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ABSTRACT

The purpose of this study was to characterize the prior conceptions of molecular structure that organic chemistry students expressed as they learned to interpret nuclear magnetic resonance spectra, and to describe the problem-solving strategies that students employ as they determine molecular structure. The two questions that frame this study focus on the development of scientific concepts and problem solving strategies. Findings indicate that students generate two-dimensional illustrations of molecular structure as a default mode and that computer modeling holds promise in helping students overcome misconceptions about molecular structure. (Contains 37 references and 15 tables.) (DDR)

The Influence of Conceptions of Molecular Structure and Patterns of Problem-Solving on the Process of Learning to Interpret Nuclear Magnetic Resonance Spectra

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INTRODUCTION

Undergraduate students with aspirations of a career in Chemistry, the health sciences, or the life sciences frequently have to take challenging prerequisites to their major course of study. These are academic fields that share a common challenge --- the organic chemistry course. In turn, one challenge in organic chemistry is understanding the impact of three-dimensional structure on the chemical and physical properties of molecules. For most undergraduates, this is their first serious encounter with this aspect of chemistry; for many, this first encounter is indeed daunting.

One of the most important skills that undergraduates learn in the organic chemistry course is how to determine the three-dimensional structural arrangement of a molecule from a given molecular formula and nuclear magnetic (NMR) spectra. Chemists use NMR as a means of characterizing compounds, monitoring chemical reactions, and verifying synthetic routes. This skill is fundamental to the practice of science in organic chemistry. Students who acquire a facility with NMR techniques must master not only the rudiments of spectroscopy, but the niceties of molecular structure. It is the intricate relationship between molecular structure and NMR spectroscopy that makes NMR spectroscopy so valuable a research tool and so daunting a challenge to the organic chemistry student.

Computer technology impacts the entire field of spectroscopy by incorporating mathematical, analytical techniques, such as Fourier Transform (FT), making it possible to interpret spectra to a greater detail than was imaginable just a few years ago. Several forms of NMR spectroscopy are more accessible to the modern scientific researcher because of computer technology. One-dimensional NMR involving isotopes of carbon-13 and fluorine-19, and most forms of two-dimensional NMR studies were once special spectral techniques, but are now fairly routine modes of analyses. The multimedia revolution in computer technology has also made possible the collection of sizable databases of NMR spectra in a compact disc format. All of these developments have enhanced the quality and quantity of research in organic chemistry.

Despite these highly touted technical advances, the process by which the undergraduate student relates the abstract lines of an FT-NMR spectrum to the equally abstract vision of the structure of a molecule is poorly understood. While technology increases the ease of accessibility and the speed of data retrieval for the practicing scientist, it does not necessarily alter the ease or speed with which the novice learns to interpret NMR spectra.

Current research in education supports a constructivist view of learning. Within this framework, rather than passively receiving knowledge, the learner actively constructs knowledge. Constructivist approaches to education recognize the impact of the learner's prior experience, and the role that social mediation plays in the learning process (Vygotsky, 1968, 1986). Cooperative learning (Totten, Sills, Digby & Russ, 1991) and metacognitive strategies (Derry, 1990; Mandinach, 1990; Wittrock, in press) are instances of pedagogic strategies based upon a constructivist viewpoint.

Studies in the domain of science education corroborate the importance of the learner's prior conceptions to the acquisition of fundamental scientific principles in physics and chemistry (Chandran, Treagust, & Tobin, 1987; Hesse, 1992; Scott, Asoko, & Driver, 1990; Staver & Jacks, 1988). However, studies such as these have not focused specifically on NMR nor on the close connection between NMR and notions of molecular structure. Characterization of the prior conceptions held by undergraduates on the nature of three-dimensional structure and its ramifications on the interpretation of NMR spectroscopy is a project of great importance to improved instructional practice. The problem-solving strategies employed while interpreting NMR spectra are also in need of examination. The challenge that the organic chemistry student faces in learning to interpret NMR spectroscopy is in turn a challenge to the science educator to discern the nature of the prior conceptions and the patterns of problem solving that influence the learning process itself. This study is an attempt to meet this challenge; an effort to describe both the notions of molecular structure and patterns of problem solving that students use in interpreting NMR spectra.

PURPOSE OF THE STUDY

The purpose of this study is to characterize the prior conceptions of molecular structure that organic chemistry students express as they learn to interpret NMR spectra and to describe the problem-solving strategies that students employ as they determine molecular structure from NMR spectra. To achieve these purposes two major questions frame this study. The first question focused on the development of scientific concepts, while the second examined problem solving strategies. The first question was an attempt to describe the students' concepts of molecular structure in relation to interpretation of NMR spectra. The second question probed the manner in which the students approached problem-solving within the context of interpretation of NMR spectra.

1. What are some of the concepts of molecular structure that undergraduates use in solving problem in NMR spectroscopy?
    - A. Do students share common conceptions or misconceptions?
    - B. Do the common conceptions have a basis in experience or chemical theory?
    - C. Are the concepts that students posit related to particular student attributes?
        - i. Academic major?
        - ii. Chemistry background?
        - iii. Cooperative group membership?
        - iv. Gender?
        - v. Race/ethnicity?
2. What problem-solving strategies do students use to determine molecular structure from NMR spectra data?
    - A. Do students employ strategies that invoke discernible patterns?
    - B. Do the strategies that the students use relate to particular student attributes?
        - i. Academic major?

ii. Chemistry background?

iii. Cooperative group membership?

iv. Gender?

v. Race/ethnicity?

