SEEING THE FOREST FOR THE TREES: AN EXPLORATION OF STUDENT PROBLEM SOLVING AND REASONING WITH ^{1}H NMR SPECTRAL FEATURES

A Dissertation
Submitted to the Graduate Faculty
of the
North Dakota State University
of Agriculture and Applied Science

By

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In Partial Fulfillment of the Requirements
for the Degree of
DOCTOR OF PHILOSOPHY

Major Programs:
Chemistry and STEM Education

April 2020

Fargo, North Dakota

North Dakota State University
Graduate School

Title

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The Supervisory Committee certifies that this ***disquisition*** complies with North Dakota State University's regulations and meets the accepted standards for the degree of

DOCTOR OF PHILOSOPHY

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ABSTRACT

Nuclear magnetic resonance (NMR) spectroscopy is vital to synthesis and provides rich problem-solving opportunities for organic chemistry students. However, little is known about ^{1}H NMR spectroscopy instruction or how students use spectral features in solving. The goal of this dissertation research was to examine how students learn about and solve ^{1}H NMR spectroscopy problems. Organic chemistry textbooks were analyzed for the ways in which spectral features were introduced and incorporated into worked examples and practice problems. Spectral features like the number of signals and chemical shift were covered by problems more frequently, while integration was covered least. Think-aloud interviews were completed to identify the operators students utilized in their problem-solving processes, and extra credit problem sets were designed and administered to students at three different universities to examine whether students could correctly perform each individual type of operator. While students could perform operators, it was unclear if students knew how and when to use the operators. To fill this knowledge gap, multiple choice assessment questions were developed and administered to students at three different large universities. Coding schemes were developed to identify and describe students' use of task features and inferences, and regression analyses were completed to discern which areas of reasoning led to success in solving. A majority of students did not identify using any critical spectral features in written explanations. Regression analyses revealed that the inferences students made, and not the task features they paid attention to, were most significantly associated with success in structural predictions; a majority of students made solely correct inferences in their reasoning explanations. When a mixture of correct and incorrect inferences were made, a majority of those students were unable to answer the questions correctly. These findings suggest that students may know enough to solve simple ^{1}H NMR spectroscopy problems, but may lack

knowledge about specific spectral features which could impact overall solving success. Students may require considerable support in deciphering the critical features in ^1H NMR spectroscopy problems and developing robust, correct inferences across all spectral features.

ACKNOWLEDGEMENTS

As I stand at the precipice of what I have so longed to attain, I consider the peculiar journey this has been. I have been brought low by the expectations I held myself to. I have been strengthened through the challenges I faced. I did not give in, although I entertained the thought many times. Yet, I “glory in tribulations also: knowing that tribulation worketh patience; And patience, experience; and experience, hope” (Romans 5:3-4, KJV) and even in moments when it felt like my hope was perpetually deferred, my strength was continually renewed. I am grateful for the joys and sorrows; I celebrate every step of my journey and the people that influenced my path. Most importantly, I know in whom my hope resides.

I have been blessed by the apt mentorship I have received, most notably from two individuals. Erika, I am forever grateful for the pathos you brought to my path, planting a seed and providing the many opportunities for me to do research that moved me, research that I cared about deeply. Jenni, you wisely facilitated the growth I needed and built upon the foundation I had. Thank you for not giving up on me (even when I thought of giving up on myself) and for empowering me with greater proficiency and confidence. I have learned so much from you. I will always stand in awe of the way you truly practice what you teach and the thoughtfulness you apply in mentorship.

I appreciate the guidance by my committee and their prudent commitment to my individual development. Under your direction, I have constantly thrived. I am also thankful to the faculty and students in NDSU’s DBER community. Our thoughtful discussions have pushed me to strive for excellence. Likewise, I greatly appreciate the support, fun, and refining by the Momsen and Offerdahl lab members. This research complied with all Institutional Review Board regulations and was supported by a STEM Education Ph.D. fellowship.

I have had the privilege of sharing each step with my loving husband. Partner does not begin to describe how knit together we were on this journey, pursuing similar paths, facing many of the same challenges, and supporting each other all along. Trent, you witnessed the worst, gave the most, and helped in ways unimaginable. Moreover, you were a source of lighthearted fun and a much needed solace. I am ever thankful for your love and care, and grateful that together we share twice the joy and half the sorrow. Your heart is true; you're a pal and a confidant.

I have always been fiercely supported by my ever-encouraging parents. Mama and Appa, as you pushed me to be the best, you truly made me believe I could accomplish anything. You are the finest examples of hard work and determination. The Lord has blessed me exceedingly abundantly above all I could ever ask by providing me with you both as my parents. My greatest goal is to be more like you. Your love and support is unmatched, and none of this would have been possible without you. If I have flourished, it is because of you.

I have been surrounded by love and support from all my family, as well as from the spiritual leaders in my life. Pastor Scheving, Pastor and Mrs. Sickmeyer, you all provided me with wise counsel and helped me calibrate my focus on things above. Thank you for being there for me at any given moment and reminding me of the love of Christ. I would not be here if not for your compassion, prayers, and guidance.

I would be remiss to not mention how thankful I am for the companionship of my dog, Arthur Earl Grey. I needed the extra doses of joy, reasons to come home, and reprieve provided by my favorite mutt and spirit animal. I look forward to taking you outside more.

Finally and foremost, I praise the Lord.

DEDICATION

There is a Korean custom to place various objects in front of a child during the celebration of their first birthday. It is believed that the object the child selects will predict their future. To the little girl that picked up a book during her 돌잔치 (doljanchi)—you brought this upon yourself.

May you continue in the things which you have learned.

"Brethren, I count not myself to have apprehended: but this one thing I do, forgetting those things which are behind, and reaching forth unto those things which are before, I press toward the mark for the prize of the high calling of God in Christ Jesus."

Philippians 3:13-14

For Mama and Appa.

