi* electrons. She subsequently drew all five of the resonance structures of furan showing delocalization of one of the lone pair on oxygen but still did not recognize aromaticity.

Abby assigned  $sp^2$  hybridization to oxygen because she counted the electrons around oxygen explaining, "there's two lone pairs, so four, and then one from each bond, so six electrons makes it  $sp^2$ ." Immediately after, she added that the carbons in benzene were  $sp^2$  because "it has three bonds." Abby did not perceive the conflict in her way of understanding hybridization until after direct instruction on the basis of

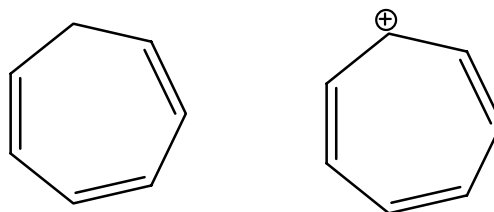


hybridization and its relationship to molecular geometry. Abby explained, “I made *O* [oxygen] be  $sp^2$  because it [refers to problem] told me it was aromatic, so it had to be  $sp^2$ . I just guessed that I count both of the lone electrons and then one from each bond because  $sp^2$  has six electrons.” In other words, Abby ignored her *counting bonds* way of understanding hybridization to account for the  $sp^2$  hybridization of oxygen.

As a result of this interaction, and her further identification of aromatic compounds, her way of understanding aromaticity at the end of Session 2 had become associated with “cyclic molecules that have *p* orbitals all around that can be filled so it can interchange between and it fits the  $4N+2$ .” This way of understanding was referred to as a *list of four characteristics*. Although Abby had an ordered list in her verbalization, it was not clear that she followed that order when she was asked to identify aromatic compounds. For some molecules, she would explain aromaticity based on resonance or *p* orbitals. The list did, however, include three critical attributes and the variable attribute,  $4N+2$ .

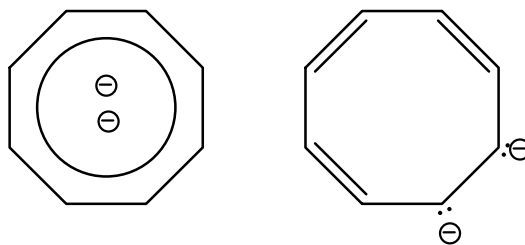
### Abby Teaching Session 3

Teaching Session 3 incorporated the final problems of Task 4 (Interview Sheet 5e) and concluded with the problems of Task 6. When solving the problems on Interview Sheet 5e (see Appendix 3), Abby was able to correctly identify the aromatic compounds, but could not distinguish between anti-aromatic and non-aromatic. She did not relate aromaticity or  $4N+2$  to the MO diagrams in Tasks 2 and 3. Instead she explained that the molecules were not aromatic and did not fit the  $4N+2$  rule, except for the structure on the left in Figure 6-10.



**Figure 6-10: Cycloheptatrienes**

Abby explained that the structure on the left in Figure 6-10 did fit  $4N+2$  but “I’m not sure if it’s too big. No. Wait! It can’t be because this doesn’t have  $p$  orbital.” Upon inquiry about her reference to the size, she explained, “it can’t be too big or it won’t be planar.” She was subsequently asked to assess the structure on the right in Figure 6-10 and she explained, “Now, I don’t know because it fits the rule but it might be too big. If I were to guess I would say, ‘yes’ because it still only has six  $\pi$  electrons, and so far everything with six  $\pi$  electrons has been aromatic. You know, if it is okay that it can delocalize the electrons in the  $p$  orbital” (sic). Abby was then asked about the aromaticity of a new structure that was drawn for her (as seen on the left, in Figure 6-11).



**Figure 6-11: Cyclooctatetraenyl Dianion**

Abby proceeded by drawing the representation on the right in Figure 6-11. After which the following dialog occurred:

**Abby:** So it's reduction. I wasn't sure if two of the carbon can have negative. It's aromatic. It does follow the rule but I'm not sure how stable it is.

**Interviewer:** Do two carbons have a negative charge?

**A:** No. The negative charge is distributed all around the ring but I wasn't sure if I could draw it like that.

**I:** Is it aromatic?

**A:** Uh. Yeah. It is. It has ten electrons.

**I:** What about the size? You said before with the other one that you were not sure because of the size and then you settled on yes because it only had six electrons. How many electrons does this one have?

**A:** It is ten. Ten *pi* electrons. Uh. I think it must be aromatic or it wouldn't happen. Two negatives in one molecule wouldn't happen unless it got some stability. So I think--yes, it is aromatic.

**I:** Because?

**A:** Because it follows the rule and the charge is delocalized around the *p* orbital and it must be stable.

The above interaction revealed that Abby considered stability as one of the characteristics of aromatic compounds. As a result of these interactions, as well as the impromptu structures in Figures 6-10 and 6-11, it was concluded that Abby considered the essential characteristics of aromatic compounds to include Hückel's Rule, *p* orbital availability, delocalization of pi electrons, resonance, planarity, stability and the cyclic nature of the ring. Her final way of understanding aromaticity was categorized as *semi-ordered list of seven characteristics favoring Hückel's Rule*. Although Abby favored the use of the variable attribute, she included six critical attributes in her Ways of understanding. The term *semi-ordered* was applied due to the fact that Abby most

likely attended to the cyclic nature as the primary factor, and then appeared to attend to Hückel's Rule. Using Hückel's Rule assisted her in determining if the structure was or was not aromatic. If it was aromatic, she then appeared to assess  $p$  orbital availability, resonance, or planarity as supporting factors.

Task 6 did not reveal further evidence of Abby's developing ways of understanding aromaticity, due to the fact that she became distracted by the mechanics of drawing resonance structures. During Session 3, Abby had not employed the explicit  $p$  orbital heuristic of Session 2. As a result, she drew non sequitur intermediates for the bromination of naphthalene, and could not attend to the aromatic characteristics of the mechanism. This indicated a regression to a way of understanding resonance as *moving symbols to produce quantity*.

#### Summary of Teaching Sessions with Abby

Abby's initial way of understanding aromaticity was a *list of three critical attributes*. Introduction of MO diagrams resulted in a change in Abby's way of understanding aromaticity to the *universal application of Hückel's Rule*. Further problem solving resulted in a revision of Abby's way of understanding to a *list of four characteristics*. These included three critical attributes and one variable attribute,  $4N+2$ , with no indication of preferred order. Upon completing Tasks 4 and 5, Abby's final way of understanding aromaticity was characterized as a *semi-ordered list of seven characteristics favoring Hückel's Rule*.

Even though Abby clearly showed preference for using Hückel's Rule prior to assessing structure characteristics, her way of understanding aromaticity was

considered more desirable than those observed in Phase I. This was due to her inclusion of six critical attributes, despite her favoring the variable attribute. Abby did not reveal the same potential as Robert for a change in her *ways of thinking* during these teaching sessions.

### **The Effect of Beliefs on WoU: Erik, Doug and Jack**

Both Robert and Abby were engaged in the problems throughout the duration of the teaching sessions. This was not the case for two of the remaining three other students who participated in the teaching interviews (Doug and Jack). In this section, the difficulty encountered with each of these students and the powerful impact that their beliefs had on their capacity to develop desirable ways of understanding the concept of aromaticity will be discussed.

All three of the remaining students exhibited NRS reasoning throughout the teaching session, as expected, without indicating potential for change. These students also demonstrated the effect that their beliefs about learning organic chemistry had on their ability to engage in the assigned task problems, and on their development of more desirable ways of understanding aromaticity. Based on their grades in past and current organic chemistry courses, these students were all relatively high achieving.

#### Summary of Teaching Sessions with Erik

Erik had great confidence in his abilities to perform well in organic chemistry. He was skilled at drawing resonance structures displaying the *moving symbols to produce quantity* way of understanding. Erik's way of understanding hybridization was characterized as *counting bonds*. These two ways of understanding, along with

other evidence throughout the teaching interview sessions, revealed that Erik used NRS reasoning without showing any potential for change in his ways of thinking. Erik tended to rely on his memory and on patterns in answers to past problems (including those done on his own) as a basis for his replies to the task problems. He exhibited behavior that revealed that explaining the reasons behind his responses was incidental. For Erik, obtaining the correct response was his primary goal. The following interaction occurred when determining the aromaticity of cyclopentadienyl cation (see Appendix 5 or Figure 4-18).

**Erik:** This one is not aromatic.

**Interviewer:** Because?

**E:** I don't remember the explanation but I remember it wasn't.

**I:** If I give you a moment, do you think you can remember the explanation?

**E:** Maybe. Is it really needed? Because I'm pretty confident that it's not aromatic.

**I:** It will help clarify something for me.

**E:** Okay. [*pauses for about 1 minute*] This carbon doesn't have any spare electrons to share in the bonding.

**I:** So you're saying there isn't any resonance?

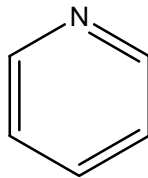
**E:** I'm saying that there wouldn't be any resonance because it doesn't have any electrons to share.

**I:** Does it have to have electrons to share for there to be resonance?

**E:** Um, [*pause*] I'm not sure, but that's kind of the trend that I saw, but it might be, like, coincidental that the molecules we use happen to be like that.

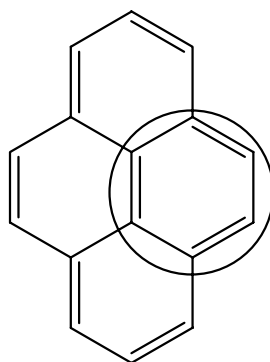
The preceding interaction is a typical example of the discourse that occurred with Erik during the teaching sessions. He relied heavily on self-observed “trends.” During problems that were designed to perturb his ways of understanding, Erik would proceed unperturbed, addressing the intended perturbation with his reliance on observed patterns. As previously stated, cyclobutadiene in Task 2 was intended to reveal the inadequacy of relying solely on the ways of understanding aromaticity, based on characteristics developed from benzene. Erik accounted for the non-aromaticity of cyclobutadiene based on ring strain, even after the MO diagrams were presented. As seen in the dialog above, he accounted for cyclopentadienyl cation as “not aromatic” because it could not form resonance structures. Cyclooctatetraene (see Figure 6-11, left structure) was not aromatic because he “remembered reading” that it was not, and it did not comply with Hückel’s Rule.

His reliance and confidence of the patterns that he recognized would frequently result in a correct response, while revealing problems in his ways of understanding foundational concepts. For example, Erik stated that nitrogen forms three bonds so, therefore, pyridine (see Figure 6-12) would not be aromatic because the bonds would take up the  $sp^2$  hybrid orbitals and the lone pair would be “in a  $p$  orbital that is sticking out away from the ring. I don’t see any room for where these electrons [*referring to lone pair*] could go, so I don’t think that they can be delocalized around the ring.”



**Figure 6-12: Pyridine**

For the problems in Task 4, identifying aromatic compounds, Erik employed primarily the *recognition of structure* way of understanding (see Figure 6-13, below) followed by the use of Hückel's Rule.



**Figure 6-13: Erik's Justification of Pyrene's Aromaticity**

When identifying the aromatic compounds (as listed on Interview Sheet 4d), Erik circled one of the rings in pyrene and explained that pyrene was aromatic because it had benzene imbedded in the structure.

Erik's way of understanding aromaticity at the end of the teaching session was characterized as an *ordered list of five factors*. The five factors included recognition, Hückel's rule, cyclic structure, resonance, and planarity. Erik's way of understanding was referred to as "ordered" because he employed the factors in that order when justifying his responses, using the process of elimination. In other words, if the application of one of the first factors did not result in a response that Erik was



confident about, he employed subsequent factors. For example, when discussing Structure D in Interview Sheet 5e (see Figure 6-7, left structure) Erik stated, “I don’t know about this one. It is not like anything I’ve seen before. It does have six electrons in the ring. I think I can draw resonance going to oxygen, but I am not sure if it’s planar. I don’t know on this one.” Erik could not be prompted to draw the resonance structures or to make a guess. If he was not confident about a response, he merely declined to respond.

Erik explicitly acknowledged his beliefs about organic chemistry. “I think what we have done so far is straightforward and not too bad. I got an A- on the midterm and I’ll probably end up with an A in the class.” For Erik, his beliefs were founded in his ability to achieve high levels of performance. His performance, at least during the teaching sessions, depended on his ability to recognize the patterns of responses in the problems, and his memory of past problems. His correct responses, however, did not correlate with the presence of a desirable way of understanding aromaticity, emphasizing the critical attributes of the concept of aromaticity.

#### Summary of Teaching Session with Doug

Throughout the teaching sessions with Doug, it became exceedingly apparent that he believed that knowledge was to be received and not created. Doug was resistant to applying excessive cognitive effort, resulting in his consistent utterance of, “I don’t know.” Even with encouragement from the researcher for Doug to attempt to solve the problems, he would reiterate his ignorance and ask to be told “the answer.” In an attempt to provide support for creating the desired knowledge, foundational

concepts were revisited, yet also met with Doug's resistance and the proclamation, "I still don't know why." During one session, the hybridization of oxygen on furan was explained, and Doug replied, "that makes sense." However, during problems in Task 4 where he had to apply the knowledge of hybridization of the heteroatoms to pyrrole, he resisted:

**Doug:** It's similar to this one [*furan*] so it could be aromatic, but I'm leaning towards not aromatic because there isn't any open *p* orbitals. *N* is  $sp^3$ .

**Interviewer:** So is it aromatic or not aromatic?

**D:** I don't know. I don't really get it. I know when it [*refers to lone pair*] adds it will create the more stable- This will move here, this will move here [*indicating movement of double bonds*]. I don't know. Something like that. I don't know. I just can't ... It will be added right there because. I don't know.

The above segment was typical for most of the interactions when Doug was asked to justify his response. Even when asked how he studied for organic chemistry, he was indifferent:

**I:** How would you tackle this normally?

**D:** I don't know. I would just learn it somehow.

**I:** Well. You got a B [*in the class*] so you have something that works for you.

**D:** I don't know. I just do it. I got a B- on the last midterm compared to the rest of the class.

**I:** What was the mean?

**D:** 67... The test was just bad because I didn't have time to finish it. It was just bad. Poorly written.

This exchange provided additional confirmation that Doug did not take responsibility for his own learning, but relied on authority to notify him on what he was required to know. He admitted that he didn't spend a lot of time studying because, "I get most of what goes on in lecture, so I just look over past exams and stuff." For Doug, running out of time on an exam did not reflect his poor preparation, but was a result of the exam being poorly written. His reliance on an authority to impart knowledge resulted in Doug's resistance to be perturbed or resolve perturbation. After the three teaching sessions it was possible to determine, however, that Doug's way of understanding aromaticity was an *ordered list of three factors*. He assessed if there were any  $sp^3$  hybridized atoms present first, then employed Hückel's Rule, and then confirmed that "it wasn't a funky one" meaning one where Hückel's Rule didn't apply or contain a heteroatom.

#### Summary of Teaching Sessions with Jack

Like Doug, Jack's beliefs about learning organic chemistry had a great impact on his development of more desirable ways of understanding. Contrary to Doug, however, Jack did not rely primarily on authority, but relied more heavily on memorization. The following discourse provided an explicit example of this limitation:

**Jack:** I really don't understand how it works. I just know that the s and p come together.

**Interviewer:** So when you have to determine hybridization...

**J:** I just memorize it.

**I:** How? So I know how it works for you?

**J:** Like this.

**I:** So you said  $sp^2$  because of the double bond.

**J:** Yeah. That's as deep as it gets.

**I:** What about molecular geometry.

**J:** Trigonal? I don't know. Maybe you should go over that again.

**I:** So you don't think about geometry at all?

**J:** No, but I should.

**I:** What about back in 140A<sup>35</sup>, did you think about geometry at all?

**J:** No. (*laughs*)

**I:** That's okay.

**J:** I have a problem with that when I study. I just memorize how to do the problems and I just kind of, you know, regurgitate it on the test. And that habit is so ingrained in me that it's kind of hard to break it.