C. Is there a relationship between the concepts that students presume and the problem-solving strategies that they employ?

THEORETICAL FRAMEWORK

The realm of constructivist views of how learning occurs is the basis for this study of students' notions of molecular structure. The learner is assumed to actively construct knowledge from personal experience and formal instruction (Vygotsky, 1968 & 1986). Studies that emanate from Leeds University and the Center for Studies in Science and Mathematics reveal that children's ideas in science are idiosyncratic, internally coherent, and persistent (Driver, Guesne, & Tiberghien, 1985). Children also exhibit a propensity to maintain certain scientific ideas from primary school to high school in the face of apparent evidence to the contrary (Carey, 1986). Strike and Posner (1992) describe the learner's unique compendium of conceptions and misconceptions in various stages of development as the "conceptual ecology." Studies of conceptual change in the chemistry domain focus on the structure of matter, notions of physical state, energy, and the distinction between chemical and physical changes (Chandran, Treagust, & Tobin, 1987; Krajcik, Simmons, & Lunetta, 1988; Staver & Jacks, 1988; Vosniadou, 1991; Hesse, 1992; Renstrom, Andersson, & Marton, 1996).

Characterization and analysis of children's understanding of the fundamental scientific concepts that are an inevitable part of common life experience is the object of most studies in the conceptual change literature. Molecular structure and NMR are not within this realm of the traditional conceptual change literature on two accounts. First, molecular structure and NMR are not usually experienced during ordinary interaction with the world. Molecules are much too small to be seen on a macroscopic level and NMR instruments too expensive for the average community college to own. Second, children are rarely, if ever, taught about molecular structure and NMR. They are introduced to it at the earliest in middle school or high school.

However, studies of students' understanding of more sophisticated scientific concepts is not without precedent in the conceptual change literature. Jensen, Wilcox, Hatch and Somdahl (1996) developed a computer program to help them assess undergraduate biology students' understanding of the concepts osmosis and diffusion. Osmosis and diffusion occur on a macroscopic level, but can only be explained in terms of molecular behavior on a microscopic level. The computer program was designed to help students consider the ramifications of molecular motion. Lawson, Baker, DiDonato, and Verdi (1993) studied the concepts of molecular polarity, bonding, and diffusion in a conceptual change study involving 77 students enrolled in a biology course for nonmajors at a suburban Arizona community college. Lawson et al. (1993) distinguish between "theoretical" and "descriptive concepts. Descriptive concepts are those that can be observed first-hand in nature and are the substance of much of the conceptual change literature. Theoretical concepts relate to imagined or unseen phenomena that are hypothesized to exist at the atomic or molecular level to explain observable behavior. Molecular structure and NMR are examples of such theoretical concepts, and worthy of study from a conceptual change perspective.

Constructivist learning principles lend a great deal of importance to those concepts that the learner constructs that are not in agreement with conventional scientific constructs. This misconception literature covers a broad spectrum of subjects including science and mathematics. The Center for Studies in Science and Mathematics research group has characterized a few of the common misconceptions that children have of atoms and molecules. Children tend to ignore particle motion, attribute bulk properties to the constituent particles, and associate intermolecular properties only with heat (Driver, Guesne, and Tiberghien, 1985). These particular conceptions of atoms and molecules were also found to be highly context-dependent. Renström, Andersson, and Marton conducted a study of 13-16- year-old students and revealed six common conceptions of matter. In order of increasing coherence with conventional notions of atoms and molecules the students viewed matter as composed of:

1. A homogeneous substance exhibiting only bulk properties.
2. Homogeneous substance units.
3. Substance units composed of small atoms.
4. An aggregation of particles.
5. Particle units
6. Systems of particles (Renström, Andersson, & Marton, 1990).

These notions of matter have some basis in the historical progression of views of the atom. From Aristotelian notions of continuous matter to more modern views of systems of atoms and molecules, all of these notions were common to the adolescents surveyed in this study.

In a related study, Griffiths and Preston (1992) interviewed thirty twelfth-grade, Canadian students about their views of the water molecule. They identified five categories of common misconceptions related to the structure, size, shape, composition , weight, bonding, and energy of water molecules. Again, this study provides evidence that students ascribe macroscopic properties to atomic or molecular behaviors. The view of matter as a continuous entity is another misconception common to the study by Renström, Andersson, and Marton. Griffiths and Preston also found that many students anthropomorphize matter; referring to molecules and atoms as being alive. Griffiths and Preston found that the range of misconceptions was the same for students no matter the extent of their background in academic science. Treagust (1988) devised a process for developing and using diagnostic tests based upon students' common misconceptions about the nature of matter.