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CHAPTER 1. INTRODUCTION

How do we know with great certainty what chemicals are present in a sample? How does a chemist know they synthesized the correct compound? How does a medical doctor determine what is ailing patient? How does law enforcement analyze substances found at a crime scene? How do we see matter and see what is unseen? All of these instances and many more are possible with the vital techniques of spectroscopy. Spectroscopy encompasses the study of the interaction of light with matter. Through spectroscopic and spectrometric methods, structural determination can be done in a matter of minutes, and in many cases without the degradation of the chemical sample. Within the last hundred years, chemists had to put an unknown chemical sample through a painstakingly many series of tests to determine the structure of the compound. Chemists would even subject themselves to the process of analysis, feeling, smelling, and tasting compounds, and would spend years to elucidate the structure (Klein, 2017). Spectroscopy is an indispensable tool that provides fundamental information on atomic and molecular levels, molecular geometry, chemical bonding, and the mechanisms of chemical reactions (Parker, 1987). Spectroscopy is heavily utilized by practicing scientists and introduces principles that are applicable to a broad variety of analytical/diagnostic techniques in other fields. It is through the development of the modern structure elucidation techniques of spectroscopy that our great and many advancements in science and medicine have been made possible.

Students typically learn about spectroscopy and structure elucidation in organic chemistry. Organic chemistry is a demanding course that is required for many majors. North Dakota State University enrolls over 700 undergraduate students annually across the two-semester sequence of organic chemistry and the survey of organic chemistry courses. Students are typically in their sophomore or junior year of study and their majors include the sciences (e.g.

biology, chemistry, physics), pre-professional and health-related fields (e.g. pre-medicine, pre-pharmacy, pre-dental), and some engineering. Within organic chemistry, and typically taught in the middle of the full curriculum, are the analytical techniques of spectroscopy. Students learn how to analyze and interpret infrared (IR) and nuclear magnetic resonance (NMR) spectra, as well as mass (MS) and ultraviolet-visible (UV-Vis) spectra. Spectral analysis has been a vital technique for synthetic chemists in characterizing and analyzing chemical compounds (Thomas, 1991) and is a routine process in learning and practicing organic chemistry. Chemists become proficient at transforming spectral representations into their respective structural representations (Kozma and Russell, 1997). Even with its crucial role in science, few studies have examined student learning of spectroscopy.

In the field of chemistry education, research has largely focused on the areas of general chemistry (Cooper and Stowe, 2018). Few studies have focused on organic chemistry, and even fewer studies have focused on the use of spectroscopic and spectrometric methods. Domin and Bodner (2000, 2012) examined the number of representations constructed by graduate students solving 2D-NMR spectra, and found that students who constructed more representations were more successful in solving the problems. While this study focused on a subtopic of NMR spectroscopy, the concepts they were measuring were for the graduate level, after spectroscopy had already been introduced and reinforced. Cartrette and Bodner (2010) examined the characteristics and differences of successful and unsuccessful solving of structures from IR and ^{1}H NMR spectra among graduate students and faculty. They found that successful solvers used consistent steps to solving the problems, were more likely to draw molecular fragments of the structures and make use of more given information, including coupling constants, and were more likely to check their final answer with the spectra or molecular formula. However, these studies only investigated problem solving by graduate students and faculty, and not by novice undergraduate organic chemistry students.

While solving ^{1}H NMR spectroscopy problems, undergraduate students have been shown to make incorrect assumptions about spectral features and resort to heuristics to make their interpretations (Connor, et al., 2019). Some students believed that the N+1 rule should hold at all times. They also found that students held incorrect assumptions on what to observe with splitting, the number of signals, and shielding. While Stowe and Cooper's (2019) students were able to mine the spectral data sufficiently enough to correctly match proton environments in their structural predictions with peaks in the ^{1}H NMR spectra when prompted, they found that their students struggled in forming evidence-based claims in their reasoning arguments and did not cite spectral data in those arguments. Additionally, it has been shown that undergraduate students do not spend their time solving by connecting spectral data with their answers. Topczewski, et al. (2017) observed experts and novices as they solved ^{1}H NMR spectroscopy problems with eye-tracking instrumentation and found that experts performed checks connecting the spectral data with the answer, while novices did not make these connections back to the spectral data. From these studies, we see that undergraduate students need further instruction and opportunities on checking and supporting their answers when solving ^{1}H NMR spectroscopy problems, and extended coverage on each of the spectral features to improve their interpretations of spectral data and prevent unchecked heuristic use. These studies have examined students solving spectroscopy problems and provide insight in the area of teaching NMR, but no studies have analyzed how the content of ^{1}H NMR spectroscopy is presented to students. Furthermore, with limited information about how students interpret the spectral features, these studies on problem solving with ^1H NMR spectroscopy all underscore a need to elucidate students' use and interpretation of spectral features.

Problem solving is a complex process, driven by a number of cognitive elements that shape the decisions made by a solver. Consequently, a study of ^1H NMR spectroscopy problem solving requires a lens wherewith the researcher can investigate how areas of cognition function in problem solving. My theoretical framework (see Chapters 3 and 4 in this dissertation) merges two theories from cognitive science to examine how students solve ^1H NMR spectroscopy problems. With ideas from Evans' (2006) heuristic-analytic theory of reasoning, I examine what the task features are for ^1H NMR spectroscopy and how they are presented to students, and the inferences formed when students reason with the task features. Furthermore, with Newell and Simon's (1972) problem-space theory, I examine the problem-solving process by studying the operators (or actions) students use in the steps taken to solve ^1H NMR spectroscopy problems. This framework, modeled in Figure 1.1 below, suggests that when students encounter a problem, they reason with the task features to form inferences, and those inferences influence the operators, or actions students take to move from one state to the next.

Figure 1.1. The general model that frames this research, depicting how notions from reasoning and problem solving work together.

With this theoretical framework, I hypothesize that as a student approaches a ^1H NMR spectrum, they will reason with the *features* of the task itself (i.e. I have a spectrum as well as a molecular formula, the scale goes up to 7 ppm, the integration of the last peak is 3, the number of neighboring protons is found from the splitting, etc.). As the student reasons with the task features and principles, they form *inferences*—conclusions on the information they possess in the problem and/or cognitively (i.e. an integration of 3 means that there are three equivalent hydrogens represented here, a quartet in splitting means there are three hydrogens neighboring this signal set, etc.). These inferences may inform further inferences, but may ultimately produce *operators*—actions to move along the problem-solving process (i.e. the student draws a CH_3 upon inferring that the three equivalent hydrogens must be a CH_3 group, etc.). This general process continues until the student is done solving the problem.