Jack realized shortly into Session 1 that the problems in the tasks of the teaching sessions revealed the superficiality of his memorized knowledge. When leaving Session 1, he exclaimed that he felt the need to go back and review several topics in organic chemistry. However, upon arriving at the subsequent session he proclaimed that he did not review any material. The above interaction occurred after revisiting the topic of hybridization. Jack developed a strong way of understanding aromaticity as the *universal application of Hückel's Rule* despite the design of several tasks to perturb this way of understanding. Jack explained that he would apply Hückel's Rule and just memorize the exceptions.

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<sup>35</sup> 140A refers to Chem 140A which is the first quarter of the three quarter organic chemistry sequence.

Jack's participation in the teaching interview sessions continued to be superficial. At the completion of the three sessions, Jack accounted for his reluctance to participate fully off-camera even though he could appreciate what was trying to be accomplished during the teaching sessions. He apologized for not being a "good student" and explained, "it is too late for me. Memorization works and I don't have a reason to change. This wasn't enough because you [*referring to the researcher*] are not writing my exams and assigning my grades." After which he returned the two movie tickets presented to all of the students as an incentive to participate.

### **Summary of Results for the Teaching Interviews Sessions**

Two of the five students who participated in the teaching interview sessions (Robert and Abby), appeared to develop more desirable ways of understanding aromaticity as a result of an instructional intervention designed to perturb students' ways of understanding. Robert's final way of understanding aromaticity was characterized as an *ordered list of seven characteristics favoring critical attributes*. Interestingly, in an e-mail sent a couple of weeks after the teaching sessions, Robert reiterated his gratitude. "I think going over aromaticity helped me greatly in this final. I saw lots of people had trouble with this concept. Thanks a lot."

Abby also developed more desirable ways of understanding aromaticity as a result of the interactions in the three teaching sessions. Abby's final way of understanding aromaticity was characterized as a *semi-ordered list of seven characteristics favoring Hückel's Rule*. Six of these seven characteristics were considered critical attributes of the concept of aromaticity (see Appendix 6). Abby

provided supporting evidence for the potential of students to develop more desirable ways of understanding through an instructional intervention designed to perturb students' ways of understanding. The fact that the remaining three students did not develop more desirable ways of understanding (relative to the students interviewed in Phase I) was a result of the effect of their beliefs about learning organic chemistry. This result could be seen as a result of the limitations of the teaching sessions, by virtue of their short duration, rather than as a failure of the instructional intervention. In fact, the principles of Harel's DNR could be utilized here to explain the reluctance of these students to participate, due to their beliefs about learning organic chemistry.

## **CHAPTER 7: DISCUSSION AND CONCLUSIONS**

This dissertation applied the constructs of Harel's DNR-based instruction (1998, 2001, in press [a]) to organic chemistry education. This final chapter will provide a brief overview of the research problem(s) and methodology used to answer the research questions. The main focus of this chapter is to summarize the results, interpret the results of all three phases as a whole, discuss the significance of the results relative to the field of organic chemistry education, and suggest areas for further research.

### **Review of the Problem Statement and Methodology**

Organic chemistry educators have long advocated that students should avoid focusing on memorization to learn, but instead focus on building a foundation of organic chemistry concepts. In particular, educators have advocated that students should focus their learning on understanding molecular structure and, through that, the reactivity of molecules. Most of the research in the field of organic chemistry education has focused on evaluating changes in curriculum solely through assessment of students' performance on exams. However, research in general chemistry education indicates that students' performance may not reflect their limited understanding of the underlying concepts. Given the research from general chemistry education, along with students' tendency in organic chemistry towards memorization, students' performance in organic chemistry likely does not provide a good indication of students' conceptual understanding. All of this suggests that curricular changes should be evaluated based on students' understanding of the foundational concepts

that we, as educators and chemists, deem as desirable, rather than their performance on exams.

The admonitions of organic chemistry educators reveal a desire to help students improve not only their conceptual understanding in organic chemistry, but also to change their beliefs—one of their ways of thinking—about learning organic chemistry. Harel's DNR-based instruction provides a theoretically grounded way in which to implement change in both students' ways of understanding and ways of thinking as indicated by the Duality Principle. Thus, Harel's DNR-based instruction (see chapter 1 for an overview of DNR) provided the theoretical framework for the research in this dissertation.

One purpose of this study was to explicate students' ways of understanding the organic chemistry concepts of aromaticity and electrophilic aromatic substitution (EAS) reactions using semi-structured clinical interviews. In addition, this study sought to quantify students' beliefs about learning organic chemistry through administration of a 46-item Likert-scale survey. Lastly, the research in this dissertation sought to demonstrate the potential for improving students' ways of understanding aromaticity through teaching interview sessions guided by the constructs of the constructivist learning theory with the intention to perturb students' existing ways of understanding (von Glasersfeld 1995).



## Summary of the Results

### Summary of Phase I Results

The analysis of the Phase I interviews revealed students' ways of understanding aromaticity and EAS reactions using the mental act of interpreting. Table 7-1 provides an overview of the categories of students' ways of understanding.

**Table 7-1: Summary of Phase I WoU Categories**

Ways of Understanding Aromaticity	<p><u>Characteristics of Aromatic Compounds</u></p> <p><i>Ordered list of three characteristics favoring Hückel's Rule</i></p> <ul style="list-style-type: none"> <li>• Hückel's Rule</li> <li>• Symbolic characteristics</li> <li>• Structural characteristics</li> </ul> <p><u>Identification of Aromatic Compounds</u></p> <ul style="list-style-type: none"> <li>• <i>Analogous Structures</i></li> <li>• <i>Structural Considerations</i></li> <li>• <i>Universal Application of Hückel's Rule</i></li> </ul>
Ways of Understanding EAS	<p><u>Bromination of Benzene</u></p> <ul style="list-style-type: none"> <li>• <i>Use of heat, light, or other reagent</i></li> <li>• <i>Need for a catalyst</i></li> <li>• <i>Bromination of Benzene reaction mechanism</i></li> </ul> <p><u>Directing Effects</u></p> <ul style="list-style-type: none"> <li>• <i>Ignored activating and deactivating effects</i></li> <li>• <i>Memorized activating and deactivating effects</i></li> <li>• <i>Activating and deactivating with meaning</i></li> </ul>

Through the ways of understanding results, two different ways of thinking were inferred: 1) non-referential symbolic (NRS) reasoning and 2) non-referential use

of terminology (NRT). NRT is likely the result of when students misinterpret chemical terminology, and is evidenced by their application of non-scientific meaning for chemical terms. For example, one third of the students in Phase I claimed that “benzene” was the common name for 1,3,5-cyclohexatriene.

NRS reasoning characterizes students’ activity when they do not give physical meaning to the symbolic representations employed in organic chemistry. For instance, some students view chemical symbols as “lines, letters, arrows and dots” instead of representations of specific molecular structures or chemical interactions. Students can be skilled in their manipulation of these symbols yielding correct responses, yet hold undesirable ways of understanding. For example, several students interviewed identified the compounds in Figure 7-1 correctly as aromatic.



**Figure 7-1: Pyrrole and pyrrole-1-ide**

For pyrrole, students employing the *counting bonds* way of understanding hybridization counted three bonds on nitrogen, designated nitrogen as  $sp^2$  hybridized, and concluded that the structure was aromatic with six pi electrons. From a chemist’s perspective, nitrogen does rearrange its geometry from  $sp^3$  to  $sp^2$  hybridization to gain the aromatic stabilization from the delocalization of the *pi* electrons; however, the reasoning that students employed, *counting bonds*, neglected the energetic gain in stabilization by ignoring the rearrangement of the geometry about the nitrogen atom.

For pyrrole-1-ide, some students viewed the negative charge as representing one lone pair of electrons in a  $p$  orbital resulting in six  $\pi$  electrons overall, thereby, designating the molecule as aromatic. Most of these students viewed pyrrole-1-ide as analogous to cyclopentadienyl anion (see Appendix 3, Structure 4c-3 or Figure 4-3) completely ignoring the fact that nitrogen, in this case, has two lone pairs of electrons.

Both of these examples demonstrate that students *do* arrive at correct solutions based on undesirable ways of understanding. In addition, these examples provide evidence of NRS reasoning, as students did not consider molecular structure in their determination of aromaticity, but instead based their determination solely on symbolic clues. NRS reasoning influences students' ways of understanding as do all ways of thinking (see chapter 1, Duality Principle). For example, students develop ways of understanding the symbolic representations in organic chemistry that focus on manipulating the symbols rather than fully appreciating the underlying concepts of molecular structure and chemical reactivity. Furthermore, according to the Duality Principle, students' beliefs associated with learning organic chemistry (another way of thinking) also directly influences their ways of understanding.

The identification of several categories of ways of understanding aromaticity and EAS reactions led to the identification of two important ways of thinking associated with these ways of understanding, as exhibited by the students interviewed in Phase I. In addition, students voluntarily discussed their beliefs about learning organic chemistry during the interviews. Beliefs, as a way of thinking, as expected

also affected students' ways of understanding. The prevalence of these beliefs was evaluated in the distribution of the Phase II survey.

### Summary of Phase II Results

The analysis of Phase II resulted in the identification of seven principal components that accounted for 51% of the variance in the Phase II survey data. Chapter 5 provides the results of this analysis, including suggestions for further research relative to the Phase II survey. Here, I will only highlight the overall results as they pertain to the results of all three phases of the research.

Of the classified principal components, students favoring a memorize-oriented way of thinking accounted for 19% of the total variance, while only one group demonstrated clear evidence of a non-memorize-oriented way of thinking, which accounted for 4% of the total variance. The results indicate students' tendency towards memorization for learning organic chemistry.

### Summary of Phase III Results

Five students completed the three teaching interview sessions. Two of those five students, Robert and Abby, demonstrated clear evidence of developing more desirable ways of understanding aromaticity. Robert also showed potential for change in his ways of thinking about organic chemistry.

Robert's way of understanding aromaticity evolved to *ordered list of seven characteristics favoring critical attributes*. Robert demonstrated clear evidence of his way of understanding aromaticity through emphasizing six critical attributes of aromatic compounds: "ring, planar,  $sp^2$  hybridized, delocalized  $\pi$  electrons and lower

bonding orbitals filled up.” He utilized Hückel’s Rule, a variable attribute, only after accounting for the presence of the six critical attributes. Despite having developed a more desirable way of understanding aromaticity, Robert did not change his undesirable way of understanding resonance, one of the foundational concepts for aromaticity.

Based on the short duration of the teaching interview sessions, I did not expect to document a change in the students’ ways of thinking. However, Robert did demonstrate a *potential* for change in his NRS reasoning. This potential was observed during Task 4 (see Appendix 5) when Robert exhibited evidence of change in his way of understanding hybridization. Robert’s way of understanding hybridization changed from *symbolic reference without counting* to *symbolic reference with structural considerations*. Although Robert still determined hybridization based on symbolic features (single bond, double bond or triple bond), he began to account for structural consequences; for example, a gain in aromatic stability, from a change in hybridization. Accounting for structural consequences only provided evidence for potential change in his ways of thinking due to the fact that Robert did not exhibit more evidence of referential symbolic reasoning. On the contrary, Robert’s persistent way of understanding resonance as *moving symbols to produce quantity* (with the quantity for Robert being limited to two structures) revealed the continued presence of NRS reasoning.

Abby did not exhibit the same potential for change in her ways of thinking, but she did exhibit behavior indicating the development of more desirable ways of

understanding aromaticity by the conclusion of the teaching interview sessions. Abby's final way of understanding aromaticity was designated as a *semi-ordered list of seven characteristics favoring Hückel's Rule*. Abby used Hückel's Rule prior to accounting for any of the six other characteristics. If the number of  $\pi$  electrons appeared to fit Hückel's Rule, Abby then used one or two of the six critical attributes to confirm aromaticity. She typically justified her determinations for up to four characteristics with Hückel's Rule being applied in each case. Her inclusion of critical attributes in her justification of aromaticity resulted in my concluding that Abby had, in fact, developed more desirable ways of understanding aromaticity relative to those observed in Phase I.

The remaining three students who participated in the teaching interview sessions did not develop more desirable ways of understanding relative to the students interviewed in Phase I. I suggest that their beliefs about learning in organic chemistry had a direct effect on the success of the teaching interview sessions, which were designed to help them develop more desirable ways of understanding aromaticity. I would not classify this result as a failure of DNR-based instruction, but rather, as a result of the limitations of the teaching interviews sessions by virtue of the short duration. The Duality Principle in Harel's DNR (1998, 2001, in press [a]) helps to explain the reluctance of these students to participate, due to their beliefs about learning organic chemistry. Students' beliefs about learning comprised one category of ways of thinking that affected students' ways of understanding. Thus, Phase III

demonstrated the importance of attending to students' beliefs when designing instruction to help develop more desirable ways of understanding.

### **Discussion of the Results**

The discussion of the results incorporates a discussion of Phase I and Phase III under the headings of “triad of determinants” and “Harel’s DNR-based Instruction” respectively<sup>36</sup>. In addition, the interpretation of the results for all three phases combined is discussed, based on the conclusions presented in previous sections. Ideas for future research and implications for teaching are also presented in each of the discussion sections. Lastly, the section discussing the overall results of all three phases includes a discussion on the limitations of this study.

#### The Triad of Determinants

The interpretation of the results of all three phases demonstrated the usefulness of incorporating the triad of determinants as an interpretive framework for analyzing students' ways of understanding and ways of thinking while problem solving in organic chemistry. Focusing on students' ways of understanding would provide educational researchers with a basis for comparison when implementing change in student learning. This study provides an example of the application of the triad of determinants as an interpretive framework. A discussion of the results of Phase I, using the triad of determinants from the DNR system, is included below, followed by suggestions for further exploratory studies.

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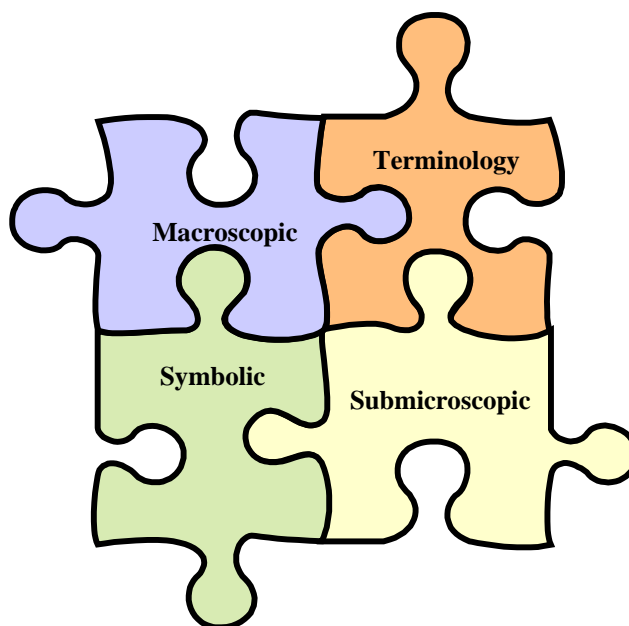
<sup>36</sup> Chapter 5 includes a discussion of the quantitative results of the Phase II survey in addition to including ideas for future research relative to the Phase II survey and the limitations of Phase II conclusions.