The vast majority of the misconception literature is based upon studies of children. The typical student learning to interpret NMR spectra is not a child, but usually in late adolescence or early adulthood. There exists within the misconception literature a body of work that addresses the misconceptions of atomic and molecular structure as manifested in secondary and post-secondary students. Gabel, Samuel, and Hunn (1987) studied pre-service elementary teachers' views of the particulate nature of matter. More than fifty percent of the pre-service teachers revealed misconceptions in the conservation and orderliness of particles. Uri Zoller, in his study of college freshmen, claims that general chemistry is the "most problematic traditional science discipline" due to abstract and nonintuitive concepts (Zoller, 1990, p. 1053). Zoller describes several major misconceptions in general and organic chemistry that are characteristic of college freshmen. Benson, Wittrock, and Baur (1993) engaged in a longitudinal study of some 1098 students from second grade to university-level chemistry targeting the particle nature of matter gases. They found three general misconceptions common across age level: the belief that matter is continuous rather than particulate, the attribution of gas behavior to the behavior of liquids, and the failure to account for empty space between gas particles. Quílez-Pardo and Solaz-Portolés (1995) characterized conceptual difficulties in the application of Le Chatelier's Principle to a chemical system at equilibrium. The subjects of this study were 170 first-year university chemistry students and 40 secondary chemistry teachers in Spain. Misconceptions in six areas are described. Harrison and Treagust (1996) interviewed 48 secondary students to describe their mental models of atoms and molecules. The students in this study prefer discrete and concrete models. Harrison and Treagust attribute their misconceptions in part to the semantic differences that exist between teacher and student language. The five studies described here demonstrate that misconceptions have significant ramifications on learning science at all age levels.

There are many explanations for the existence of common scientific misconceptions. The historical development of science and its correlation to the development of scientific concepts in the individual is one of the explanations often offered. Griffiths and Preston (1992) refer to this in their analysis of students' views of water molecules. Renström, Andersson, and Marton (1990) warn that science education itself may serve as the source for some misconceptions (p. 567). Logan and Logan (1993) concur with this finding to the extent that words used in science have different meanings when used in the vernacular. For example, the notion of "resonance hybrid" bonds in a benzene molecule is confusing to students because "resonance" has connotations of vibrations from physics and "hybrid" has connotations of inherited characteristics from biology. Students faced with learning a new vocabulary may build erroneous notions on the basis of the meanings of identical words in other contexts.

Cognitive psychology offers an extensive literature on the distinction between the thought processes of novices and experts. Experts are considered to be those persons who possess highly developed skills or who are unusually knowledgeable in a given domain. Experts have the facility to process information pertinent to a given problem in chunks rather than as discrete data. Although experts exhibit better recall of information from within their domain of expertise, studies have shown that they do not have a better memory in general (Bruer, 1993). "Studies have shown that experts know how to select and manipulate information for the problem at hand: selecting useful material, making appropriate inferences, and organizing relationships for a problem" (Hawkins, Mawby, & Ghitman, 1985). The novice employs different criteria for categorizing and approaching a problem. The distinction between the novice and expert problem solving methods reveals the inherent differences in the their conceptual frameworks.

Cognitive scientists conduct novice-expert studies in a wide variety of domains, but have not included the domain of molecular structure determined by interpretation of NMR spectra. Interpretation of NMR spectra is analogous to the process by which medical professionals interpret x-ray films to produce a clinical diagnosis; a process which has been studied by cognitive scientists. NMR and x-ray interpretation both require expertise in a complex skill. Both integrate several fields of knowledge with distinct organizing principles. They both involve a substantial perceptual component as well as a formal knowledge component. Studies of medical residents ability to interpret x-rays reveal that the acquisition of expertise depends upon the refinement of schemata developing through a subtle form of generalization and discrimination. A strong parallel exists between the acquisition of the complex skill of x-ray diagnosis and general cognitive development. Experts are able to build mental representations of patient anatomy from x-rays; they evoke pertinent schema efficiently; and they take account of possible diagnoses as they arise (Lesgold, Rubinson, Feltovich, Glaser, Klopfer & Wang, 1988). Similar behavior may be expected of experts in NMR interpretation.

In studies of other problem-solving situations in chemistry, novices are found to work more slowly, use more incorrect formulas, group similar problems by topic, and use fewer modes of representing a problem (Heyworth, 1989, & Bruer, 1993). A study of graduate students solving problems in organic synthesis by Bourne, Dominowski, and Loftus (1979) resulted in a model for problem solving that is particularly salient to this study. According to this model, problem solving is regarded as a nonlinear, iterative process that involves preparation, production, and evaluation of a solution to the problem.

Methods

This study took place on the campus of the University of California, Los Angeles. UCLA is a large, public university serving a highly diverse student body. The sample consisted of thirty-two students randomly drawn from the sophomore organic chemistry laboratory course in the Department of Chemistry and Biochemistry. Data were collected over a six-week interval in one academic quarter (see Table 1). A written PreLab Quiz surveyed students' prior conceptions of eight target concepts of molecular structure and notions of problem solving. Demographic data was self-reported by the students on the PreLab Quiz (see Table 2). After the PreLab Quiz was complete, students solved two NMR problems using an interactive computer program, "FT-NMR Problems" (Chapman & Russell, 1989). Students worked in unstructured groups of three or independently at the computer. The groups and individual students were selected to have equal representation by males and females. The students completed a worksheet describing their procedure for solving each problem at the end of the computer session. The computer session was videotaped. The computer sessions lasted approximately ninety minutes.

The students solved two problems in the Beginner level of the FT-NMR Problems program. The first problem, *p*-xylene, involved a planar geometry, aromaticity, resonance, and two lines of symmetry in its structure (see Figure 1). The second problem, a-cyclohexanone, required that the students consider a nonplanar geometry in a six-membered carbon ring, the influence of the ketone functional group, and an apparent lack of symmetric elements (see Figure 2).