Let's say a student encounters the ^1H NMR spectrum shown below in Figure 1.2, and their task is to interpret the spectrum to determine the structure of the compound represented. In this case, the compound represented is ethyl acetate (the structure is shown in Figure 1.3). The goal is for that student to come up with the chemical structure of ethyl acetate from looking at the spectrum given. The student may start out by noticing the *task feature* of the set of peaks at 4.0 ppm. By accessing their prior knowledge on the *spectral feature*, chemical shift, the student may make an *inference* that the hydrogens represented by that peak are quite deshielded. The student may also make an *inference* that there must be an electronegative atom nearby that group of hydrogens, such as an oxygen. That last inference may lead the student to drawing a fragment of the whole compound, an oxygen attached to a CH_2 group—this action of drawing a fragment is an *operator* that moves the student to a new state in their problem-solving process. Again, this process continues, but as noted in this example, the student made a couple inferences without applying an operator. Every inference does not necessarily produce an operator. A person's inference could potentially lead to further inferences, but this and other nuances in the theories will be described in more detail in the theoretical framework.

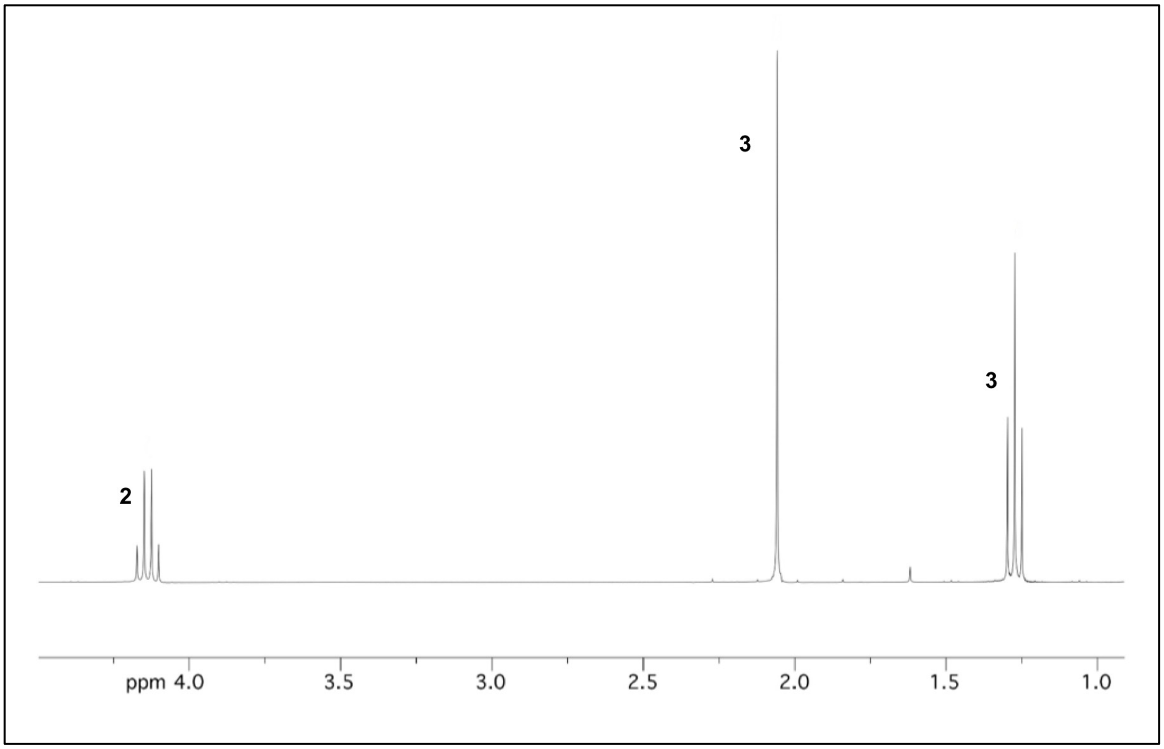

Figure 1.2. An example of a ^{1}H NMR spectrum, the ^{1}H NMR spectrum of ethyl acetate.

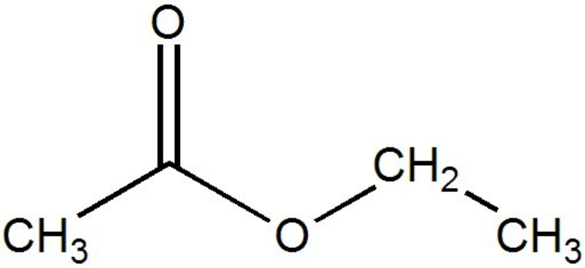

Figure 1.3. The structure of ethyl acetate, represented in the spectrum above.

The purpose of this dissertation is to examine how students learn about and solve ^{1}H NMR spectroscopy problems. I investigated students' solving of ^{1}H NMR spectroscopy problems through the lens of the general model presented above (Figure 1), specifically in three areas: the solver's interaction with the task features, the operators a solver can use to move from one state to another with ^{1}H NMR spectroscopy problems, and the specific inferences students make when reasoning with the spectral and task features. In this dissertation, each data chapter probes an area of the model. Specifically, I explored the following research questions:

Study 1: Task features (Chapter 2)

1. What ^{1}H NMR spectral features do textbook worked examples and practice problems focus on?
2. How do textbook worked examples and practice problems show evidence of interleaving and blocking with ^{1}H NMR spectral features?

Study 2: Operators (Chapter 3)

1. What operators do students use in their problem-solving processes with ^{1}H NMR spectroscopy problems?
2. To what extent do students correctly perform each operator in solving ^{1}H NMR spectroscopy problems?

Study 3: Inferences (Chapter 4)

1. What are the task features and inferences students utilize in their problem-solving processes with ^{1}H NMR spectroscopy problems and how well do these task features align with the inferences students made?
2. To what extent do students pay attention to the critical spectral features necessary to solve the problem?
3. What is the relationship between problem solving success and students' use of task features and inferences? How does the presence of correct and/or incorrect inferences impact solving?