### Discussion for Phase I Results: Conceptual Understanding in Chemistry Redefined

By focusing on the mental act of interpreting, I was able to categorize students' ways of understanding aromaticity and electrophilic aromatic substitution reactions. Based on the categorization of these ways of understanding, two different ways of thinking were identified: non-referential symbolic (NRS) reasoning and non-referential use of terminology (NRT). Results from this study revealed that the definition of "conceptual understanding" (see Chapter 1) should be redefined.

Recall that "conceptual understanding" in chemistry incorporated three different representational levels: the symbolic, submicroscopic and microscopic (see Figure 1-1). The definition of conceptual understanding in chemistry (and organic chemistry) should be revised to incorporate an additional representational level, the use of terminology. Figure 7-2 represents the diagram for conceptual understanding in chemistry, in general. The research in this dissertation is in the realm of organic chemistry, however, the significance for the results of this study have implications beyond that of organic chemistry, extending into general chemistry education research. As a result, a diagram relative to the broader audience of chemistry education was chosen.





**Figure 7-2: Conceptual Understanding in Chemistry Redefined**

Figure 7-2 shows the redefinition of conceptual understanding in chemistry incorporating terminology as a fourth representational level. The terminology representational level in chemistry refers to both chemical vocabulary and the uses of common language in the scientific sense. The chemical vocabulary includes nomenclature of chemical compounds, and terminology of chemical concepts, including the use of common words in a chemical context. For example, chemists use the word “strong” in association with acids and bases referring to the complete dissociation into the ionic components. Therefore, the use of common language with scientific meaning is also part of the terminology representation level.

Terminology follows an analogous purpose as that of the symbolic representational level. Both of these representational levels emphasize *communicating* in chemistry. In the example from chapter 1 used to define each of the three

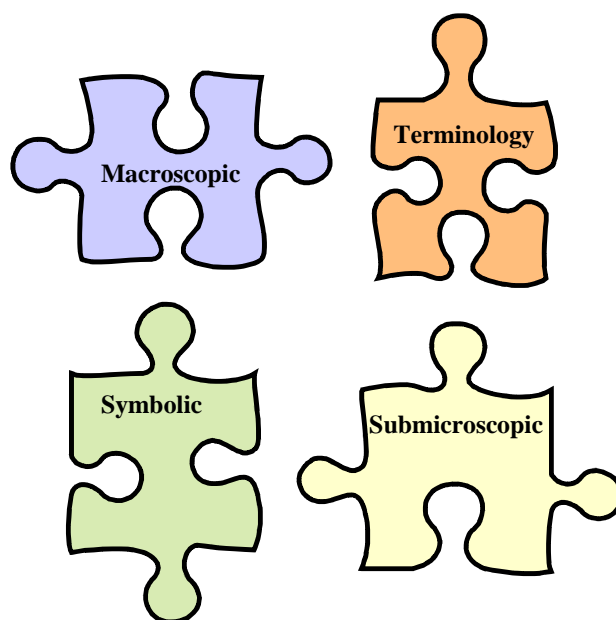
previously mentioned levels (see chapter 1, “Conceptual Understanding in Chemistry” section), the letter sequence NaCl represented the symbolic representational level. Similarly, “sodium chloride” is the linguistic equivalent to the symbolic representation. When chemists write NaCl, they verbalize the name representative of these symbols with the appropriate nomenclature. Likewise in organic chemistry, each symbolic representation (or skeletal structure) has a formal name. For example, Figure 4-1 is a skeletal structure with the formal name of “benzene.”

The incorporation of terminology into the definition of conceptual understanding portrays a more complete view of conceptual understanding. In addition, this incorporation communicates the importance of including referential use of terminology in the building of students’ conceptual understanding in chemistry. Although Figure 7-2 reflects the terminology piece as independent of the symbolic puzzle piece (because they are diagonal from each other) this is not the case. Their position in the diagram reflects their analogous ability to communicate ideas in chemistry in a different way. Therefore, terminology and symbols are intricately related and, thus, communicate the same chemical concepts through different representations.

It is important to note that the four pieces in Figure 7-2 do not represent desirable ways of understanding from a DNR perspective. Rather, chemists interrelate each of the four representational levels portrayed by Figure 7-2. In other words, they have a connected view of these four representational levels. Thus, “multi-relational representations” is a *way of thinking* characterizing chemists’ mental act of relating or

connecting these four representational levels. Students, on the other hand, do not portray this connected way of thinking, as verified by the prevalence of the non-referential symbolic reasoning demonstrated by the students in this study. Students rarely related the symbolic representation to the actual molecular structure (submicroscopic level) or chemical reactivity (macroscopic level). Therefore, students exhibited a very fragmented way of thinking about the different representations in chemistry.

To illustrate this point, the puzzle pieces of Figure 7-2 could be separated into four different representations, independent of each other (see Figure 7-3). The cognitive objective in educating chemistry students then becomes the development of the connected puzzle pieces, a “multi-relational representations,” way of thinking.



**Figure 7-3: Unconnected Conceptual Understanding in Chemistry**

### Future Exploratory Studies Using The Triad of Determinants

The research in this dissertation used the mental act of interpreting as the lens through which to determine ways of understanding, and through those ways of understanding, infer ways of thinking. Future research could extend interpreting using other chemical concepts. This research revealed that concepts originating from general chemistry—resonance and hybridization—influence students' ways of understanding aromaticity. Therefore, focusing on ways of understanding and ways of thinking in general chemistry could provide important information and a foundation for students' ways of understanding organic chemistry concepts.

In addition, future research could incorporate analyses of ways of understanding and ways of thinking using other mental acts. Problem solving is a large component of students' learning in organic chemistry. Research focused on students' approaches to problem solving would not only reveal students' ways of understanding associated with that mental act, but also students' ways of thinking. For example, one of the three categories of ways of thinking from mathematics is “problem solving approaches.” Research on problem solving approaches in chemistry using the DNR framework could extend the research on problem solving processes already conducted by Bodner and Bowen (1991). These researchers looked at problem solving approaches of graduate students and their use of various representational systems. This research focused on documenting the representational systems employed by graduate students, rather than analyzing their problem solving approaches. Using the DNR system, I suggest conducting studies on *undergraduate* students' problem solving

approaches, rather than graduate students. The majority of undergraduate students taking organic chemistry will not become organic chemistry graduate students. As a result, research on undergraduate student learning that examines problem solving approaches could provide a valuable evidence for curricular change or change in the types of problems that we ask students to solve.

Another category of ways of thinking Harel (1998, 2001, in press a) identifies are “proof schemes”. Although organic chemistry does not employ the use of a “proof scheme” per se, research in organic chemistry applying the constructs of the DNR system could reveal the organic chemistry counterpart. For instance, Harel and Sowder (1998) provided results from exploratory studies revealing three categories of proof schemes, each with several subcategories. One of these categories, external conviction proof schemes, had three subcategories: ritual, authoritarian, and symbolic. The symbolic proof scheme was essentially the non-referential symbolic (NRS) reasoning proof scheme. The research in this dissertation showed that NRS reasoning had an analogous counterpart in organic chemistry; students solved problems in organic chemistry manipulating symbols without attending to the physical meaning that the symbols represented.

Further research in problem solving in organic chemistry would most likely reveal several other analogous counterparts. For example, Phase III of this research revealed that Doug believed that knowledge was *received*, and not *created* by him. As a result, I would propose that he had an “external conviction” justification scheme with a clear dependence on authority, either instructor-based authority, or textbook-

based. Thus, exploratory studies in organic chemistry problem solving attending to several different mental acts could provide an analogous classification of students' problem solving approaches as well as "justification schemes<sup>37</sup>."

That being said, further research may reveal that there are more categories of ways of thinking in organic chemistry. The categories revealed as ways of thinking in mathematics would have to be established and redefined for science and, in the case of this research, for organic chemistry.

In summary, utilizing the triad of determinants from Harel's DNR-based instruction (1998, 2001, in press [a]) in exploratory studies could explicate students' ways of understanding various organic chemistry (and general chemistry) concepts, as well as provide chemical analogies to the categories of ways of thinking identified in mathematics. In addition, application of the constructs of the DNR system in chemistry could reveal ways of thinking categories unique to science, chemistry and/or organic chemistry.

#### Harel's DNR-Based Instruction

The Phase III teaching interview sessions were analyzed using constructs of Harel's DNR-based instruction, ways of understanding and ways of thinking. Even though there were only three teaching sessions, two students developed desirable ways of understanding aromaticity, with one of those two also demonstrating potential for change in his ways of thinking.

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<sup>37</sup> The term "justification schemes" is referred to here in quotations since this category has not yet been established as a category of ways of thinking in chemistry or science.

Furthermore, Phase III revealed the effect that ways of thinking have on the development of students' ways of understanding as explained by the Duality Principle. Three of the students participating in the teaching interviews did not develop more desirable ways of understanding as a result of their ways of thinking. Doug repeatedly resisted engaging in the task problems as a result of his authoritative belief about learning organic chemistry. His continued use of the phrase "I don't know" and the resulting time waiting (for answers), indicated that he believed that he learned organic chemistry by authority figures telling him what he needed to know. One of the questions that arose as a result of my interactions with Doug was the question of intellectual need. More precisely, what constitutes intellectual need for organic chemistry students? In Doug's case, his beliefs about learning affected his engagement. He did not engage in the problems, nor was he puzzled by them. In fact, he showed some frustration at being asked to solve a problem where he did not have a provided method of solution. For Doug, the teaching intervention in Phase III did not result in creating an internal need to resolve the problem situations presented to him.

The original intent of Phase III was to demonstrate the potential for students' development of desirable ways of understanding, guided by all three instructional principles of DNR. However, upon analysis of the data, I found that students did not engage in all of the problems as originally intended. For example, the original intent of the first task was designed to create a need for students to develop a classification of aromatic compounds. The task was based on historical evidence, and had created puzzlement in chemists in the past. This first task did not create the same puzzlement

in students. In fact, students were not puzzled at all. They simply calculated the difference in the predicted heat of hydrogenation versus the experimental value, without exhibiting *any* internal conflict about the difference. They simply waited for the researcher to explain the difference. Thus, what constituted intellectual need for chemists did not create intellectual need in the students in this study.

Therefore, one area of future research would be to explore the issue of intellectual need for organic chemistry students. I believe that a study evaluating intellectual need must occur at the very early stages of a year-long organic chemistry sequence before students become aware of the sufficiency of their existing undesirable ways of thinking, as demonstrated by Doug. The tasks designed for the teaching sessions in Phase III were based mainly on the historical development of the concept of aromaticity. In the past, these problems created puzzlement for chemists. However, the problems that created puzzlement in chemists cannot be presumed to create the same puzzlement for organic chemistry students, most of whom will not become chemists. A study investigating intellectual need in students could reveal an area in which the problem tasks pose real puzzlement. Since most of these students plan on careers in the health sciences, I would begin an investigation of intellectual need in organic chemistry with problems based on the applicability of organic chemistry concepts associated with the medical field.

A longitudinal study of students' learning in organic chemistry, with curricula designed to create intellectual need, would provide more compelling evidence of the effects of DNR-based instruction on student learning. One way to incorporate DNR-



based instruction, without making radical changes to the traditional teaching format, would be to incorporate DNR with the Peer-Led-Team-Learning (PLTL) approach to running discussion sections (see chapter 2). One area of research in chemistry education that also extends into organic chemistry education is PLTL where student performance and retention has improved as a result of peer led group study sessions. These sessions generally meet weekly and are in lieu of the traditional recitation section for large chemistry courses. The PLTL researchers have developed a series of PLTL guidebooks, handbooks and suggested problems for students to solve during the sessions (Kampmeier et al. 2001; Roth et al. 2001; Gosser et al. 2001; Varma-Nelson et al. 2001). Prior to developing problems for the teaching sessions for this dissertation, I evaluated the suggested problems from the PLTL researchers in the area of aromaticity and electrophilic aromatic substitution reactions. The suggested problems from PLTL were similar to those problems found at the end of textbook chapters and on typical exams. In other words, the problems were similar to those kinds of problems solved by students prior to participating in this study.

One study involving the PLTL instructional approaches could assess students' ways of understanding that developed as a result of incorporating PLTL into the students' courses. Previous studies of PLTL have focused on student performance and retention. As reported in the results of this dissertation, student performance should not be equated with students' development of desirable ways of understanding. Rather than assess students' ways of understanding each organic chemistry concept, I would propose a study of students' ways of understanding symbolic representations as a

result of DNR-based instruction, instead of merely using textbook or PLTL problems. Using DNR-based instruction, in conjunction with the PLTL format of discussion sections, would provide evidence for students' ways of understanding.

The Phase III teaching sessions with Jack, as discussed in chapter 6, reinforced the need for future investigations of student learning in organic chemistry in the first weeks of the organic chemistry sequence. Jack had found a learning strategy that resulted in relatively high performance on exams, despite weak conceptual understanding. During the teaching sessions, Jack admitted that he had weak conceptual understanding. Rather than work to resolve his understanding of concepts such as hybridization and resonance, Jack engaged only superficially in problem tasks. When the superficiality of his engagement revealed non sequitur structures, Jack merely stated that he knew it was wrong but that, "I would never have to do this on a real exam."

Therefore, how and what we assess in organic chemistry appears to be the driving force for the focus in student learning. Because assessment of organic chemistry concepts also occurs outside of the organic chemistry course (for example, on the Medical College Admissions Test, MCAT), studies of assessment should probe beyond the organic chemistry sequence. A collaborative effort between organic chemistry instructors, medical college admissions faculty, and educational researchers, could result in a study that would not only transform the questions posed on assessments, but re-evaluate the purpose of the organic chemistry course for students seeking careers in the health care fields.

### Discussion of the Overall Results

In chapter 3, during the discussion of the purpose of each phase of this study, I proposed that Phase I would demonstrate the effect of ways of thinking on ways of understanding (see Figure 3-2). In addition, I proposed that Phase III would reveal the effect of ways of understanding on ways of thinking (see Figure 3-3). Although the results of Phase III demonstrated the potential for change in ways of thinking as a result of change in ways of understanding for one student (Robert), the overall effect of the intervention was as expected, with no change in ways of thinking for the four other students. The results of Phase III portrayed additional information about the very powerful effect that ways of thinking (including beliefs about learning) have on ways of understanding. Even though I did not expect to show change in students' ways of thinking, I did expect to see the potential for change in a greater number of students.

One reason that this effect was not demonstrated could be the short duration of the teaching sessions, as previously explained. However, another reason not yet discussed is the timing of the study in relation to the organic chemistry course sequence. The concept of aromaticity was presented in the middle of a year-long organic chemistry sequence. Aromaticity was chosen not only because it is an important concept, but also because planar aromatic compounds were thought to avoid any issues related to spatial visualization. One issue that was not anticipated before the study was the very strong effect of students' ways of understanding foundational concepts, including spatial visualization, of molecular structure.

The results of Phase I revealed that students did, in fact, have problems with visualizing the molecular structure. This became apparent when students had to determine whether several compounds were aromatic or not. Very few students mentioned the non-planarity of the molecular structure as a reason for it not being aromatic. As stated in chapter 4, most students relied on Hückel's Rule and superficial symbolic features (see Figure 7-1 and its discussion). One example of a non-aromatic compound is cyclooctatetraene (See Figure 6-4). Even though this structure was presented in the textbook (Vollhardt and Schore 2003) as not planar and, therefore, not aromatic, half of the students still referred to the number of *pi* electrons as eight, not fitting Hückel's Rule and, therefore, not aromatic.