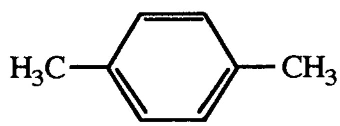

Figure 1. FT-NMR Problem 7. *p* -Xylene

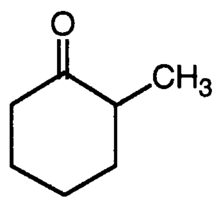

Figure 2. FT-NMR Problem 12. α-Methylcyclohexanone

During the tenth week of the academic quarter, half of the original thirty-two students participated in an exit interview. The students completed another concept survey and solved an additional NMR problem without using the computer. The exit session was videotaped. The semi-structured interviews lasted about forty-five minutes. The researcher served as a participant observer for the problem sessions and exit interviews.

Data were subject to qualitative and quantitative analyses. All of the videotaped sessions were transcribed. The PreLab Quiz, problem worksheets, videotaped problem sessions, and videotaped exit interview were all subject to analysis. The coding scheme for the data included means for the analysis of the concepts that the students invoked and the strategies that they employed. Eight concepts were targeted for analysis based upon data collected in a prior pilot study. These eight concepts were chosen because they are commonly invoked in solving NMR problems. The concepts chosen were: *aliphatic*, *aromatic*, *benzene*, *chemical shift*, *cyclohexane*, *degrees or sites of unsaturation*, *resonance*, and *symmetry*. In the written instruments the students were asked to describe and illustrate these terms.

The responses were categorized by the completeness of the concept in relation to theoretical notions of the concept in chemistry. The textbook assigned to the students in the lecture course was used as a source for ascertaining the historical development of these concepts in theory (Solomons, 1992). The illustrations of the concepts were categorized by common patterns in shape, dimension, and detail. Based upon a scheme used by Westbrook and Marek (1991), the concept explanations and illustrations were assigned to one of four categories: blank, misconception, partial, and complete (see Appendix A). Responses were assigned a blank code when no attempt was made to generate an explanation or illustration. A response was considered to be a misconception if the target concept was explained or illustrated using unrelated concepts. Responses coded as partial conceptions are those that involve an incomplete notion of the target concept, often accompanied by a misconception. Those responses that indicated a thorough linking of a target concept to its accepted theoretical foundation were coded as complete conceptions.

The strategies that the students used to solve the NMR problems were subjected to analysis from a theoretical perspective proposed originally by Bourne, Dominowski, and Loftus (1979). According to this model, problem-solving is a nonlinear process involving preparation for a solution, production of a solution and evaluation of a solution. In this study, solution preparation was presumed to be related to the information available from a given molecular formula, calculation of degrees of unsaturation, and the various carbon and hydrogen spectra for each problem. Students took the information presented and decomposed it into information segments that could be used as an element in producing a solution to the problem --- a structure for a molecule. *Analysis* is the term adopted in this study to describe this type of activity. Solution production, or *synthesis*, is the process by which the students exploited the information available in the problem and composed a solution from the information segments. *Verification* describes any act whereby students sought to evaluate a possible solution. A coding scheme was devised for the solution of NMR problems that took into consideration not only solution analysis, synthesis, and verification, but the order in which the processes appeared in the solution process (see Appendix B).

The validity of the methods employed in this study was safeguarded in two ways. First, in as many ways as possible, participants for the study were randomly selected. The entire sample itself was taken from an existing course population. The laboratory sections were the result of student self-selection in enrollment. While these facts could have interfered with overall validity, probability does play a role in enrollment. The teaching assistants selected to administer the PreLab NMR Quiz to two lab sections were chosen randomly. Within each lab section the students who participated in the study were chosen randomly by the teaching assistant. A coin was flipped to determine the gender of the triad and singleton participants (see Appendix C). The reliability of the coding scheme was verified by triangulation and inter-rater reliability methods. Cross tabulation analyses were triangulated with inferences from student discourse.

RESULTS

The data in Tables 3-7 indicate that the students did express shared conceptions and misconceptions of the eight concepts on the PreLab Quiz. The ideas reported do have a basis in the theory of chemistry and in student experience. The concepts that proved to be the most troublesome to the students on the PreLab Quiz are the terms *aliphatic* and *chemical shift*. The most frequent response for both the explanation and the illustration for these two concepts is a lack of response. In the case of the concept *aliphatic* the result is surprising. Aliphatic hydrocarbons are introduced at the beginning of the organic chemistry course while chemical shift is introduced at the time that NMR spectroscopy is addressed. The lack of response on the PreLab Quiz may be due to a lack of familiarity with a new concept in the case of *chemical shift*, while a failure to respond for the term *aliphatic* may be due to insufficient review of past concepts.

During the course of the study, students had the opportunity to experience growth in their understanding of NMR as a process and in their understanding of basic concepts in molecular structure. The students in the Exit Interview were polled regarding their explanation and illustration of the same concepts that appeared on the PreLab Quiz. It is well documented in the literature that misconceptions are highly resistant to change (Driver, Guesne & Tiberghien, 1985; Carey, 1986; Clough & Driver, 1986). It is not surprising, therefore, that there is little change in the student patterns of response to the concept survey for this reason. The results from the PreLab Quiz and the Exit Survey indicate that there is an association in the explanation response that students provided for four out of the eight target concepts. There is one concept that indicates an association between illustrations on the PreLab Quiz and Exit Survey. The four explanations that are stable are either complete or partial concepts. The stable illustration was a blank for the concept *aliphatic*. However, students are continuously learning. The four concepts whose explanations differed between the PreLab Quiz and the Exit Survey were: *aliphatic*, *chemical shift*, *cyclohexane* and *resonance*. For the concept, *aliphatic*, there was a decrease in the frequency of blank responses and an increase in partial and complete conceptions. For *chemical shift* there is an increase in the frequency of misconception and partial responses and a decrease in the blanks. The explanations for *cyclohexane* tended to shift from partial conceptions on the PreLab Quiz to a small increase in blanks and misconceptions. For *resonance*, the explanations tended to shift from partial conceptions to an increased frequency of complete conceptions. It is possible that the six-week interval between the PreLab Quiz and the Exit Survey allowed some students to experience conceptual development, but not for others.