In the first study, I analyzed organic chemistry textbooks for the ways in which spectral features were introduced and incorporated into worked examples and practice problems. The study develops a means to comparatively examine the sequencing and progression of textbook problems across a chapter. In the second study, broken into two smaller studies, think-aloud interviews were completed to develop a coding scheme of operators students utilized in their problem-solving processes, and extra credit problem sets were designed and administered to students at three different universities to examine if students could correctly execute each individual type of operator. In the third study, multiple choice assessment questions were developed and administered to students at three different large universities to explore students' reasoning with ^{1}H NMR spectroscopy problems. Coding schemes were developed to annotate students' use of task features and inferences, and regression analyses were completed to discern which areas of reasoning led to success in solving. The results of this dissertation research inform future research on student learning and solving of spectroscopy problems, as well as the instruction on the area of ^{1}H NMR spectroscopy.

CHAPTER 2. SUPPORT FOR INSTRUCTIONAL SCAFFOLDING WITH ^{1}H NMR SPECTRAL FEATURES IN ORGANIC CHEMISTRY TEXTBOOK PROBLEMS[1]

Introduction

Nuclear magnetic resonance (NMR) spectroscopy is an indispensable tool for chemists to characterize unknowns and synthesized products. Spectroscopy provides fundamental information on atomic and molecular levels, molecular geometry, chemical bonding, and the mechanisms of chemical reactions (Parker, 1988). Spectral analysis is a vital technique for synthetic chemists in characterizing and analyzing chemical compounds (Thomas, 1991) and is a routine process in learning and practicing organic chemistry. Chemists are proficient at transforming spectral representations into their respective structural representations (Kozma and Russell, 1997).

As a result of NMR spectroscopy's importance to chemists and its vital role in synthesis, interpreting these spectra and identifying unknown compounds with spectra serve as a component of organic chemistry instruction. In undergraduate organic chemistry, students learn about both ^{1}H and ^{13}C NMR spectroscopy, along with other spectroscopic and spectrometric methods. While all methods can be used together in the characterization of organic compounds, ^{1}H NMR spectroscopy provides enough information by itself to deduce the whole structure of an unknown organic compound. Instructors often note—anecdotally—that students struggle with ^{1}H NMR spectroscopy, but systematic research exploring these concerns is lacking. Research on student understanding of NMR spectroscopy has focused on the characteristics of graduate-level

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[1] The material in this chapter was co-authored by Shannon Anderson, Whitney Ong, and Dr. Jennifer Momsen and is published as Anderson, Ong, and Momsen (2020). Shannon Anderson designed the study, contributed to the data collection, completed the data analyses, drafted this chapter, and contributed to revisions of this chapter. Whitney Ong contributed to the data collection. Dr. Jennifer Momsen contributed to the data analysis and revisions of this chapter.

solvers (Bodner and Domin, 2000; Cartrette and Bodner, 2010; Domin and Bodner, 2012) and on how undergraduate students approach such problems (Topczewski, et al., 2017; Connor, et al., 2019; Stowe and Cooper, 2019).

While solving ^{1}H NMR spectroscopy problems, undergraduate students have been shown to make incorrect assumptions about spectral features and resort to heuristics to make their interpretations (Connor, et al., 2019). While students have been shown to possess adequate procedural knowledge on approaching ^{1}H NMR spectroscopy problems, they have been found to lack reasoning to support their answers (Stowe and Cooper, 2019). Likewise, it has been shown that undergraduate students do not spend their time solving by connecting spectral data with their answers; students lack the checking procedures that experts utilize (Topczewski, et al., 2017). Connor and Shultz (2018) examined the pedagogical content knowledge (PCK) in ^{1}H NMR spectroscopy with teaching assistants and found that PCK increased with experience in teaching the subject of NMR. Additionally, they found that TAs struggled to identify what would make similar problems difficult and to provide teaching strategies for those problems, indicating that PCK with NMR may be specific to certain problems and topics. From these studies, we see that undergraduate students need further instruction and opportunities on checking and supporting their answers when solving ^{1}H NMR spectroscopy problems, and extended coverage on each of the spectral features to improve their interpretations of spectral data and prevent heuristic use. These studies have examined students solving spectroscopy problems and provide insight in the area of teaching NMR, but to our knowledge no studies have analyzed how the content of ^{1}H NMR spectroscopy is presented to students.

Textbooks are a reliable resource for learners, created by experts in the field, assigned by professors, and made available to all students. A number of studies have examined undergraduate chemistry textbooks, and have shown that textbooks are important to teaching and learning chemistry (Gkitzia, et al., 2011), often guiding the organization of a course's curriculum (Koppal and Caldwell, 2004). Just as different general chemistry textbooks have been shown to present the same concepts differently in the narrative (Pyburn and Pazicni, 2014), in practice problems (Dávila and Talanquer, 2010), and with representations (Nyachwaya and Gillaspie, 2016), we can likewise discern and establish the different ways students are being presented with content on ^{1}H NMR spectroscopy. We therefore focused our research on the potential of textbooks to support instruction on ^{1}H NMR spectroscopy.

Background

Instructional scaffolding can support the learning of spectroscopy

Scaffolded instruction is an idea that emerges from Vygotsky's zone of proximal development (Vygotsky, 1962, 1978). Scaffolding is an interactive process between the instructor and student, whereby the instructor provides supports to the student so they can accomplish a task that might otherwise be too difficult. Well-designed scaffolding adjusts to meet the needs of each student; the support gradually fades to allow the student to complete the task without any instructional scaffolds (van de Pol, et al., 2010). While most research on scaffolding does not examine the aspects and benefits of fading (Lin, et al., 2012), fading is still regarded as a crucial step of scaffolding. Students with faded support outperform those with either continuous or no support (McNeill, et al., 2006). Scaffolding as a whole reduces cognitive load by allowing learners to master the individual steps in the problem-solving process, prior to attempting a problem involving all those steps. In spectroscopy, scaffolding might involve the mastery of one spectral feature before learning and combining multiple spectral features. For example, a student might be presented with how to interpret chemical shift before advancing to using chemical shift and integration together to make an inference on the structure of a compound.