The predominant way of thinking identified in Phase I was non-referential symbolic (NRS) reasoning. Students with this way of thinking did not attend to the three-dimensional structure and, therefore, avoided utilizing their spatial ability. The study by Ferk et al. (2003) revealed that students generally had more difficulty solving tasks that used a more abstract schematic molecular structure. These abstract representations required the students to build the three-dimensional mental image in their minds, as apposed to visualizing molecular modeling kits or computer animations. Students in this study generally attended to non-structural features (Hückel's Rule), rather than visualize the molecule as a planar structure with delocalized *pi* electrons.

One of the reasons I chose to evaluate students' ways of understanding the concept of aromaticity was to avoid issues with spatial ability because of the effect

spatial ability has on student performance (see chapter 2). Although I did not assess spatial ability skills in this dissertation, in future research I would consider the students' spatial ability skills an integral part of any study in organic chemistry, due to the fact that *any* visualization of three-dimensional structures requires the students to use their spatial ability skills. In determining aromaticity, students must be able to assess the relative planarity of a molecule in three-dimensional space. Although not mentioned in the results chapters, some students admitted that they had problems visualizing molecules in three-dimensional space and avoided it at all cost. This is not surprising for students with NRS reasoning, because they do not attend to the physical meaning of the symbolic representations. However, if educators wish to change students' ways of thinking, then ignoring spatial ability for any concept in organic chemistry would be a mistake.

Another issue discovered in this study was the influence that underlying concepts had on developing understanding of a new concept. Concepts from general chemistry, such as hybridization and resonance, proved difficult, as expected, based on pilot study data. However, the effect of students' ways of thinking, as a result of their past experience in organic chemistry, was not anticipated. Students had found success using NRS reasoning within a variety of topics over the course of the approximately fifteen weeks that they had been enrolled in organic chemistry. The attempt to even show potential change resulted in only relative success. Most of the students in Phase III had already built problem solving strategies that had proved successful for them, and, therefore, they did not have enough incentive to change based solely on this

research project. Thus, further research in organic chemistry education would need to begin early in the year-long sequence in order to aid students in developing more desirable ways of thinking.

The findings in this study reveal that it is important for organic chemistry educators to recognize that students develop robust ways of thinking relative to organic chemistry by mid-year and most likely sooner. Students build these robust ways of thinking based on their ways of understanding that evolve during problem solving. As a result, we, as educators need to provide students with different types of problems in order for them to develop more desirable ways of understanding and ways of thinking. All of this suggests that curricular changes should be evaluated based on students' understanding of the foundational concepts that we, as educators and chemists, deem as desirable, rather than their performance on exams.

## APPENDIX 1: VOLUNTARY SURVEY FOR PARTICIPATION IN A CHEMICAL EDUCATION RESEARCH PROJECT

Thank you for taking the time to fill out this brief background questionnaire for the research in students' understanding of organic chemistry. The researcher, Anne Duffy, is a graduate student working on a PhD in chemistry education with an interest specifically in organic chemistry. The data of this study will be used in her PhD dissertation. The interview phase of the study will provide important background information for a subsequent phase that will be geared toward improving students' understanding in organic chemistry. Some students who fill out this form will be asked to participate in an interview. The interview will last about an hour and will be scheduled at your convenience during the last two weeks of class. There will be a small compensation for your time. You have the right to not answer any question on this questionnaire that you do not choose to answer. All information on the questionnaire and obtained during the interview will remain confidential and will not affect your grade in Chemistry 140B. In order to contact you to schedule an interview, you need to provide your name and some way to contact you in the next couple of weeks.

**Please return this form immediately after class or to Gail McNabb in York 4010.**

Name: \_\_\_\_\_

Phone: \_\_\_\_\_

E-mail: \_\_\_\_\_ Do you prefer to be reached by phone or e-mail?

---

For the following question, circle your response or fill in your response wherever appropriate.

- 1) Are you a current student at UCSD?    No            Yes  
If not, what is your home university? \_\_\_\_\_
- 2) What is your current major? \_\_\_\_\_  
(If undeclared, just write UND)
- 3) What is your reason for taking organic chemistry? Circle all that apply.
  - a) General interest
  - b) Major requirement
  - c) Professional school requirement
  - d) Other: Explain \_\_\_\_\_
- 4) What is your gender?    Male    or    Female
- 5) Which age range best describes you?
  - a) under 19    b) 19-22    c) 22-27    d) Over 27
- 6) What grade did you receive in Chemistry 140A (or equivalent)?  
\_\_\_\_\_
- 7) What grade do you expect to receive in Chemistry 140B?  
\_\_\_\_\_

- 8) Which study method(s) best describes you? Circle all the apply.
- a) I work through problems in order to understand what I am learning.
  - b) I work as many problems as I can to make sure I am prepared for any problem I see on an exam.
  - c) I try to memorize as much as I can.
  - d) I read the text sections close to the time we cover the topic in class.
  - e) I work through example problems as I read the text.
  - f) I cram as much information as possible before an exam.

PLEASE WRITE YOUR AVAILABILITY ON THE BACK OF THIS PAGE.

INCLUDE ALL TIMES MON-SAT WHERE YOU ARE AVAILABLE.



## APPENDIX 2: PHASE I INTERVIEW PROTOCOL

### Interview check list

1. Introduce myself and thank participant. \_\_\_\_\_
  2. Go over consent to act as a research subject and consent to be videotaped forms. Make sure that the participant knows that he/she is allowed to discontinue the interview at any time. \_\_\_\_\_
  3. Inform the participant that they will be asked to complete a series of tasks and to solve the tasks in the best way that they can. The interviewer will not interrupt or ask for clarification until the participant indicates that he/she is done. The participant may choose to talk out loud during problem solving or remain quiet.
  4. \_\_\_\_\_ Thank the participant again and give movie ticket for helping. \_\_\_\_\_
- 

#### Task 1:

- A. For the first problem, I would like you to draw the skeletal structure of bromobenzene.
- B. [When complete ask] Can you explain to me why you chose to draw the structure that way? Is there another way to draw it?
- C. What is the hybridization of each of the carbon atoms? What is the hybridization of the bromine? Can you explain to me how you think about hybridization?
- D. Show me how could you make bromobenzene starting with benzene and any other starting materials?
- E. [When complete reaction ask] What do we call this reaction?
- F. [If FeBr<sub>3</sub> is used as a catalyst ask] Can you explain why you chose to use FeBr<sub>3</sub>? Why does Br<sub>2</sub> not work without a catalyst? Can you show me the mechanism?
- G. [If FeBr<sub>3</sub> is NOT used ask] Can you show me the mechanism? How would you brominate an alkene? Does this same mechanism work in the case of benzene?
- H. Can you synthesize *p*-bromobenzoic acid from bromobenzene?

- I. If so, how would you proceed? Can you explain the directing effects of bromine? Can you show me the mechanism?
- J. If not, why? How would you synthesize *p*-bromobenzoic acid? Can you show me the mechanism?

Ask any necessary follow-up questions to gain clarification if there is something the subject does or says that requires further probing.

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**Task 2:**

- A. Let's discuss aromaticity. Can you explain how you think about aromaticity?
- B. Can you draw me an example of an aromatic compound that is not benzene?
- C. [After example] How do you know that this compound is aromatic? Can you draw a compound that is non-aromatic?
- D. [After example] How do you know that this compound is non-aromatic? Can you draw a compound that is anti-aromatic? Can you explain to me how you think about non-aromatic and anti-aromatic compounds?
- E. [In case of confusion of terms non- and anti- ask] What is the difference between non-aromatic and anti-aromatic? What does the  $4n$  rule tell us about a compound?
- F. What is special about a compound being aromatic?
- G. How does being aromatic aid or help in reactions with benzene? For example, is it easier to add a substituent to benzene than to add across an alkene? Why or why not?
- H. Can you tell me anything about the energetics behind aromaticity?
- I. Can you draw 1,3,5 cyclohexatriene? Does this molecule exist? Why or why not?
- J. For the following groups of molecules and ions classify each compound as aromatic, anti-aromatic or non-aromatic. Explain your reasoning.

[Hand the subject Interview Sheet 4a, then 4b, 4c and 4d]

(see back pages for interview sheets in order)

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**Task 3:**

I am going to ask you to solve several electrophilic aromatic substitution problems. I would like you to solve them the best you know how. You can either talk out loud as you solve or you can wait until you are done and then we will discuss your response. For each compound that I ask you to synthesize, you will start with benzene and use any other necessary reagents. If you have trouble remembering which reagents to use make your best guess.

1. How would you synthesize 1,2-dichloro-4-nitrobenzene?
2. How would you synthesize *p*-Chloroaniline?
3. How would you synthesize 4-chloro-2-nitroaniline?
4. How would you synthesize *m*-Hexylbenzenesulfonic acid?
5. How would you synthesize *m*-nitrotoluene?
6. How would you synthesize 1,3,5-Tribromobenzene?

- 
- Make sure to probe into how the students think about the problem. For example, if they sigh- ask what makes you sigh?
  - After each problem ask the student to explain how they thought about the problem in general and then at any point where they seem to get stuck.
- 

[5 and 6 require diazotizing aniline-this may not be covered in the subjects' lecture. If this is the case, then do not let the subject fret over these two problems for long]

**Task 4:**

1. Explain to me how you think about substituents that are activating. ...deactivating.
2. Explain the directing effects (ortho/para or meta) of certain substituent. How do you keep track of which substituents direct to which positions?

3. Phenols, anilines, alkylbenzenes, phenyl ethers and phenoxides are activating or deactivating? Explain.
4. Give an example of each of the above compounds [repeat] and set them in order of activating strength? Explain why you chose this order.
5. Can you tell me the directing effects of these compounds?
6. Using phenol, show me why this is ortho- para- directing.[If Subject can not ask for resonance structures]
7. Are all ortho-para directors activators? [or deactivators if that is what the subject thinks] If not, give an example and explain the rationale.
8. Are meta- directors activating or deactivating? Why?

---

THE NEXT TWO TASKS MAY PROVE TOO DIFFICULT OR MAY NOT BE INCLUDED DUE TO TIME CONSTRAINTS

**Task 5:**

Other aromatic compounds can also undergo electrophilic aromatic substitution. Complete the following problems using the given aromatic compound and any other necessary reagents.

1. Using naphthalene [give the structure if necessary] show the following products
  - a. Of bromination.
  - b. Sulfonation
  - c. Nitration
  - d. Alkylation using chloroethane.

Why did you choose to substitute naphthalene in the position you chose? Show me the mechanism of one of these reactions.

2. Using furan [give structure only if subject needs it] show the mechanism for bromination at the number 2 and number 3 position. Based on your mechanisms, which is the primary product of bromination of furan?
-

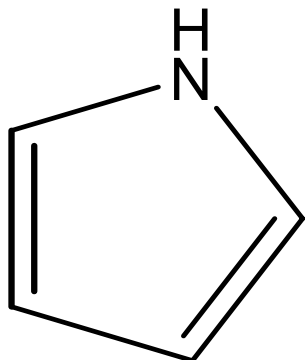
**Task 6:**

[The structure of the following compounds will be given if necessary-these question should only be asked if there is time left over]

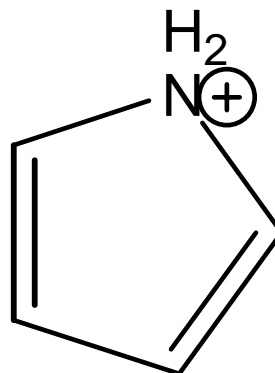
1. Using anthracene, show your prediction of the product of bromination and justify your prediction.
2. Using phenanthrene, show your prediction of the result of bromination and justify your prediction.

APPENDIX 3: INTERVIEW SHEETS

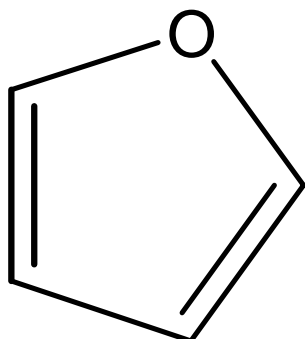
Interview Sheet 4a



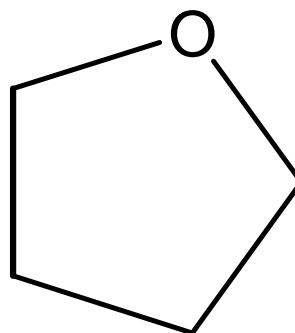
Structure 4a-1



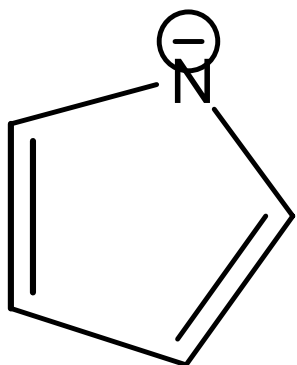
Structure 4a-2



Structure 4a-3

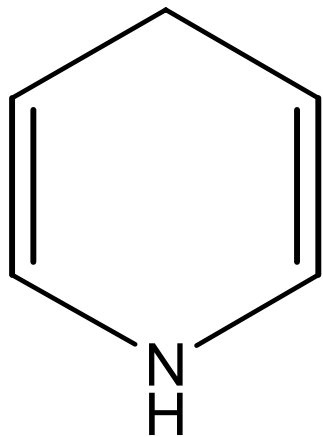


Structure 4a-4

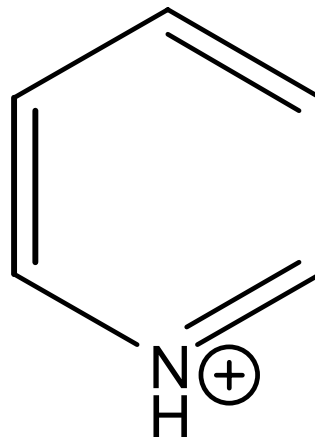


Structure 4a-5

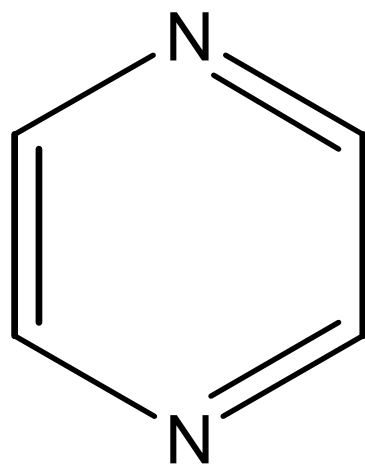
## Interview Sheet 4b



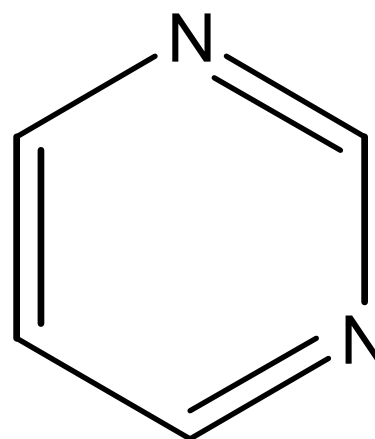
Structure 4b-1



Structure 4b-2

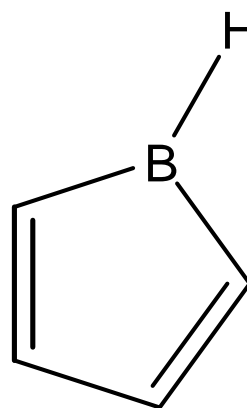
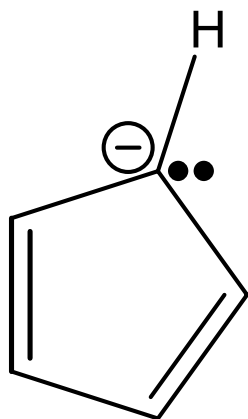
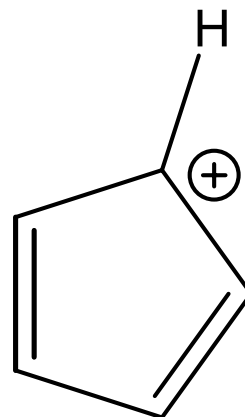
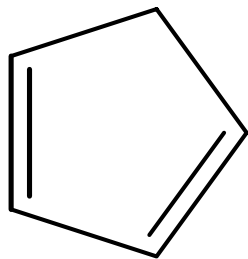