Four of the eight target concepts have no association to academic major, background in chemistry, gender, or ethnicity (see Tables 8-9). There is only one association between a student's conceptions and membership in cooperative group. This could mean that students are not unduly influenced by others. Working in a group is not detrimental to learning. However, the benefits of cooperative work are not apparent. The associations that are significant are for the most part questionable. The small numbers of students that constitute cohorts in academic major and chemistry background cast doubt on the apparent associations. More study is required to investigate the possible influence of these particular student attributes.

The molecular concepts that students declare do have a basis in their experience, particularly in their prior instruction. Tables 3, 4, 6, and 7 summarize the most frequent response for explanations and illustrations on the PreLab Quiz and the Exit Interview. On the PreLab Quiz the most frequent substantive response for the concept, *aromatic*, is pi orbital overlap. Students learn about pi orbital overlap in the organic chemistry course. At the time of the PreLab Quiz pi orbital instruction is fresh in students' minds. Students frequently draw illustrations of concepts that have no three-dimensional detail. For example, the common illustration for *cyclohexane* is a hexagon. The hexagon is a two-dimensional figure that does not reveal the true geometry of the molecule. When asked about this during the Exit Interview students refer to their prior instructional experience as a reason for drawing two-dimensional representations of molecules.

Researcher: ... do you envision it as two or three dimensional?

Triad: Two. (All respond at once.)

Researcher: OK. When you do two dimensions... Why do you think of it in two dimensions first?

Brent: Because I am thinking of it on paper, not...(The answer trails off.)

Researcher: OK. Doug.

Doug: Yeah. I think the first step is to think the most basic way, and I

> think two dimensions is just the more basic than three. So, it's easier, once you try to learn about something and they tell you it's a different way.

Doug's final statement reflects the tension between the economy of the two-dimensional view and the cognitive demand that the additional information from a three-dimensional view requires. There is little evidence that students' notions of the eight target concepts have a link to personal experience. The students rarely use analogies to link their notion of a concept to a personal understanding of the world. Chemical theory is also reflected in the quality of the explanations and illustrations that students produce for the eight target concepts. The coding scheme inferred from the data is categorized by the historical progression of chemical theory: structural, valence, resonance, and molecular orbital. It appears that there may be a confounding of prior experience and chemical theory.

Four of the eight target concepts have no association to academic major, background in chemistry, gender, or ethnicity (see Tables 8-10). There is only one association between a student's conceptions and membership in cooperative group. This could mean that students are not unduly influenced by others. Working in a group is not detrimental to learning. However, the benefits of cooperative work are not apparent. The associations that are significant are for the most part questionable. The small numbers of students that constitute cohorts in academic major and chemistry background cast doubt on the apparent associations. More study is required to investigate the possible influence of these particular student attributes.

There is evidence that students employ a pattern of problem-solving strategies to determine molecular structure from NMR spectra. The pattern of problem solving may be primarily described as iterative. Students tend to work forward without strict adherence to trial and error and algorithmic methods. Students develop a pattern for the order in which the various spectra are addressed. Analysis is more frequent in the spectra with which students are most familiar. Synthesis and verification are rare events during the solution process. There is a critical mass of data that students require before attempting to produce trial solutions and check them (see Tables 11 and 12).

In general, there is insufficient evidence to support the contention that the problem-solving strategies that students employ in the determination of molecular structure from NMR spectra is related to student attributes such as academic major, chemistry background, cooperative group assignment, gender, and ethnicity. Significant associations to academic major and chemistry background are compromised by the small number of students in the sample. It is also possible that chemistry background and group membership are confounded.

The data also do not indicate that there is a relationship between the concepts that students hold and the strategies that they employ in the context of solving NMR problems. Less than 10% of all possible associations are significant (see Tables 13-15). Most of the significant cross tabulations link superficial understandings of concepts to failure to attempt strategies across the databases. Students use more databases and strategies in the Exit Interview than in the PreLab Quiz. This is possible evidence that learning has occurred. It is worthy of further research to investigate why *benzene* did not have any significant cross tabulations on the Exit Interview for both explanations and illustrations. If students use naive concepts in conjunction with algorithmic strategies, they may not be confronted with cognitive discrepancies. This allows the students to apply their current understanding of a concept to their current knowledge of a strategy.

EDUCATIONAL IMPORTANCE OF THE STUDY

The results of this study have implications for the chemistry curriculum. The complexity involved with learning to interpret NMR spectra is exacerbated by a tension between the students' and the instructor's understanding of fundamental concepts of molecular structure. Although both may use the same words, they do not always share the same meanings. This study presents evidence for this phenomenon, in particular the concepts *aliphatic* and *chemical shift*. Most students are unable to generate explanations or illustrations for these two concepts throughout the six-week study. The important question for educators is how to create a common ground of understanding. Instructors need to be aware of some of the common meanings that students are likely to hold and to confront these meanings in their instructional practice.