While scaffolding holds promise in enabling students to master activities such as problem solving with spectroscopy, the term scaffolding itself has been interpreted and used in different ways. Research has depicted scaffolding as involving an instructor providing structures to support a student's performance (Wood, et al., 1976; Rosenshine and Meister, 1992), becoming a participant in a student's learning process (Bruner, 1983; Mercer and Littleton, 2007), helping a learner accomplish a task that they would not have been able to accomplish on their own (Bruner, 1974; Maybin, et al., 1992), and systematically devising the sequencing of prompted content, tasks, and support to optimize student learning (Dickson, et al., 1993). Most simply stated, scaffolding is a support for learning (as inferred from its metaphor to construction). However, descriptions of scaffolding in practice—and what it looks like in the classroom—are limited. Synthesizing research on scaffolding, van de Pol, et al. (2010) proposed a framework to characterize instructional scaffolding. Drawing from research by Tharp and Gallimore (1988) and Wood, et al. (1976), van de Pol, et al. (2010) describes a scaffolding strategy as involving two dimensions, means and intentions (Table 2.1). The means of a scaffolding strategy include clear pedagogical moves like providing feedback or demonstrating a particular skill. The second dimension of a scaffolding strategy is the intention, that is the purpose of the scaffolding strategy. The intention can include actions that help the student stay on task or organize their thinking. van de Pol, et al. (2010) proposed that scaffolding is comprised of both an intention and means, where the means of scaffolding act to implement the intentions of scaffolding. For example, an instructor may want to aid a student in staying on task toward the current goal (direct maintenance) by the act of asking the student a question (questioning).

Table 2.1. Scaffolding intentions and means (van de Pol, et al., 2010).

		Definition
Intentions	Direct maintenance	Keep the student on target and ensure the student is working toward a particular objective
	Cognitive structuring	Help the student organize and justify areas of the task
	Reduction of the degrees of freedom	Take over parts of the task that the student cannot yet complete in order to simplify the task
	Recruitment	Get students interested in the task
	Contingency management	Provide incentives to keep students motivated
	Frustration control	Minimize or prevent a student's frustration
Means	Feeding back	Providing students with information on their performance
	Giving hints	Providing clues or suggestions to aid the students in progressing forward
	Instructing	Explaining how something must be done and why
	Explaining	Providing more detailed information or clarification
	Modeling	Demonstrating skills and offering the students actions they can adopt or imitate
	Questioning	Asking students questions that require an active answer

Although the broad use of the term scaffolding has been criticized for being vague and meaning nothing more than support (Pea, 2004; Puntambekar and Hubscher, 2005), the framework of scaffolding as proposed by van de Pol, et al. (2010) addressed these criticisms by clearly defining the intentions and means of scaffolding strategies in instruction. We propose that scaffolding is essential to learning ^{1}H NMR spectroscopy because the task is complex, with multiple steps and spectral features dependent on the diverse characteristics of a compound. As shown by van de Pol, et al., scaffolding strategies can be infused at different curricular levels, such as the course, unit of instruction, or even the individual item. In fact, Stowe and Cooper (2019) investigated scaffolding at the item level by guiding students' argumentation to different extents through item prompts. They found that scaffolding at the level of the prompt showed no impact on students' abilities to construct evidence-based arguments behind their ^{1}H NMR spectroscopy problem solving. We hypothesize that learning ^{1}H NMR spectroscopy could benefit from scaffolding on the level of the unit as a whole, where intentions like reducing the degrees of freedom would provide students with problems requiring the use of the chemical shift, before encountering problems requiring the use of the chemical shift and the splitting.

Undergraduate organic chemistry students learn about several spectral features (in particular, the number of signals, chemical shift, integration, and splitting), are expected to correctly interpret those features and then use those spectral features together to determine the structure of the compound represented. With intentions (or goals) like direct maintenance, focused cognitive structuring, and reducing the degrees of freedom, an instructor can directly reduce the cognitive demand on a student while interpreting ^{1}H NMR spectra. Furthermore, through means such as instructing, explaining, and modeling, an instructor can show a student how to approach their interpreting of ^{1}H NMR spectra.

Textbooks are reliable instructional tools that can support scaffolded instruction

While textbooks do not accomplish the task of instructional scaffolding alone, they are designed with features to support an instructor when scaffolding content on ^{1}H NMR spectroscopy. Textbook chapters on spectroscopy typically include rich NMR data sets, worked examples, practice problems, figures depicting the instrument and spectra, along with descriptions and applications of the spectral features. As a result, instructors of introductory organic chemistry often rely on textbooks to structure curriculum, reinforce lecture topics, and provide worked examples and practice problems (Justi and Gilbert, 2002; Mikk, 2000; Chiappetta, et al., 1991). Students then use textbooks to reinforce or clarify lecture material, explore applications, and evaluate their own problem-solving abilities. Instructors may also rely on worked examples and practice problems to demonstrate critical components and steps of the spectroscopy problem-solving process; learners may use those same worked examples to develop their own problem-solving skills. Textbooks are, therefore, viewed by students and instructors as reliable resources that support, enhance, and reinforce students' learning of critical spectral features (Knight, 2015). As a consequence, textbooks can have a substantial impact on instructional scaffolding and by extension, student learning.

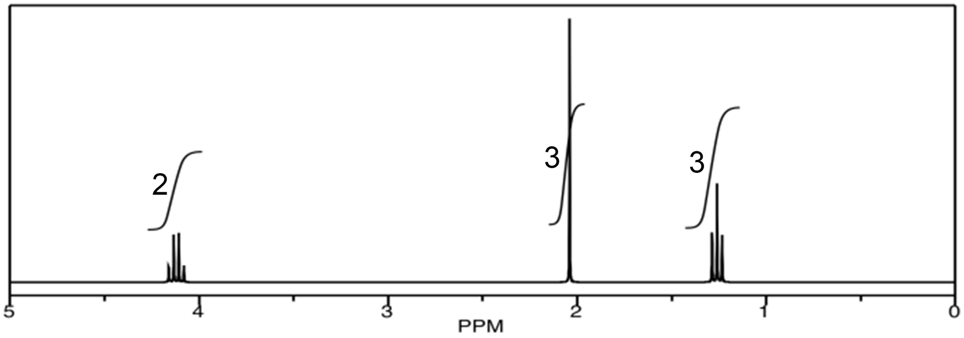
Although textbooks are resources unto themselves, scaffolding is a process between the instructor and student. Therefore, textbooks have the potential to support instructional scaffolding, but how textbooks function as part of the scaffolding process is highly instructor-dependent. For example, an instructor may use a textbook to introduce spectroscopy before going over the information in class. An instructor may also have students refer to the textbook upon introducing the subject in class, where the textbook provides students with clarification and practice on the task. An instructor may also use the textbook problems, both within the chapter and at the end of the chapter, as formative or even summative assessment. Regardless of what an instructor chooses to do, textbooks have the potential to explicitly support scaffolded instruction in the areas of *cognitive structuring* and *reducing the degrees of freedom* through content that *explains* and *models*, and can *fade* that support through the order and structure of problems (van de Pol, et al., 2010).