Structure 4b-3



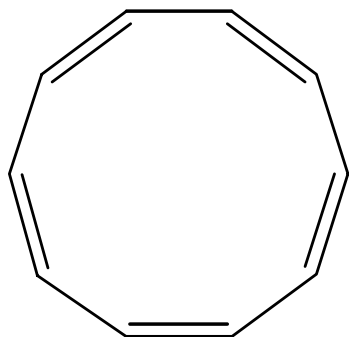
Structure 4b-4

## Interview Sheet 4c

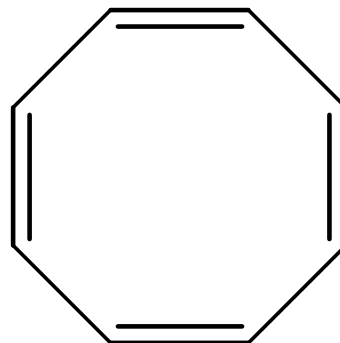




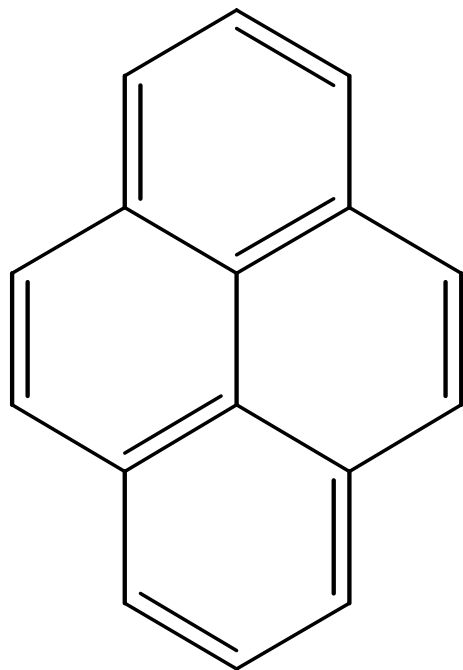
## Interview Sheet 4d



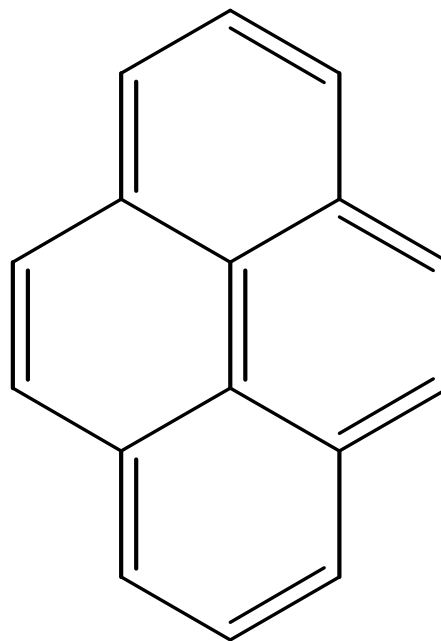
Structure 4d-1



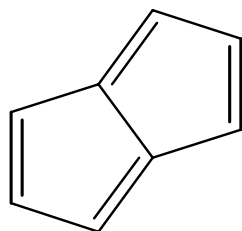
Structure 4d-2



Structure 4d-3



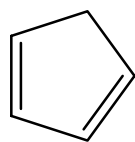
Structure 4d-4



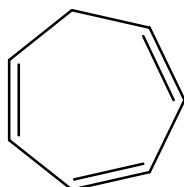
Structure 4d-5

**Task 4: Identifying Aromatic Compounds**

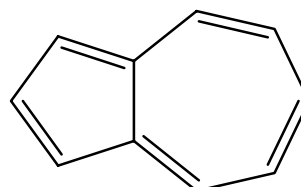
## Interview Sheet 4e



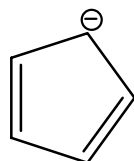
4e-1



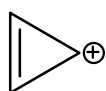
4e-2



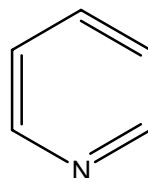
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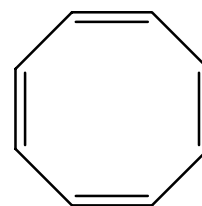
4e-4



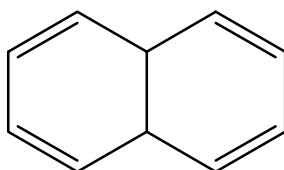
4e-5



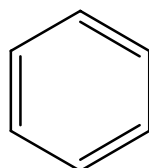
4e-6



4e-7



4e-8



4e-9



4e-10

#### APPENDIX 4: PHASE II SURVEY

DO NOT WRITE YOUR NAME. Thank you for taking the time to fill out this anonymous survey evaluating your attitudes and beliefs regarding organic chemistry. Answer as honestly as possible to help inform a study to improve learning in organic chemistry. Circle one response per question.
1. To understand most of the basic ideas in this course, I read the text, work most of the problems, and pay close attention in class.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
2. I go over my class notes carefully to prepare for tests in this course.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
3. To me, problem solving in organic chemistry basically means remembering which reactions will lead to the desired product.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
4. I think the best way to learn the reactions is to memorize them.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
5. I spend a lot of time figuring out and understanding the organic chemistry reactions by understanding the mechanisms.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
6. The best way for me to learn organic chemistry is by solving many problems rather than by carefully analyzing a few in detail.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
7. A good grade in this course is necessary to achieve my career goals. A good understanding in organic chemistry is not essential.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
8. Knowledge in organic chemistry consists of many pieces of information each of which applies primarily to a specific situation.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
9. My grade in this course is primarily determined by how familiar I am with the material. Insight and creativity has little to do with it.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree

10. Learning organic chemistry is a matter of acquiring knowledge that specifically has to do with molecular structure, reactivity, and organic synthesis.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
11. In solving problems in organic chemistry, I depend a great deal on my knowledge of pKa's.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
12. Only very few specially qualified people are capable of really understanding organic chemistry.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
13. An important part of learning organic chemistry is a matter of acquiring knowledge that specifically has to do with spectroscopy.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
14. To understand organic chemistry, I sometimes think about what I have learned in previous science courses in order to relate what I am currently learning to what I already know.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
15. The most crucial thing in solving an organic synthesis problem is remembering the right reagents to use.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
16. If I don't remember a particular reaction mechanism for an exam, there's nothing much that I can do (legitimately!) to come up with it.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
17. Organic chemistry is related to the real world and it sometimes helps me to think about the connection, but it is rarely essential for what I have to do in this course.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
18. The main skill I get out of this course is how to solve organic synthesis problems.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
19. The results of an exam don't give me any useful guidance to improve my understanding of the course material. All the learning associated with an exam is in the studying I do before it takes place.	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
20. When I solve problems in organic chemistry, I think about the influence of the molecular structure(s).	Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree

21. Understanding organic chemistry basically means being able to recall something that you've read in the text or been shown in class.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
22. Learning organic chemistry means memorizing a lot of new vocabulary.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
23. Spending a lot of time (20 minutes or more) on a problem is a waste of time. If I don't make progress quickly, I'd be better off asking someone who knows how to solve the problem.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
24. A significant problem in this course is being able to memorize all the information I need to know.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
25. The main skill that I get out of this course is to learn how to reason logically in the context of organic chemistry.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
26. I use the mistakes I make on homework and on exam problems as clues to what I need to focus on to understand the material better.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
27. It is possible to pass this course (get a "C" or better) without understanding organic chemistry very well.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
28. Learning organic chemistry requires that I substantially rethink, restructure and reorganize the information that I am given in class and/or the text.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
29. In order to do well in organic chemistry, I need to attend nearly every lecture and take good notes.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
30. Understanding organic chemistry will help me become better informed on issues in current events (environmental, medical and health issues).
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
31. I depend a lot on having a good instructor in order to do well in organic chemistry.
Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree

32. I depend a lot on having a good T.A. to help me understand what we are learning in class.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
33. I skip over things that I don't understand and hope that they will not be on an exam.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
34. Working on problems in study groups outside of class really helps me understand the material better.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
35. Using the molecular model kits helps me better understand organic chemistry. If I didn't use a model kit, I would have had a hard time making it through organic chemistry.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
36. Using computer software has helped me to visualize the three-dimensional structures.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
37. I work hard at learning "electron pushing." I feel like being able to "push" electrons will help me better understand organic chemistry.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
38. In order to do well in this course, I need to be familiar with the instructor's expectations and the types of problems he or she writes.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
39. Organic chemistry concepts build upon each other. When new concepts are introduced, I look for ways to understand the new material based on what I already know from past concepts.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree
40. Learning organic chemistry takes a lot of time. In order to do well, I need to budget my time wisely.  Strongly Agree   Agree   Neither Agree Nor Disagree   Disagree   Strongly Disagree

41. Please indicate your gender.				
	Female		Male	
42. Please circle the age range that best describes you.				
< 19	19-20	21-24	25-29	>29
43. Please indicate the department that you are affiliated with.				
Biology	Chemistry	Other-Science	Psychology	Other-Non science
44. Please circle the grade that you expect to receive in this course.				
A	B	C	D	F
45. My grades on organic chemistry exams are not representative of my knowledge in organic chemistry.				
Strongly Agree	Agree	Neither Agree Nor Disagree	Disagree	Strongly Disagree
46. Rate the organic chemistry course for level of difficulty compared with other courses.				
One of the Most Difficult	Difficult	Neither Difficult nor Easy	Easy	One of the Easiest

## APPENDIX 5: TEACHING INTERVIEW TASKS

### Task 1 Problems

Problem 1-A: The hydrogenation of cyclohexene is exothermic releasing 28.6 kcal/mol of heat, a value expected for the hydrogenation of a cis double bond. Based on this information, calculate the expected heat of hydrogenation for 1,3-cyclohexadiene.\* Discuss the structure of cyclohexene.

Problem 1-B: The actual heat of hydrogenation for 1,3-cyclohexadiene is  $-54.9$  kcal/mol. How would you account for the difference between your calculated value and the actual value? \* Discuss the structure of 1,3-cyclohexadiene.

Problem 1-C: Based on the information provided, calculate the expected heat of hydrogenation for the compound 1,3,5-cyclohexatriene.

Problem 1-D: The actual experimental result for the heat of hydrogenation of benzene is  $-49.3$  kcal/mol. How do you account for this difference from the expected calculated value?

Problem 1-E: How is benzene different than the other two molecules? How is benzene the same? Draw the resonance structures of benzene. What is the difference between benzene and 1,3,5-cyclohexatriene?

\*\*\*\*\*

### Task 2 Problems

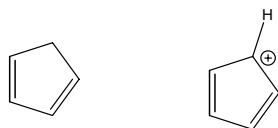
Problem 2-A: Draw the structure of 1,3-cyclobutadiene.

Does this molecule have resonance forms? Do you think it is aromatic?

Problem 2-B: Draw the molecule orbital diagrams for benzene and 1,3-cyclobutadiene.



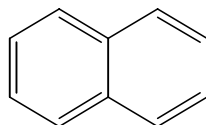
**Problem 2-C:** Do the following structures have resonance? If so, draw the resonance structures. Are these structures aromatic? What do the MO diagrams look like for these molecules?



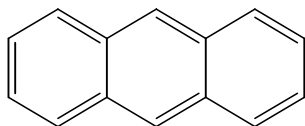
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### Task 3 Problems

**Problem 3-A:** Predict the MO diagrams for the following compounds. Are these compounds aromatic?



Naphthalene



Anthracene

**Problem 3-B:** Compare the MO diagrams for benzene, naphthalene and anthracene. What trend do you observe?

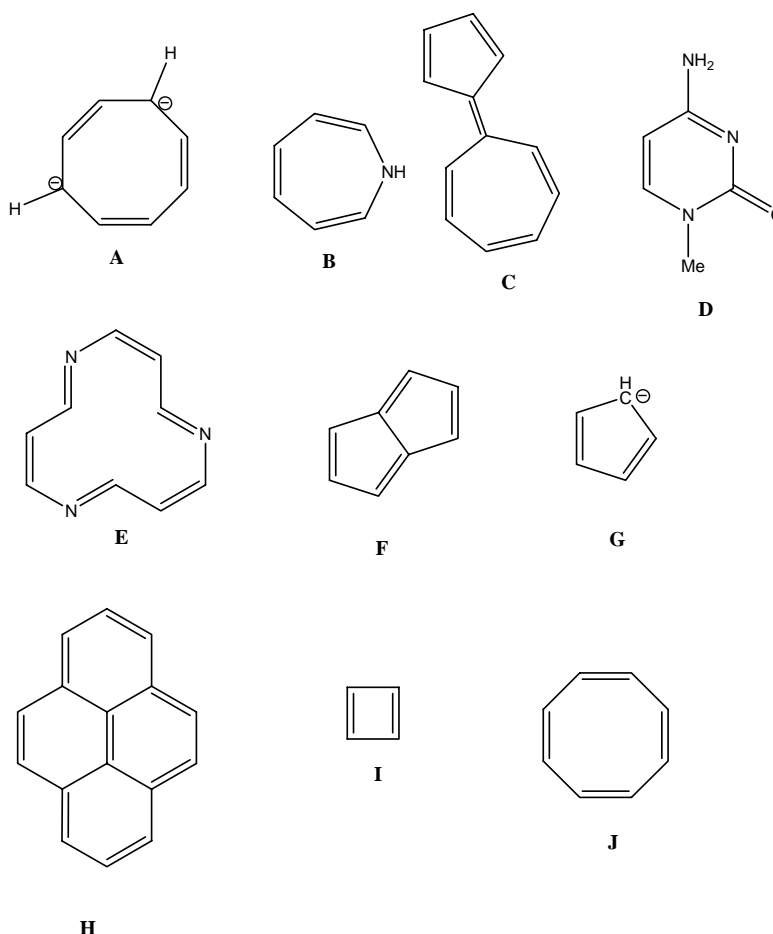
**Problem 3-C:** What does the MO diagram for cyclopropenyl cation look like? If all of these molecules are considered aromatic, what is the trend observed from their MO diagrams?

### Task 4 Problems

**Problem 4-A:** Using Interview Sheet 4a and 4b (See Appendix 3) From these compounds, please tell me which ones are aromatic, anti-aromatic, non-aromatic and why.

**Problem 4-B:** Using Interview Sheets 4d and 4e. From these compounds, please tell me which ones are aromatic, anti-aromatic, non-aromatic and why.

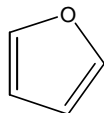
**Problem 4-C:** Using the following compounds, please tell me which ones are aromatic, anti-aromatic, non-aromatic and why. (From Dr. O'Connor's past exam problems)



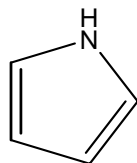
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### Task 5 Problems

Problem 5-A: Explain the aromaticity of the heterocycle, furan, (see below) in terms of the rule that you have established for aromaticity. Using resonance theory, account for the relatively large resonance energy of 16 kcal/mol that has been measured for furan?