Students generate two-dimensional illustrations of molecular structure as a default mode. This propensity is in part the result of years of exposure to books, blackboards, and screens used for instruction. Organic chemistry requires a facility in visualization of molecules in three-dimensions. This is particularly true when a tool such as NMR is used. Students must develop the facility to interchange views. A recent study demonstrated that high school students overcome misconceptions about the structure of water molecules by using computer-generated simulations (Hakerem, Dobrynina & Shore, 1993). In another unrelated study, Williamson and Abraham (1995) found that students who view molecular animations earn higher test scores than students who viewed still images of the same situations. With this kind of evidence pointing to the efficacy of computer modeling, chemistry instructors might consider allowing students to have access to a molecular modeling program while solving NMR problems.

Table 1.

Research Calendar

Week	Location	Activity
1-2		Preparation for data collection
3	Young Hall Labs	Attendance at TA Meeting Distribution of TA Instructions
	Young Hall	Attendance at NMR lecture Recording of field notes
4	Physical Sciences Learning Center	Pre-Lab Quiz Administration Videotaping of sessions Recording of field notes Collection of FT-NMR Worksheets
5	Young Hall Labs	Collection of NMR Spectrum Analysis
6-8		Transcription of videotapes Analyses of the data
9	Young Hall Labs	Scheduling of interviews
10	Physical Sciences Learning Center	Key Concept Survey administered Videotaping of exit interviews

Table 2

Baseline and Study Group Demographics

Demographic Data	Baseline Group % N=38	Study Group % N=32
Gender		
Female	50.00	50.00
Male	44.74	50.00
No response	5.26	
Ethnicity		
African American	2.63	0.00
Asian	47.37	40.62
Hispanic/Latino(a)	10.53	18.75
Pacific Islander	2.63	0.00
White	18.42	31.25
Other	2.63	0.00
No Response	15.79	9.38
Academic Major		
Chemistry/Biochemistry	10.53	12.50
Life sciences	47.37	43.75
Nonscience	21.05	34.38
Physical sciences	2.63	0.00
No response	18.42	9.38
Background in Chemistry		
AP Chemistry	18.42	12.50
No AP Chemistry	71.05	78.13
Not sure	5.26	6.25
No response	5.26	3.13

Table 3

Most Frequent Responses for Concept Explanation of the PreLab Quiz

Concept Explanation	Code (N = 32)	Frequent Responses	Frequency in Percent
Aliphatic	Blank	No Response	59.4%
	Misconcep	Polarity	21.9%
	Partial	Nonaromatic hydrocarbon	18.8%
Aromatic	Blank	No Response	6.3%
	Misconcep	Consecutive double bonds	25.0%
	Partial	Alternating double bonds	18.8%
	Complete	π orbital overlap	50.0%
Benzene	Blank	No Response	6.2%
	Misconcep	More than one electron arrangement	3.1%
	Partial	Unsaturated C_6H_6 ring	68.8%
	Complete	π orbital overlap	21.9%
Chemical Shift	Blank	No Response	40.6%
	Misconcep	Shift electron to positive site	18.8 %
	Partial	Change in signal due to neighbors	28.1%
	Complete	Shielding/Deshielding	12.5%
Cyclohexane	Blank	No Response	6.3%
	Misconcep	Antiaromatic, 4n pi electrons	3.1%
	Partial	Six-membered ring, C_6H_{12}	84.4%
	Complete	Chair/boat conformations	6.3%
Degrees of Unsaturation	Blank	No Response	18.8%
	Misconcep	Empty valence, missing electrons	18.8%
	Partial	Carbon with four hydrogens	9.4%
	Complete	Number of multiple bonds or rings	53.1%
Resonance	Blank	No Response	9.4%
	Partial	Stabilization of molecule or ion	71.9%
	Complete	π orbital overlap	18.8%
Symmetry	Blank	No Response	6.3%
	Misconcep	Same pull on both sides	9.4%
	Partial	Molecule with similar sides	40.6%
	Complete	Similar atom environments	43.8%

Table 4

Frequent Responses for Concept Explanation on the Exit Survey

Concept Explanation	Code (N = 16)	Frequent Responses	Frequency in Percent
Aliphatic	Blank	No Reponse	37.5%
	Misconcep	Negative and positive charge	31.3%
	Partial	Carbon has four bonds to hydrogen	25.0%
	Complete	Carbon has maximum single bonds	6.3%
Aromatic	Blank		
	Misconcep	Ring 2n+2 elecs/Converged ring	12.5%
	Partial	Alternating double bonds	25.0%
	Complete	π orbitals, overlap	62.5%
Benzene	Partial	Unsaturated C_6H_6 ring	75.0%
	Complete	π orbitals	25.0%
Chemical Shift	Blank	No Response	18.8%
	Misconcep	where peaks appear	25.0%
	Partial	Change in signal due to neighbors	50.0%
	Complete	Shielding/deshielding	6.3%
Cyclohexane	Blank	No Response	12.5%
	Misconcep	Five-membered carbon ring	12.5%
	Partial	C_6H_{12} ring with no double bonds	75.0%
	Complete		
Degrees of Unsaturation	Blank	No Response	6.3%
	Misconcep	Error in Z formula	12.5%
	Partial	Calculate Z value	25.0%
	Complete	Number of multiple bonds or rings	56.3%
Resonance	Blank	No Response	12.5%
	Misconcep		
	Partial	More than one Lewis structure	56.3%
	Complete	π orbitals, overlap	31.3%
Symmetry	Blank	No Response	6.3%
	Misconcep		
	Partial	Similar carbon, hydrogen sites	43.8%
	Complete	Axis/plane of symmetry	50.0%