Learning to interpret ^{1}H NMR spectra is a complex task, one that benefits from instructional scaffolds. Students must be able to comprehend and interpret each spectral feature, use all the spectral features together, and be able to move forward or backward in that interpretation process (either by predicting what a spectrum should look like based on the compound or by inferring what is represented by a given spectrum). Ideally, textbooks should provide material sufficient for mastering all areas of interpretation. Specifically, textbooks should provide support for cognitive structuring with features to instruct and explain each spectral feature of ^{1}H NMR spectroscopy and then reduce the degrees of freedom by modeling areas of interpretation. Building student understanding of these spectral features one at a time, then moving to two or three spectral features together, before moving to all four spectral features together slowly introduces more degrees of freedom into the problem-solving process. Once all spectral features have been practiced alone and together, practice problems can fade the support further when the arrangement of problems does not foreshadow the approach to take. For example, an organic chemistry textbook could provide examples and questions for the number of signals, chemical shift, integration, and splitting individually and then together, modeling how to use all the spectral features alone and in concert to interpret a full spectrum. Worked examples and practice problems allow textbooks to accomplish this support to instructional scaffolding.

Worked examples and practice problems demonstrate potential support for instructional scaffolding

Effective scaffolding supports students' learning of how and *why* to do a task (Hmelo-Silver, 2006). Worked examples, with their written explanations (Figure 2.1A) are one textbook tool that can convey that information, although the extent to which they actually scaffold learning is unknown. Worked examples consist of a problem statement and the appropriate steps to the solution (Kalyuga, et al., 2001). The level of solution detail varies among textbooks, but each worked example must provide a problem statement, answer, and some description of the solution pathway. The description of the solution can vary, where the specific steps are described in detail or briefly. Considering van de Pol's framework, worked examples are particularly useful in supporting learning in scaffolded instruction as they address two intentions of scaffolding: cognitive structuring through organizing and justifying ways to problem solve, and the reduction of degrees of freedom by showing the steps to solve a problem and the solution, allowing the students to focus on those individual details rather than generating a solution path as well as reflecting on the steps they took. Furthermore, worked examples supply two scaffolding means to support learning with explanations on how steps should be done and why, and with the process to solve the problems modeled for the students.

Reducing cognitive load, worked examples can help students in identifying how and why steps are taken in a path to solve a problem by allowing them to focus exclusively on the characteristics of that path, rather than both creating a solution path *de novo* and then evaluating the accuracy or correctness of that path. For the novice solver, evaluating the accuracy or correctness of a path may be cognitively taxing. Evidence from mathematics and the learning sciences demonstrates that worked examples can reduce cognitive load (Cooper and Sweller, 1987; Paas, 1992; Paas and van Merriënboer, 1994; van Gerven, et al., 2002; Paas, et al., 2006). Moreover, reducing cognitive load functions analogously to the reduction of the degrees of freedom in scaffolding. In ^{1}H NMR spectroscopy, worked examples can reduce cognitive load by allowing the learner to focus on the interpretations that can be made with each individual spectral feature and then use all the spectral features together to come to a solution.



A. Sample of a worked example using the spectrum above:

What is the structure of the compound represented by the spectrum above?

Step 1. Determine the number of different kinds of protons. The number of NMR signals equals the number of different types of protons. This molecule has three signals and therefore three types of protons.

Step 2. Use the integration data to determine the number of hydrogen atoms giving rise to each signal. Two equivalent Hs usually indicates a CH_2 group. Three equivalent Hs typically indicates a CH_3 group. There are likely two CH_3 groups and one CH_2 in this compound. Don't forget to consider that the integration could represent more (or less) hydrogens of the same ratio shown.

Step 3. Use individual splitting patterns to determine which carbon atoms are bonded to each other. Start with the singlet. The singlet is due to a CH_3 group with no adjacent nonequivalent hydrogen atoms. Possibilities include the CH_3 adjacent to an oxygen, a carbonyl, or a quaternary carbon. The triplet in the spectrum indicates that there must be two hydrogens on the adjacent carbon(s), likely an adjacent CH_2 group. The quartet indicates that there must be three hydrogens on the adjacent carbon(s), likely a CH_3 group. The groups from the triplet and the quartet could go together to make an ethyl group.

Step 4. Use chemical shift data to complete the structure. Put the structure together in a manner that preserves the splitting data and is consistent with the reported chemical shifts. There are two possible arrangements: one with the oxygen directly attached to the CH_2, or one with a carbonyl attached to the CH_2. If the carbonyl were directly attached to the CH_2, then the CH_3 singlet would be attached to the oxygen, making that CH_3 signal absorb furthest downfield. If the oxygen were directly attached to the CH_2, then the CH_2 would absorb furthest downfield. Because the CH_2 is furthest downfield, the oxygen is directly attached to the CH_2. All chemical shifts match up with a structure where an ethyl group is attached to an oxygen that is attached to a carbonyl that is attached to a methyl group, giving us the structure of ethyl acetate.

B. Sample of practice problems for the spectrum above:

What is the structure of the compound represented by the spectrum above?

How many types of nonequivalent hydrogens are present in the compound represented by the spectrum above?

Figure 2.1. Worked example and practice problem samples.

In contrast, practice problems (Figure 2.1B) provide a problem statement, but do not provide the answer or goal state. Left as an unknown, students must have a developed problem-solving approach to find the goal state. Thus, practice problems have a very different learning goal, namely to provide students with opportunities to practice, refine, and expand problem-solving approaches. Practice problems serve as an implicit part of the scaffolding process because they do not explicitly indicate which spectral features to use when solving a problem. Practice problems support scaffolded instruction as a diagnostic that addresses areas in need of continued cognitive structuring, and serve as a form of faded support that increases the degrees of freedom. Moreover, the systematic order and combination of problems can implicitly function as a means of scaffolded instruction.