Problem 5-B: Explain the larger resonance energies observed for pyrrole (the N analog of furan- see below) and thiophene (the S analog) at 21 kcal/mol and 28 kcal/mol respectively?

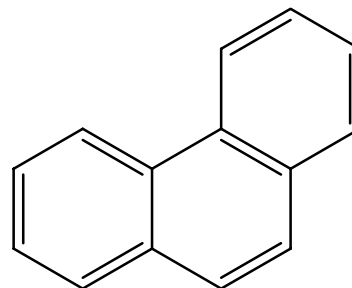
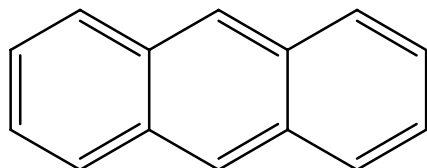
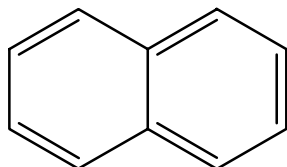


Problem 5-C: On the following Interview Sheets, 4a and 4b, (See Appendix 3) please tell me if the compound is aromatic, anti-aromatic or non-aromatic.

\*\*\*\*\*

### Task 6 Problems

Problem 6-A: Given the bromination of benzene, in which position would substitution occur for the following compounds. Justify your response.



## APPENDIX 6: CONCEPT ANALYSIS OF AROMATICITY

### Definition:

The concept of aromaticity is multidimensional and thus an exact definition will not be provided. See the critical attributes as well as the variable attributes for an outline of the concept. These were developed predominantly based on the reviews of Krygowski et al. (2000) and Balaban et al. (2004).

### Critical Attributes:

C1: Compound must be largely planar. (Small deviations from planarity have little effect but larger deviations decrease aromaticity significantly)

C2: Compound must be a cyclic structure.

C3: Pi electrons must be delocalized throughout the cyclic structure.

C4: Aromatic systems contain  $sp^2$  hybridized atoms that form a delocalized pi electron aromatic closed shell.

C5: The delocalized pi electrons generate an electric current, a ring current, when in the presence of an external magnetic field. In H-NMR, H's attached to aromatic rings appear downfield at approximately 7-9 ppm.

C6: Aromatic structures have added thermodynamic stability due to electron delocalization (resonance energy) as compared to an analogous structure with localized double bonds.

C7: Molecular Orbital energy levels reveal a cyclic pi system is stabilized relative to the acyclic system with the same number of pi bonds. (Larger gap between the HOMO-LUMO orbitals.)

C8: There exists equalization of bond lengths between those of typical single and double bonds.

C9: Show higher energy UV/Vis spectral bands.

C10: Large symmetry in IR spectra.

### Variable Attributes:

V1: The number of pi electrons must obey Hückel's rule,  $4N + 2$ . (True only for monocyclic systems of 1<sup>st</sup> row elements)

V2: Heteroatoms present in the ring structure and will arrange lone pairs in order to be  $sp^2$  hybridized and allow for electron delocalization throughout the ring. (Excessively high or low electronegativity results in destabilization)

V3: Bond lengths are all equal in an aromatic ring. ( $C_{60}$  and Radialene are counterexamples both with equal bond lengths but not aromatic.)

V4: Aromatic compounds undergo substitution reactions (aromatic substitution) more easily than addition reactions. (Anthracene, the 1,4-addition becomes more important than substitution and dominates in pentacene. Furan in Diels-Alder cycloadditions. 2-pyridone undergoes addition reactions as well.)

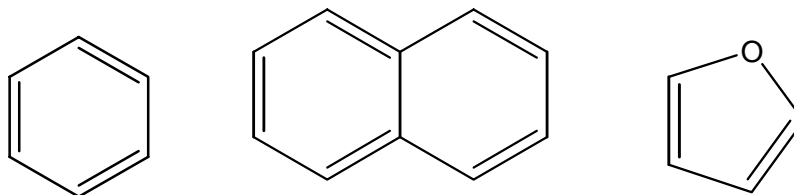
V5: Kinetic stability is not analogous with thermodynamic stability. Aniline is very reactive towards EAS. It is thermodynamically stable but kinetically unstable.

**Supraordinate Concept:** Molecular geometry and structure, resonance, hybridization,

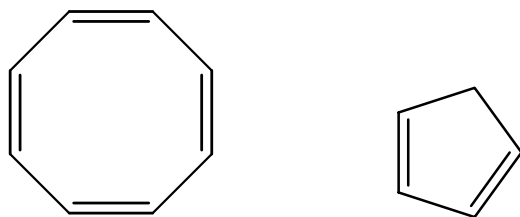
**Coordinate Concept:** Chemical reactivity.

**Subordinate Concept:** Heterocyclic pi systems, polycyclic pi systems, monocyclic pi systems.

**Examples:** Benzene, naphthalene (see below), furan (see structure with oxygen below)

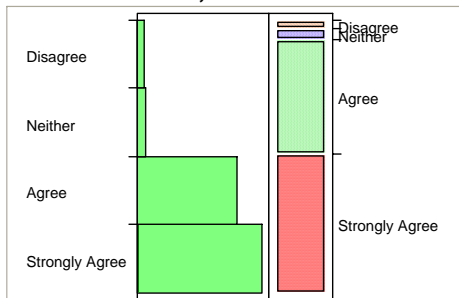


**Nonexamples:** Cyclooctatetraene (see below) other noncyclic systems.



## APPENDIX 7: FREQUENCY DISTRIBUTIONS FOR PHASE II SURVEY

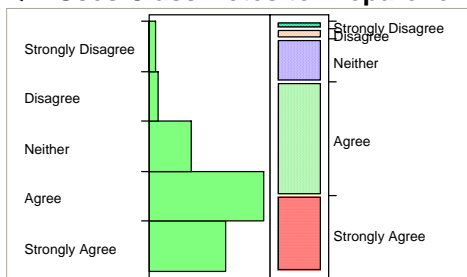
### Q1: Reads Text, Works Problems and Pays Attention in Class



**Frequencies: Mean = 1.58**

Level	Count	Prob
Strongly Agree	52	0.51485
Agree	42	0.41584
Neither	4	0.03960
Disagree	3	0.02970
Total	101	1.00000

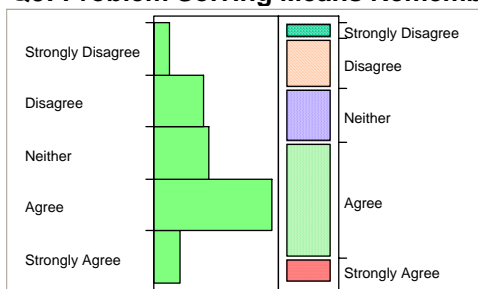
### Q2: Uses Class Notes to Prepare for Exams



**Frequencies: Mean = 2.03**

Level	Count	Prob
Strongly Agree	31	0.30693
Agree	46	0.45545
Neither	17	0.16832
Disagree	4	0.03960
Strongly Disagree	3	0.02970
Total	101	1.00000

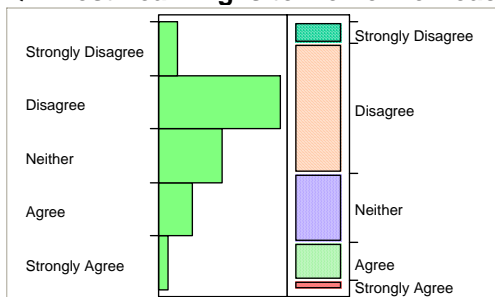
### Q3: Problem Solving Means Remembering Reactions



**Frequencies: Mean = 2.66**

Level	Count	Prob
Strongly Agree	10	0.09901
Agree	45	0.44554
Neither	21	0.20792
Disagree	19	0.18812
Strongly Disagree	6	0.05941
Total	101	1.00000

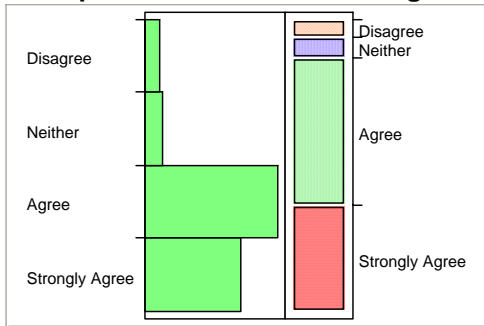
### Q4: Best Learning is to Memorize Reactions



**Frequencies: Mean = 3.42**

Level	Count	Prob
Strongly Agree	4	0.03960
Agree	14	0.13861
Neither	26	0.25743
Disagree	49	0.48515
Strongly Disagree	8	0.07921
Total	101	1.00000

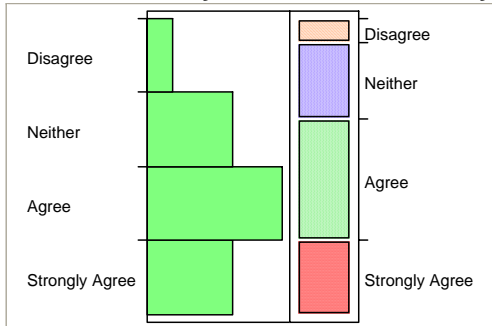
**Q5: Spends Time Understanding Mechanisms**



**Frequencies: Mean = 1.82**

Level	Count	Prob
Strongly Agree	37	0.36634
Agree	51	0.50495
Neither	7	0.06931
Disagree	6	0.05941
Total	101	1.00000

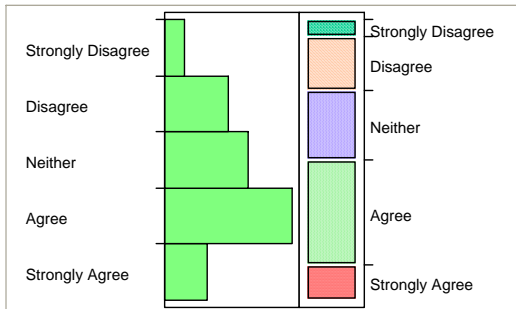
**Q6: Solves Many Problems Over Analyzing a Few**



**Frequencies: Mean = 2.15**

Level	Count	Prob
Strongly Agree	26	0.25743
Agree	41	0.40594
Neither	26	0.25743
Disagree	8	0.07921
Total	101	1.00000

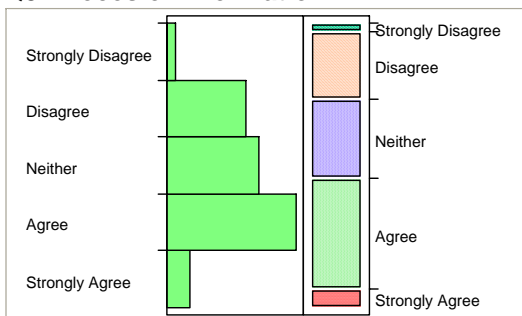
**Q7: Good Grade Better then Good Understanding**



**Frequencies: Mean = 2.89**

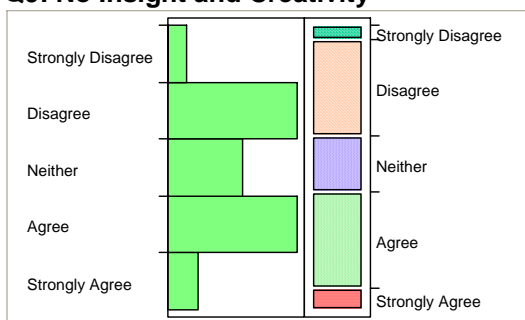
Level	Count	Prob
Strongly Agree	13	0.12871
Agree	38	0.37624
Neither	25	0.24752
Disagree	19	0.18812
Strongly Disagree	6	0.05941
Total	101	1.00000

**Q8: Pieces of Information**

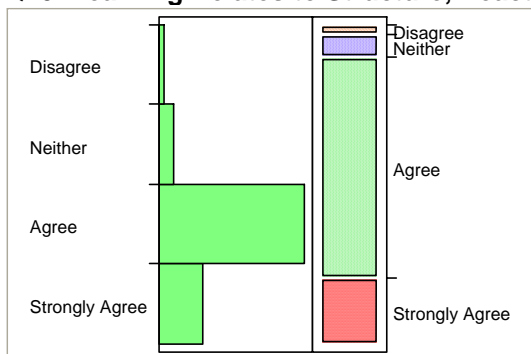


**Frequencies: Mean = 2.72**

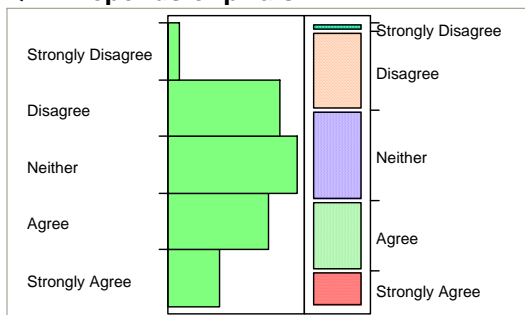
Level	Count	Prob
Strongly Agree	7	0.06931
Agree	39	0.38614
Neither	28	0.27723
Disagree	24	0.23762
Strongly Disagree	3	0.02970
Total	101	1.00000

**Q9: No Insight and Creativity****Frequencies: Mean = 2.86**

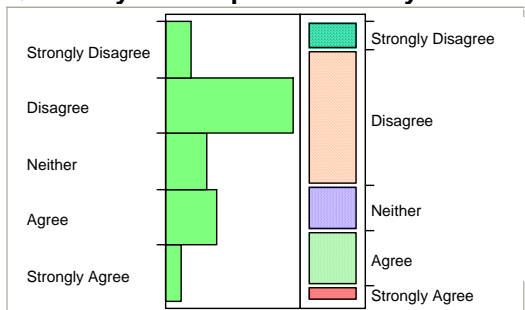
Level	Count	Prob
Strongly Agree	8	0.07921
Agree	34	0.33663
Neither	20	0.19802
Disagree	34	0.33663
Strongly Disagree	5	0.04950
Total	101	1.00000

**Q10: Learning Relates to Structure, Reactivity and Synthesis****Frequencies: Mean = 2.07**

Level	Count	Prob
Strongly Agree	21	0.20792
Agree	70	0.69307
Neither	7	0.06931
Disagree	3	0.02970
Total	101	1.00000

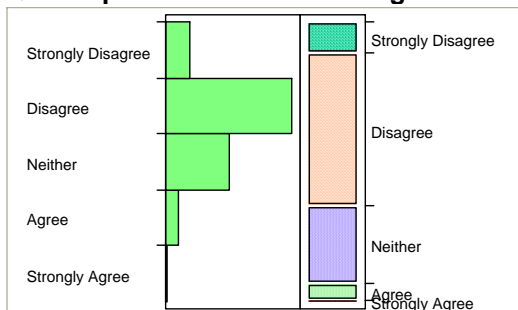
**Q11: Depends of pKa's****Frequencies: Mean = 3.22**

Level	Count	Prob
Strongly Agree	13	0.12871
Agree	25	0.24752
Neither	32	0.31683
Disagree	28	0.27723
Strongly Disagree	3	0.02970
Total	101	1.00000

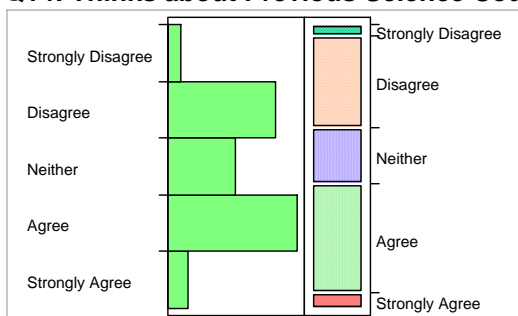
**Q12: Only Few Capable of Really Understanding****Frequencies: Mean = 3.37**