Table 5

Comparison of Concepts in PreLab Quiz and Exit Survey

Concept	Code Common Response	Common Response	X^2	df	p
Aromatic Explanation	Complete	π orbital overlap	13.80	6	0.03*
Benzene Explanation	Partial	Unsaturated C_6H_6	9.33	2	0.01*
Degrees Unsat Explanation	Complete	Multiple bonds/rings	18.59	9	0.03*
Symmetry Explanation	Partial	Similar C/H sites	14.23	4	0.01*

*p<0.05

Table 6

Most Frequent Responses for Concept Illustration of the PreLab Quiz

Concept Illustration	Code (N = 32)	Frequent Responses	Frequency in Percent
Aliphatic	Blank	No Reponse	65.6%
	Misconcep	Fragments	15.6%
	Partial	Alkane and alkene or alkyne	3.1%
	Complete	Alkane	15.6%
Aromatic	Blank	No Response	25.0%
	Misconcep	Alternating double bonds in diene	21.9%
	Partial	Alternating double bonds	18.8%
	Complete	π orbitals, overlap	34.4%
Benzene	Blank	No Response	6.3%
	Misconcep	Hexagon	3.1%
	Partial	Hexagon, three double bonds	68.8%
	Complete	Circle inscribed in hexagon	21.9%
Chemical Shift	Blank	No Response	50.0%
	Misconcep	Proton migration	6.3%
	Partial	Schematic H or C scale	28.1%
	Complete	Peaks shifted from TMS	15.6%
Cyclohexane	Blank		
	Misconcep	Octatriene	3.1%
	Partial	Hexagon	81.3%
	Complete	Chair/Boat conformations	15.6%
Degrees of Unsaturation	Blank	No Response	40.6%
	Misconcep	Unsaturated sites labelled saturated	15.6%
	Partial		
	Complete	Line formula alkene or alkyne	43.8%
Resonance	Blank	No Response	6.2%
	Misconcep	Keto-enol structures	25.0%
	Partial	Conjugated alkenes	15.6%
	Complete	Benzene	53.1%
Symmetry	Blank	No Response	9.4%
	Misconcep		
	Partial		
	Complete	Molecule, axis/plane of symmetry	90.6%

Table 7

Frequent Responses for Concept Illustration of the Exit Survey

Concept Illustration	Code (N=16)	Frequent Responses	Frequency in Percent
Aliphatic	Blank	No Response	56.3%
	Misconcep	Protein zwitterion/hexagon	12.5%
	Partial	Line alkane and alkene or alkyne	12.5%
	Complete	Zig zag alkane	18.8%
Aromatic	Blank	No Response	6.3%
	Misconcep	Alternating double bonds in chain	6.3%
	Partial	Hexagon, alternating double bonds	43.8%
	Complete	Inscribed circle in hexagon	43.8
Benzene	Blank		
	Misconcep	Hexagon	6.3%
	Partial	Hexagon, alternating double bonds	56.3%
	Complete	Hexagon, inscribed circle	37.5%
Chemical Shift	Blank	No Response	31.3%
	Misconcep	Bond migration/Primary alcohol	12.5%
	Partial	Schematic C/H scale	43.8%
	Complete	Peaks shifted from TMS	12.5%
Cyclohexane	Blank		
	Misconcep	Pentagon	12.5%
	Partial	Hexagon	68.8%
	Complete	Chair/boat configuration	18.3%
Degrees of Unsaturation	Blank	No Response	62.5%
	Misconcep		
	Partial		
	Complete	Condensed or line, alkene or alkyne	37.5%
Resonance	Blank	No Response	18.8%
	Misconcep	Double bond shift/Keto-enol error	25.0%
	Partial	Conjugated alkenes, inorganic ions	18.8%
	Complete	Benzene molecule	37.5%
Symmetry	Blank	No Response	12.5%
	Misconcep		
	Partial		
	Complete	Molecule, with line/plane symmetry	87.5%

Table 8

Significant Cross tabulations for Concepts in PreLab Quiz

Concept	Variable	X^2	df	p
Explanations				
Resonance Explanation	AP Chem	16.40	6	0.01*
Symmetry Explanation	AP Chem	17.52	9	0.04*
Illustrations				
Aliphatic Illustration	AP Chem	34.18	9	0.00*
Aliphatic Illustration	Major	18.26	9	0.03*

*p<0.05

Table 9

Significant Cross tabulations for Concepts in Exit Survey

Concept	Variable	X^2	df	p
Explanations				
Benzene Explanation	Group	7.20	2	0.03*
Degrees of Unsaturation Explanation	Major	21.45	9	0.01*
Resonance Explanation	Major	14.27	6	0.03*
Illustrations				
Degrees of Unsaturation Illustration	Major	9.60	3	0.02*

*p<0.05

Table 10

Cross Tabulation for Chemistry Background by Aliphatic Illustration

	Blank	Misconception	Partial	Complete	
No AP Chem	16	5		4	25 78.1%
No response			1		1 3.1%
Not sure	2				2 6.3%
AP Chem	3			1	4 25.0%
	21 65.6%	5 15.6%	1 3.1%	5 15.6%	32 100%