The sequencing of practice problems through interleaving and blocking can impact scaffolding

As practice problems reintroduce degrees of freedom, the sequencing of practice problems with the strategies of interleaving and blocking can reduce or increase the degrees of freedom and thereby add support or fade support in solving. Interleaving deliberately intermixes problems and solving strategies to help learners distinguish between similar concepts and solution pathways. In contrast, blocking drills a single strategy through repetition (Rohrer, 2012). Interleaving may help students develop discrimination skills, thereby supporting their ability to identify an appropriate strategy, rather than having the order of the problems dictate which strategy to use. In contrast, blocking drills a single strategy or concept in a block of questions, with the next question set drilling another strategy. Research in mathematics has found that interleaving promotes students' problem solving (Rohrer, et al., 2014). Although interleaving has been broadly applied to areas like art, language learning, and animal classification, these studies have focused on categorization and identification tasks (Kornell and Bjork, 2008; Vlach, et al., 2008; Wahlheim, et al., 2011). To our knowledge, there is no research exploring how interleaving might impact students' use of spectral features when solving spectroscopy problems.

The interpretation of spectral features to solve ^{1}H NMR spectroscopy problems may not be directly comparable to the problem-solving approaches in the literature on interleaving and blocking, but the material could benefit from interleaving. In ^{1}H NMR spectroscopy, the strategy or approach does not change between problems: as students interpret spectra, they should attend to all four spectral features each time. However, in each problem, a specific spectral feature or a few spectral features may lead to the structure solution; those spectral features vary with each problem. Additionally, the order in which a solver attends to each spectral feature may differ with the problem and/or the person solving. No matter the order used in solving the problem, the student should still use and interpret all four spectral features. Finally, while there is no evidence that students confuse one spectral feature of ^{1}H NMR spectroscopy with another, interleaving could still be a useful tactic to help students discern *how* and *when* to use the spectral features and make the practice problems more diagnostic in nature, so a student knows which spectral feature(s) they do not understand.

Outside the context of categorization and identification tasks, we hypothesize that blocking and interleaving could work together to promote mastery in problem solving. Blocking supports the mastery of a single spectral feature, while interleaving supports mastery of the overall problem-solving process. Blocking can function to aid the student in mastering the interpretations and uses of specific spectral features, and with support from the text, blocking can reduce the degrees of freedom regarding the determination of which spectral features to pay attention to. Students can, therefore, focus on mastering interpretation with one spectral feature at a time. Moreover, interleaving allows for further mastery of problem solving by fading that support, letting students develop and evaluate the solution pathway. While research on interleaving has purported the use of interleaving over blocking, according to van de Pol's framework, the intentions of scaffolding apply to both blocking and interleaving. Thought should go into using both blocking and interleaving to build the problem-solving pathway.

Through the ordering of spectral features within worked examples and practice problems found in organic chemistry textbooks, students are provided with multi-faceted opportunities to develop their knowledge of ^{1}H NMR spectroscopy and problem solving. Systematically examining the worked examples and practice problems for the presence of these spectral features of ^{1}H NMR spectroscopy provides evidence of how textbooks can support the scaffolded instruction of ^{1}H NMR spectroscopy. In this study, we characterized the potential for supporting scaffolded instruction in worked examples and practice problems found in organic chemistry textbooks commonly used in undergraduate instruction. Specifically, we asked:

1. What ^{1}H NMR spectral features do textbook worked examples and practice problems focus on?
2. How do textbook worked examples and practice problems show evidence of interleaving and blocking with ^{1}H NMR spectral features?

Methods

Textbook selection and sampling

We used a convenience sample of eight organic chemistry textbooks commonly used at many institutions; six of the selected textbooks were listed in the top 20 organic chemistry books based on sales on Amazon.com in February 2015 (Table 2.2). Within each textbook, we identified and analyzed the sections pertaining to ^{1}H NMR spectroscopy. Any problem on ^{1}H NMR spectroscopy within the spectroscopy chapters was analyzed, including worked examples. The number of worked examples and practice problems were counted for each textbook. There was a wide range in the total number of practice problems presented in the textbooks, from 42-

154, with a median of 76.5 (Table 2.3). There was also a wide range in the number of worked examples presented in the textbooks, from 1 to 31 (Table 2.3), with a median of 7. Further, some textbooks presented many practice problems while presenting few worked examples. Because some textbooks presented a limited number of worked examples, we chose to constrain our examination of the scaffolding of spectral features to the four textbooks that provided the most worked examples (shown in bold in Table 2.3). Even with their differences, most textbooks have been found to be variations of the same underlying design. Textbook design and structuring emerged over time, guided by personal empiricism (Cooper and Stowe, 2018), where scientists went with gut instinct and personal experience with what had been done before, instead of being driven by empirical evidence. Raker and Holme (2013) in their analysis of organic chemistry curricula through ACS exams, found that little has changed since the 1970s. Cooper, et al. (2019) submit that undergraduate organic chemistry textbooks and curricula have not changed in those 50 years, as textbooks use the presentation of synthesis and reactivity of functional groups and the use of electron pushing formalism to show how electrons move in those reactions to guide the compounds formed. With such similarity among undergraduate organic chemistry textbooks, our narrowing down to these four textbooks was further supported by examining the patterns in presenting the spectral features of ^{1}H NMR in each textbook (Table 2.4). Each of the four selected textbooks reflects a different pattern in the ordering of spectral features.

Table 2.2. Surveyed textbooks.

Title	**Authors**	**Edition**	**Publisher**
Organic Chemistry	Brown, W.H.; C.S. Foote; B.L. Iverson; and E. Anslyn	5th edition	Cengage Learning
Organic Chemistry	Bruice, P.Y.	4th edition	Prentice Hall
Organic Chemistry	Carey, F.A. and R.M. Giuliano	8th edition	McGraw-Hill
Organic Chemistry	Jones Jr., M. and S.A. Fleming	5th edition	W. W. Norton & Company
Organic Chemistry	McMurry, J.E.	8th edition	Cengage Learning
Organic Chemistry	Smith, J.G.	3rd edition	McGraw-Hill
Organic Chemistry	Solomons, T.W.G. and Fryhle, C.B.	9th edition	Wiley
Organic Chemistry	Wade, Jr., L.G.	5th edition	Prentice Hall

Table 2.3. Number of practice problems and worked examples provided by each textbook.