Level	Count	Prob
Strongly Agree	6	0.05941
Agree	20	0.19802
Neither	16	0.15842
Disagree	49	0.48515
Strongly Disagree	10	0.09901
Total	101	1.00000

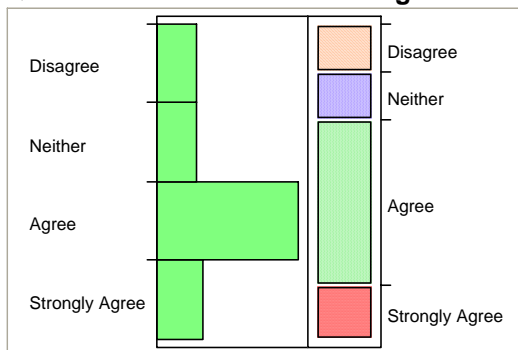


**Q13: Important Part of Learning O Chem: Spectroscopy****Frequencies: Mean = 3.68**

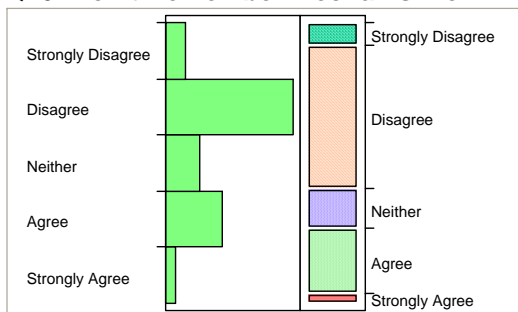
Level	Count	Prob
Strongly Agree	1	0.00990
Agree	6	0.05941
Neither	28	0.27723
Disagree	55	0.54455
Strongly Disagree	11	0.10891
Total	101	1.00000

**Q14: Thinks about Previous Science Courses****Frequencies: Mean 2.90**

Level	Count	Prob
Strongly Agree	6	0.06000
Agree	38	0.38000
Neither	20	0.20000
Disagree	32	0.32000
Strongly Disagree	4	0.04000
Total	100	1.00000

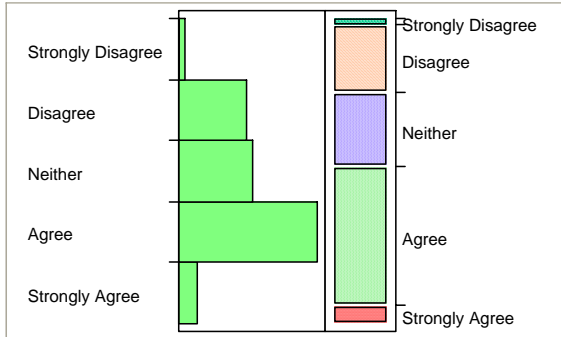
**Q15: Crucial to Problem Solving is Remembering Reagents****Frequencies: Mean = 2.28**

Level	Count	Prob
Strongly Agree	17	0.17172
Agree	52	0.52525
Neither	15	0.15152
Disagree	15	0.15152
Total	99	1.00000

**Q16: Don't Remember Mechanism on Exam, Can't Do it****Frequencies: Mean = 3.36**

Level	Count	Prob
Strongly Agree	4	0.04000
Agree	23	0.23000
Neither	14	0.14000
Disagree	51	0.51000
Strongly Disagree	8	0.08000
Total	100	1.00000

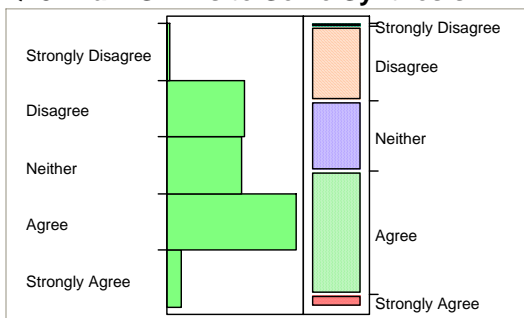
**Q17: Connection Between Real World Rarely Essential**



**Frequencies: Mean = 2.69**

Level	Count	Prob
Strongly Agree	6	0.06061
Agree	45	0.45455
Neither	24	0.24242
Disagree	22	0.22222
Strongly Disagree	2	0.02020
Total	99	1.00000

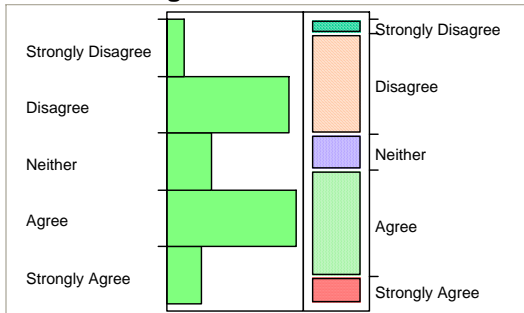
**Q18: Main Skill is to Solve Synthesis**



**Frequencies: Mean = 2.75**

Level	Count	Prob
Strongly Agree	5	0.05000
Agree	43	0.43000
Neither	25	0.25000
Disagree	26	0.26000
Strongly Disagree	1	0.01000
Total	100	1.00000

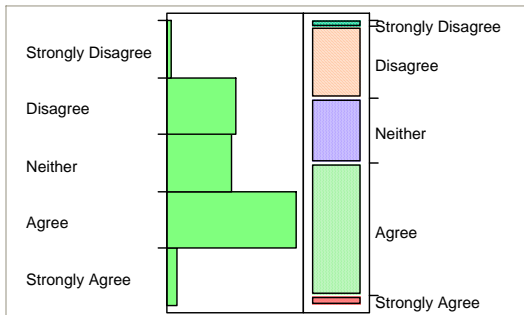
**Q19: Learning Occurs Before Exam**



**Frequencies: Mean = 2.88**

Level	Count	Prob
Strongly Agree	10	0.10000
Agree	37	0.37000
Neither	13	0.13000
Disagree	35	0.35000
Strongly Disagree	5	0.05000
Total	100	1.00000

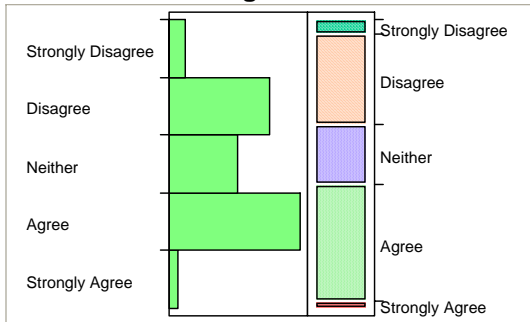
**Q20: Thinks of Influence of Molecular Structure**



**Frequencies: Mean = 2.75**

Level	Count	Prob
Strongly Agree	4	0.04000
Agree	46	0.46000
Neither	23	0.23000
Disagree	25	0.25000
Strongly Disagree	2	0.02000
Total	100	1.00000

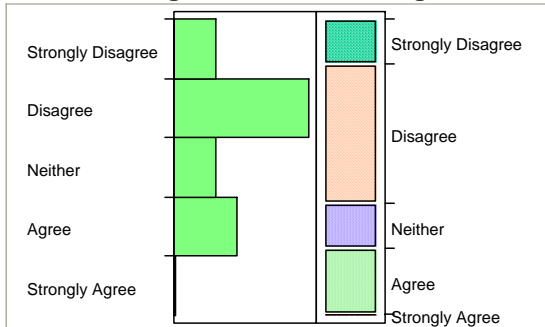
**Q21: Understanding Means Recall**



**Frequencies: Mean = 2.95**

Level	Count	Prob
Strongly Agree	3	0.03000
Agree	40	0.40000
Neither	21	0.21000
Disagree	31	0.31000
Strongly Disagree	5	0.05000
Total	100	1.00000

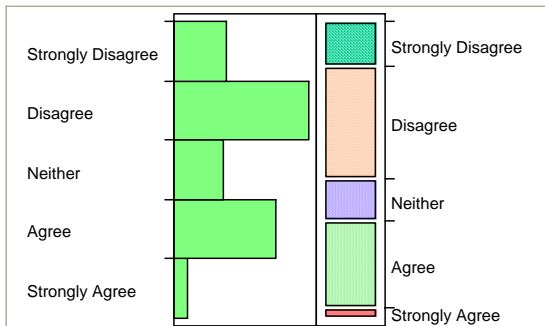
**Q22: Learning Means Memorizing Vocabulary**



**Frequencies: Mean = 3.53**

Level	Count	Prob
Strongly Agree	1	0.01000
Agree	22	0.22000
Neither	15	0.15000
Disagree	47	0.47000
Strongly Disagree	15	0.15000
Total	100	1.00000

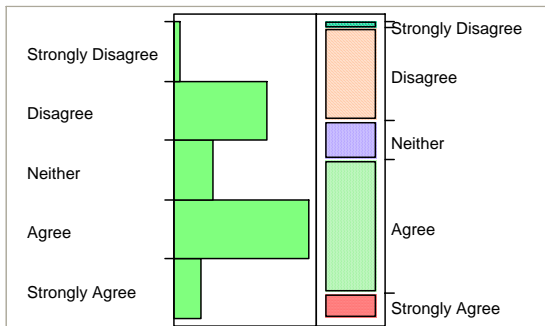
**Q23: Too Much Time on Task is Wasteful**



**Frequencies: Mean = 3.31**

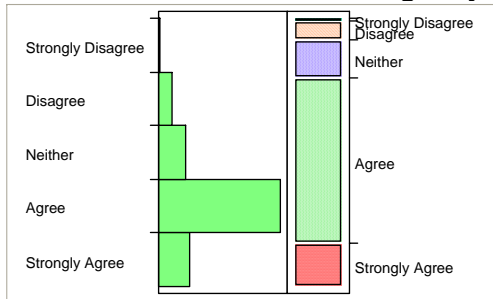
Level	Count	Prob
Strongly Agree	4	0.04000
Agree	29	0.29000
Neither	14	0.14000
Disagree	38	0.38000
Strongly Disagree	15	0.15000
Total	100	1.00000

**Q24: Problem with Course is Need to Memorize All**

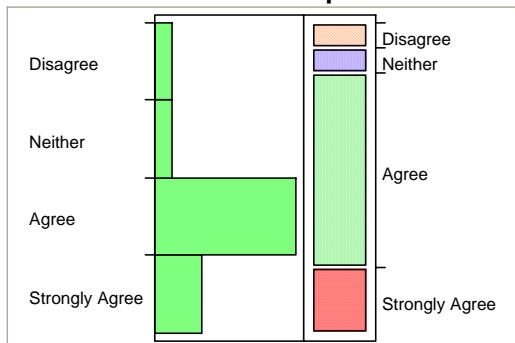


**Frequencies: Mean = 2.72**

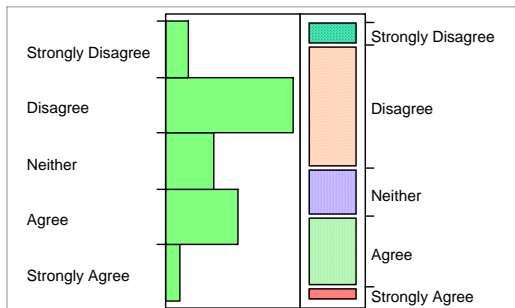
Level	Count	Prob
Strongly Agree	9	0.09000
Agree	45	0.45000
Neither	13	0.13000
Disagree	31	0.31000
Strongly Disagree	2	0.02000
Total	100	1.00000

**Q25: Main Skill is to Reason Logically about O Chem****Frequencies: Mean = 2.15**

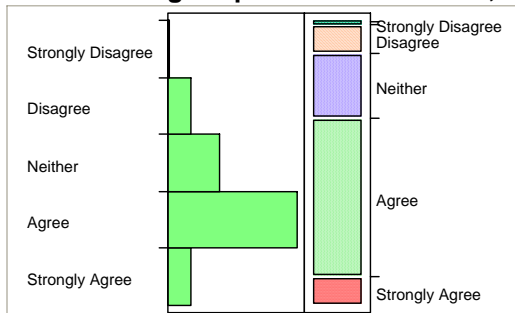
Level	Count	Prob
Strongly Agree	16	0.16162
Agree	61	0.61616
Neither	14	0.14141
Disagree	7	0.07071
Strongly Disagree	1	0.01010
Total	99	1.00000

**Q26: Uses Mistakes to Improve Understanding****Frequencies: Mean = 2.03**

Level	Count	Prob
Strongly Agree	21	0.21212
Agree	62	0.62626
Neither	8	0.08081
Disagree	8	0.08081
Total	99	1.00000

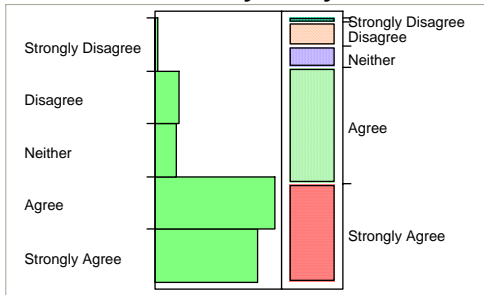
**Q27: Can Pass the Course Without Understanding****Frequencies: Mean = 3.25**

Level	Count	Prob
Strongly Agree	5	0.05051
Agree	25	0.25253
Neither	17	0.17172
Disagree	44	0.44444
Strongly Disagree	8	0.08081
Total	99	1.00000

**Q28: Learning Requires me to Rethink, Restructure and Reorganize****Frequencies: Mean = 2.36**

Level	Count	Prob
Strongly Agree	10	0.10309
Agree	54	0.55670
Neither	22	0.22680
Disagree	10	0.10309
Strongly Disagree	1	0.01031
Total	97	1.00000

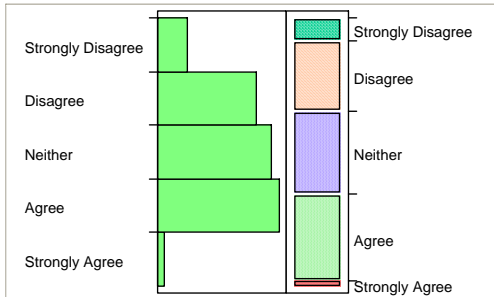
**Q29: Attends Nearly Every Lecture**



**Frequencies: Mean = 1.92**

Level	Count	Prob
Strongly Agree	37	0.37755
Agree	43	0.43878
Neither	8	0.08163
Disagree	9	0.09184
Strongly Disagree	1	0.01020
Total	98	1.00000

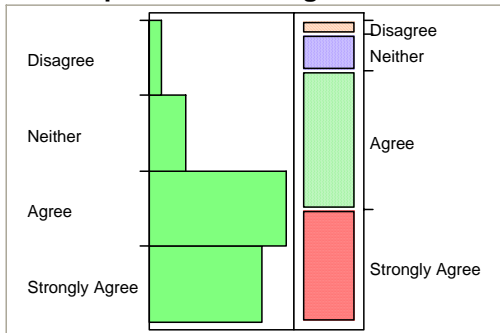
**Q30: Better Informed on Current Events**



**Frequencies: Mean = 3.06**

Level	Count	Prob
Strongly Agree	2	0.02041
Agree	32	0.32653
Neither	30	0.30612
Disagree	26	0.26531
Strongly Disagree	8	0.08163
Total	98	1.00000

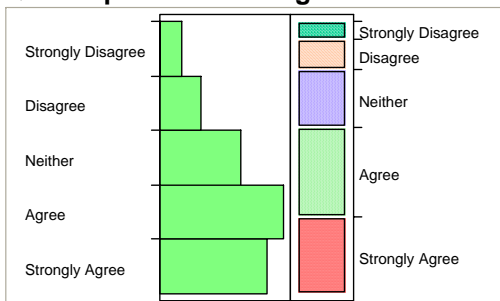
**Q31: Depends on Having Good Instructor**