$X^2(12, N = 32) = 21.87, p = .04$

Table 11

Frequent Responses for PreLab Quiz Strategies

	Order		Analysis		Synthesis		Verification	
Strategy	Response	*Percent Frequency	Response	*Percent Frequency	Response	*Percent Frequency	Response	*Percent Frequency
Saturation	0	53.1%	No Resp	53.1%	No Resp	90.6%	No Resp	100.0%
	1	43.8%	Mention	21.9%	Fragment	6.3%		
Molecular Formula	0	93.8%	No Resp	93.8%	No Resp	93.8%	No Resp	100.0%
	1	6.3%	Predict	6.3%	Fragment	3.1%		
					Structure	3.1%		
PDC	0	40.6%	No Resp	40.6%	No Resp	93.8%	No Resp	96.9%
	2	34.45	Unique Carbons	18.8%	Fragment	3.1%	Carbon spectra	3.1%
	1	21.9%			Connect	3.1%		
DEPT	0	81.3%	No Resp	81.3%	No Resp	100.0%	No Resp	100.0%
	2	12.5%	H's on C	15.6%				
GDC	0	100.0%	No Resp	100.0%	No Resp	100.0%	No Resp	100.0%
COSY	0	96.9%	No Resp	96.9%	No Resp	100.0%	No Resp	100.0%
	4	3.1%	Interact H	3.1%				
HETCOR	0	96.9%	No Resp	96.9%	No Resp	100.0%	No Resp	100.0%
	3	3.1%	C to H	3.1%				
H-NMR	0	34.4%2	No Resp	31.3%	No Resp	75.0%	No Resp	93.8%
	3	28.1%	Chm Shf	15.6%	Fragment	9.4%	C Spectra	3.1%
	1	18.8%	Multiple	15.6%	Structure	9.4%	H Spectra	3.1%

*N = 32

Table 12

Frequent Responses for Benzaldehyde Exit Problem Strategies

	Order		Analysis		Synthesis		Verification	
Strategy	Response	*Percent Frequency	Response	*Percent Frequency	Response	*Percent Frequency	Response	*Percent Frequency
Saturation	2	68.8%	No Resp	37.5%	No Resp	75.0%	No Resp	75.0%
	4	18.8%	Multiple	25.0%	H Spectra	12.5%	Multiple	12.5%
	0	12.5%	Calculate	18.8%	C Spectra	6.3%	C Spectra	12.5%
			Predict	12.5%	Spectra	6.3%		
			Other	6.3%				
Molecular Formula	1	81.3%	No Resp	68.8%	No Resp	93.8%	No Resp	93.8%
	3	18.8%	Clues	25.0%	Multiple	6.3%	Mol For	6.3%
			Multiple	6.3%				
PDC	3	93.8%	Ch Shift	37.5%	No Resp	50.0%	No Resp	43.8%
	1	18.8%	Multiple	31.3%	Structure	31.3%	C Spectra	25.0%
	4	18.8%	Unique C	12.5%	Fragment	12.5%	Multiple	25.0%
	2	6.3%	No Resp	12.5%	Multiple	6.3%	Mol For	6.3%
			Symm C	6.3%				
DEPT	4	50.0%	Unique C	100.0%	No Resp	87.5%	No Resp	75.0%
	2	25.0%			Fragment	6.3%	C Spectra	18.8%
	3	25.0%			Structure	6.3%	Multiple	6.3%
GDC	0	100.0%	No Resp	100.0%	No Resp	100.0%	No Resp	100.0%
COSY	0	68.8%	No Resp	75.0%	No Resp	100.0%	No Resp	75.0%
	5	18.8%	Mention	18.8%			H Spectra	12.5%
	6	12.5%	C to H	6.3%			Multiple	12.5%
HETCOR	0	62.5%	No Resp	75.0%	No Resp	100.0%	No Resp	93.8%
	5	18.8%	Mention	18.8%			2-D Spec	6.3%
	6	18.8%	C to H	6.3%				
H-NMR	0	68.8%	No Resp	68.8%	No Resp	100.0%	No Resp	93.8%
	5	31.3%	Splitting	18.8%			H Spect	6.3%
			Ch Shift	6.3%				
			Integrate	6.3%				

*N = 16

Table 13

<u>Significant Cross Tabulations for Strategies in PreLab Quiz</u>

Strategy	Variable	X^2	df	p
PDC Analysis	AP Chem	31.78	18	0.02*

Note: Strategies independent of gender, group, ethnicity, and major

Table 14

<u>Cross Tabulation for Chemistry Background by PDC Analysis for PreLab Quiz</u>

	Mention	Unique C	Symm C	Chemical Shift	# C Signals	More than once	No Response	Row Total
No AP	3	6		4	1	1	10	25
No Resp						1		
Not sure			1				1	
AP Chem						2	2	
Col Tot	3	6	1	4	1	4	13	32

X^2 (18, N = 32) =31.78, p = .02

Table 15

<u>Significant Crosstabulations for Strategies in Benzaldehyde Exit Problem</u>

Strategy	Variable	X^2	df	p
Saturation Order	Group	7.27	2	0.03*
PDC Synthesis	Group	11.73	3	0.01*
DEPT Synthesis	Group	6.86	2	0.03*
COSY Order	Group	7.27	2	0.03*
COSY Verification	Group	7.11	2	0.03*

*p<0.05

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