**Frequencies: 1.83**

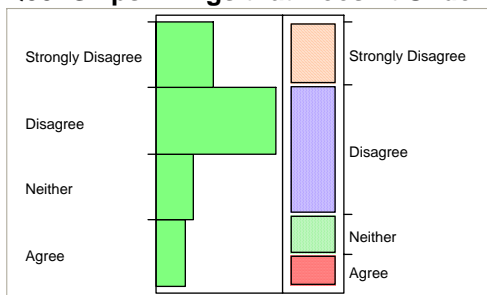
Level	Count	Prob
Strongly Agree	37	0.37755
Agree	45	0.45918
Neither	12	0.12245
Disagree	4	0.04082
Total	98	1.00000

**Q32: Depends of Having Good TA**

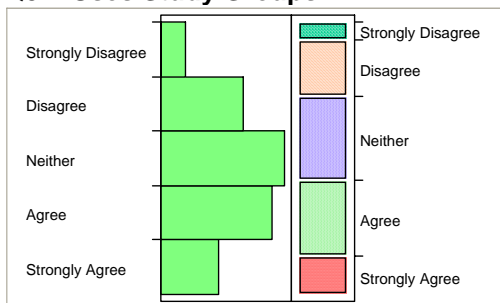


**Frequencies: Mean = 2.34**

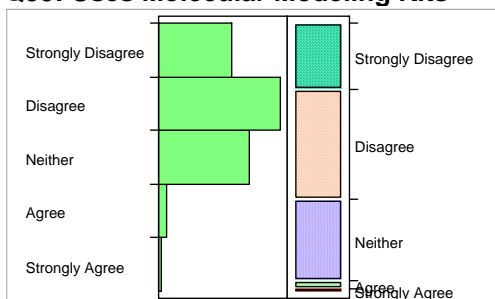
Level	Count	Prob
Strongly Agree	28	0.28571
Agree	32	0.32653
Neither	21	0.21429
Disagree	11	0.11224
Strongly Disagree	6	0.06122
Total	98	1.00000

**Q33: Skips Things that Doesn't Understand and Hopes not on Exam****Frequencies: Mean = 3.84**

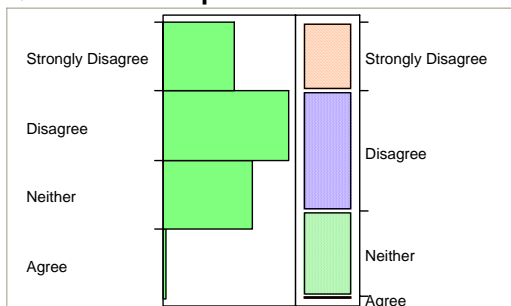
Level	Count	Prob
Agree	12	0.12245
Neither	15	0.15306
Disagree	48	0.48980
Strongly Disagree	23	0.23469
Total	98	1.00000

**Q34: Uses Study Groups****Frequencies: Mean = 2.76**

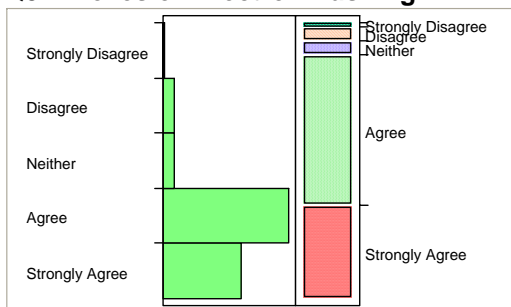
Level	Count	Prob
Strongly Agree	14	0.14433
Agree	27	0.27835
Neither	30	0.30928
Disagree	20	0.20619
Strongly Disagree	6	0.06186
Total	97	1.00000

**Q35: Uses Molecular Modeling Kits****Frequencies: Mean = 3.85**

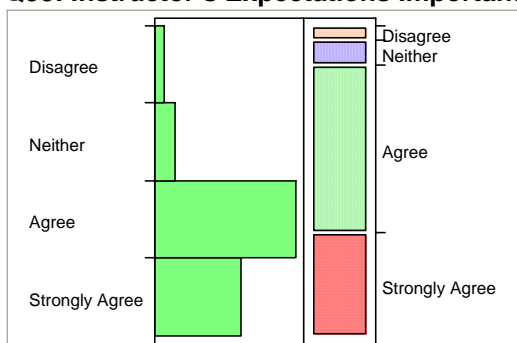
Level	Count	Prob
Strongly Agree	1	0.01020
Agree	3	0.03061
Neither	30	0.30612
Disagree	40	0.40816
Strongly Disagree	24	0.24490
Total	98	1.00000

**Q36: Uses Computer Software****Frequencies: Mean = 3.92**

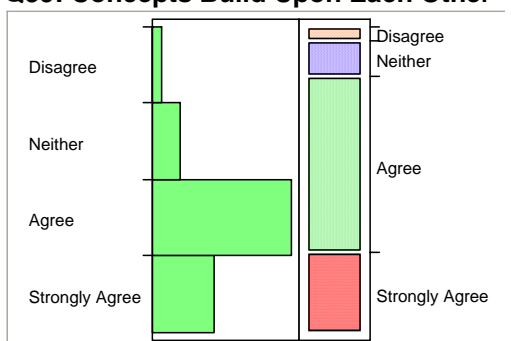
Level	Count	Prob
Agree	1	0.01031
Neither	30	0.30928
Disagree	42	0.43299
Strongly Disagree	24	0.24742
Total	97	1.00000

**Q37: Relies on Electron Pushing****Frequencies: Mean = 1.85**

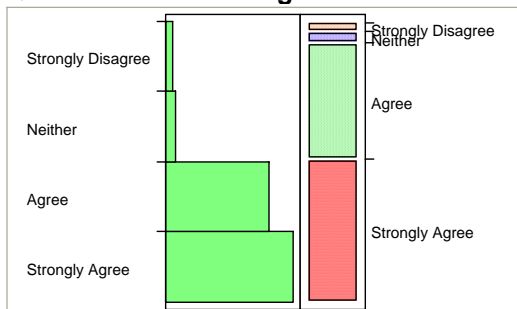
Level	Count	Prob
Strongly Agree	33	0.34021
Agree	53	0.54639
Neither	5	0.05155
Disagree	5	0.05155
Strongly Disagree	1	0.01031
Total	97	1.00000

**Q38: Instructor's Expectations Important for Success****Frequencies: Mean = 1.83**

Level	Count	Prob
Strongly Agree	32	0.33333
Agree	52	0.54167
Neither	8	0.08333
Disagree	4	0.04167
Total	96	1.00000

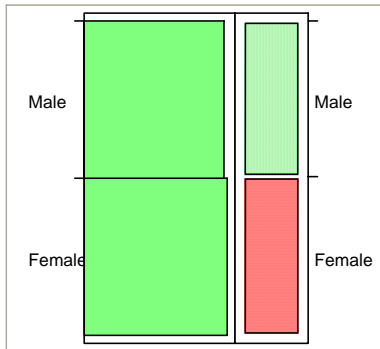
**Q39: Concepts Build Upon Each Other****Frequencies: Mean = 1.94**

Level	Count	Prob
Strongly Agree	25	0.26316
Agree	55	0.57895
Neither	11	0.11579
Disagree	4	0.04211
Total	95	1.00000

**Q40: O Chem Learning Takes Lots of Time****Frequencies: Mean = 1.63**

Level	Count	Prob
Strongly Agree	49	0.51042
Agree	40	0.41667
Neither	4	0.04167
Strongly Disagree	3	0.03125
Total	96	1.00000

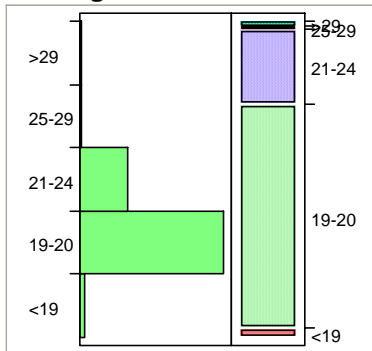
**Q41: Gender**



**Frequencies:**

Level	Count	Prob
Female	48	0.50526
Male	47	0.49474
Total	95	1.00000

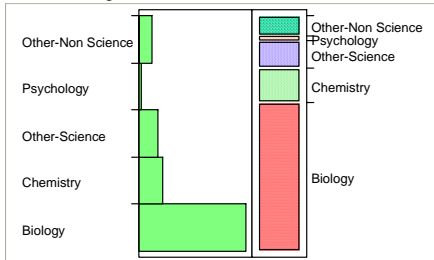
**Q42: Age**



**Frequencies**

Level	Count	Prob
<19	3	0.03125
19-20	68	0.70833
21-24	23	0.23958
25-29	1	0.01042
>29	1	0.01042
Total	96	1.00000

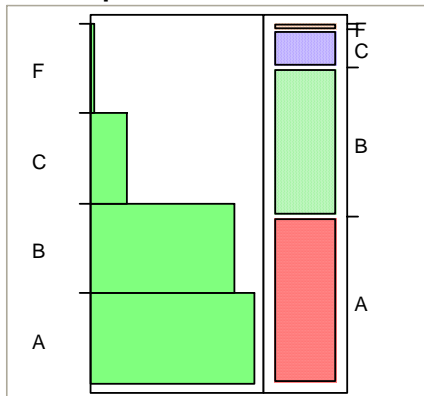
**Q43: Major**



**Frequencies**

Level	Count	Prob
Biology	61	0.63542
Chemistry	14	0.14583
Other-Science	11	0.11458
Psychology	2	0.02083
Other-Non Science	8	0.08333
Total	96	1.00000

**Q44: Expected Course Grade**

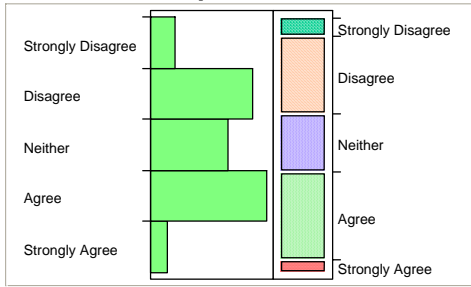


**Frequencies: Mean = 1.72**

Level	Count	Prob
A	44	0.46809
B	39	0.41489
C	10	0.10638
F	1	0.01064
Total	94	1.00000



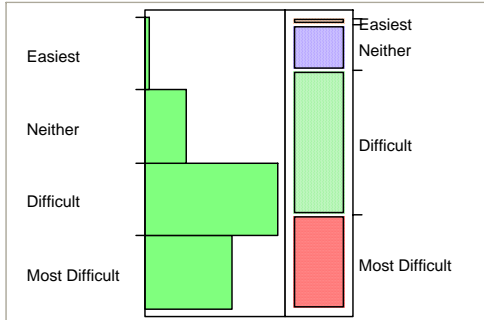
**Q45: Exams Representative of Knowledge**



**Frequencies: Mean = 3.0**

Level	Count	Prob
Strongly Agree	5	0.05208
Agree	33	0.34375
Neither	22	0.22917
Disagree	29	0.30208
Strongly Disagree	7	0.07292
Total	96	1.00000

**Q46: Course Level of Difficulty**



**Frequencies: Mean = 1.89**

Level	Count	Prob
Most Difficult	31	0.32632
Difficult	47	0.49474
Neither	15	0.15789
Easiest	2	0.02105
Total	95	1.00000

## APPENDIX 8: PARTIAL 40 X 40 CORRELATION MATRIX

Partial 40 x 40 Correlation Matrix for Survey Data

	PCA1	PCA2	PCA3	PCA4	PCA5	PCA6	PCA7
F1	-0.18591	0.173647	0.247475	-0.10839	0.062023	-0.11854	-0.0285
F2	-0.14975	0.142661	0.200717	-0.19627	-0.16594	-0.07714	0.045861
F3	0.158015	0.128732	0.121271	-0.24471	-0.03781	0.080737	0.276417
F4	0.21434	0.068213	0.154803	-0.26297	-0.02183	-0.11327	0.169308
F5	-0.23494	0.048637	0.132966	-0.01713	0.208721	-0.07538	0.15593
F6	-0.0323	0.186835	0.024415	0.045288	0.081041	-0.31963	-0.05023
F7	0.202074	0.045843	0.1272	0.021486	0.02525	-0.08252	-0.13371
F8	0.092775	0.219565	0.072767	-0.1248	0.03773	-0.07326	0.049359
F9	0.145535	0.020117	0.156067	-0.00843	0.34042	-0.18991	0.038797
F10	0.09899	0.137751	0.253346	0.03351	-0.04391	0.282206	-0.15367
F11	-0.21051	0.10368	-0.04019	-0.0207	0.113158	0.210535	0.132174
F12	0.19118	0.170408	-0.0475	-0.12559	-0.05231	0.020272	-0.40223
F13	0.076538	0.226637	-0.06161	-0.31135	0.209982	-0.02217	-0.00237
F14	-0.01476	0.087838	-0.17699	-0.27559	0.063011	0.315011	-0.24473
F15	0.179334	0.1274	0.116535	0.062881	0.088725	0.2072	-0.09925
F16	0.227026	0.123083	0.041988	0.079502	-0.09727	-0.10345	-0.08851
F17	0.190929	0.092233	0.310925	0.023661	0.025321	0.153289	0.054133
F18	0.116307	0.149467	-0.00894	0.195721	0.249671	-0.04538	-0.22675
F19	0.149959	-0.01524	0.163748	0.271909	0.259901	0.166631	0.044309
F20	-0.18958	0.168592	0.073356	-0.13043	0.099651	0.162971	0.171429
F21	0.248657	0.112885	0.140522	0.084358	0.10522	-0.02298	0.24489
F22	0.138578	0.169499	-0.15045	-0.21864	0.002159	-0.0667	-0.05156
F23	0.215002	0.126695	0.110772	0.023329	-0.01764	0.08353	0.091195
F24	0.190717	0.212829	-0.10176	-0.08803	-0.15593	-0.00524	-0.13095
F25	-0.16975	0.132099	0.07315	0.148098	0.10056	0.205325	0.037472
F26	-0.24788	0.150822	0.19546	0.04236	-0.06869	0.151138	-0.11145
F27	0.149407	-0.07662	-0.06603	0.070147	-0.08739	0.284685	0.380315
F28	-0.1772	0.191074	-0.07326	-0.08885	0.066607	-0.00936	0.05278
F29	-0.09104	0.29367	0.030953	0.06763	0.026848	-0.20253	0.11033
F30	-0.12202	0.195181	-0.19548	-0.2581	-0.15091	0.122921	0.171797
F31	-0.0159	0.280396	-0.11681	0.18078	-0.22571	-0.04367	-0.07896
F32	0.035228	0.205443	-0.18543	0.141773	-0.32014	-0.11612	0.066861
F33	0.22991	-0.01064	-0.2122	0.041289	-0.1373	0.096599	0.013438
F34	-0.03005	0.078596	-0.13727	0.17783	0.200929	-0.29888	0.012425
F35	0.089535	0.127106	-0.34517	0.134145	0.272567	0.142841	0.116982
F36	0.068658	0.169487	-0.37005	0.075238	0.255107	0.05593	0.194651
F37	-0.08928	0.155255	-0.0103	0.229993	-0.0471	0.219305	-0.10328
F38	-0.0061	0.172174	0.149051	0.289782	-0.28707	0.071832	0.118996
F39	-0.21471	0.207505	-0.00689	0.082281	0.14454	0.11085	-0.2585
F40	-0.05922	0.230244	-0.02018	0.218144	-0.17794	-0.17198	0.178629

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