Textbook	**Practice problems at end of chapter**	**Practice problem within narrative**	**Worked examples**
Brown, et al.	**30**	**12**	**15**
Bruice	57	97	3
Carey, Giuliano	**34**	**30**	**31**
Jones, Fleming	**62**	**11**	**14**
McMurry	50	35	2
Smith	**82**	**55**	**8**
Solomons, Fryhle	28	28	1
Wade	34	46	6

Table 2.4. Pattern of spectral feature introduction.

	First feature	**Second feature**	**Third feature**	**Fourth feature**	**Textbook(s) following the pattern**
Pattern 1	#S	CS	INT	SPL	Bruice, **Smith**, Solomons, McMurry*
Pattern 2	CS	#S	INT	SPL	**Carey**, Wade
Pattern 3	#S	INT	CS	SPL	**Brown**
Pattern 4	INT	CS	SPL		**Jones**

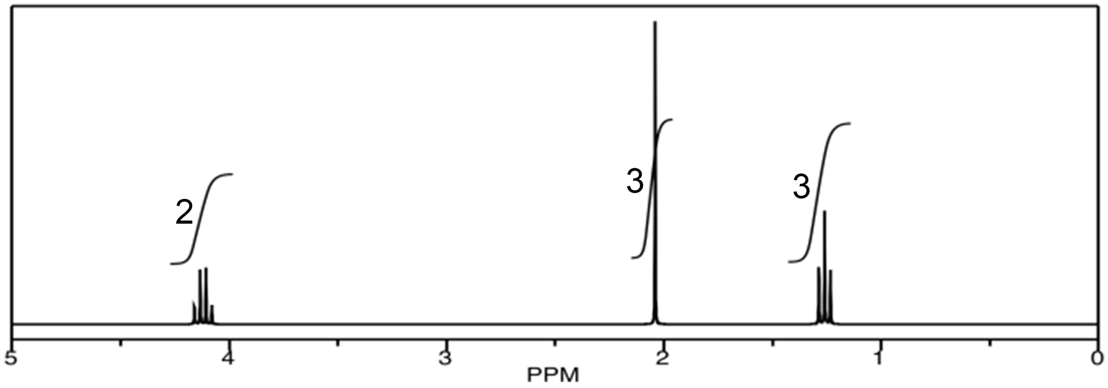
*Note: McMurry briefly introduced the feature of chemical shift in terms of NMR spectroscopy in general and with ^{13}C NMR spectroscopy before more explaining the topic in depth with respect to ^{1}H NMR spectroscopy.

Coding and analysis

Within each ^{1}H NMR spectroscopy chapter, two researchers coded all eight textbooks together to categorize the content as narrative, figures, hints, worked examples, and practice problems. Worked examples and practice problems emerged from the analysis as primary resources existent in all the textbooks in supporting the learning of problem solving with ^{1}H NMR spectroscopy, as they offered opportunities to practice problem solving with the spectral features. A worked example was classified as a problem when it contained both an answer and an explanation and/or steps to arrive to the answer. Practice problems were defined as containing a problem statement, without an explanation or steps to arrive at the answer. Practice problems included problems within and at the end of the chapter.

To determine which ^{1}H NMR spectral features were the focus of worked examples and practice problems, each problem and worked example was coded for the specific spectral feature(s) indicated by the problem. Those spectral features were the number of signals/proton equivalency (#S), chemical shift (CS), integration (INT), and splitting (SPL). The *number of signals* in the spectrum indicates the number of equivalent proton groups the compound has and is equal to the number of different types of protons. The *chemical shift*, or the position of a signal, is determined by shielding and deshielding effects, where shielding shifts an absorption upfield and deshielding shifts an absorption downfield. *Integration* is the area under a signal and is proportional to the number of absorbing protons. *Splitting,* the pattern of absorption peaks resulting from spin-spin splitting of nuclei, can be used to determine how many protons reside on the carbon atoms near the absorbing proton. The number and nature of adjacent protons determines the observed splitting pattern. These four spectral features were examined because they encompass the information on ^{1}H NMR spectroscopy most readily and universally available in undergraduate organic chemistry instruction. While some undergraduate courses may cover spectral features like spin-spin coupling and diastereotopic protons, the four spectral features we examined are because they pertain to a baseline of features covered in undergraduate instruction. An *a priori* coding scheme of the spectral features was established by two researchers, and one researcher independently coded all worked examples and practice problems. The second researcher took a random sample of worked examples and practice problems, comprising 25% of the total sample, and coded them to establish reliability (Cohen's kappa: 0.945).

Once the practice problems and worked examples were coded for the four outlined ^{1}H NMR spectral features (see example in Figure 2.2 below), the scaffolding of problems was examined in terms of the ordering and combinations of those spectral features. The ordering of the spectral features for the in-text practice problems and worked examples was compared to the ordering of the spectral features in the narrative. To support our goal of identifying evidence of blocking and interleaving, we used sunburst diagrams to visualize the spatial distributions of spectral features in worked examples and practice problems. We modified a typical sunburst diagram to show the progression of spectral features used in worked examples and practice problems.



A. Sample of a worked example using the spectrum above:

What is the structure of the compound represented by the spectrum above?

All four spectral features, as highlighted below:

Step 1. Determine the number of different kinds of protons. The number of NMR signals equals the number of different types of protons. This molecule has three signals and therefore three types of protons.

Number of signals

Step 2. Use the integration data to determine the number of hydrogen atoms giving rise to each signal. Two equivalent Hs usually indicates a CH_2 group. Three equivalent Hs typically indicates a CH_3 group. There are likely two CH_3 groups and one CH_2 in this compound. Don’t forget to consider that the integration could represent more (or less) hydrogens of the same ratio shown.

Integration

Step 3. Use individual splitting patterns to determine which carbon atoms are bonded to each other. Start with the singlet. The singlet is due to a CH_3 group with no adjacent nonequivalent hydrogen atoms. Possibilities include the CH_3 adjacent to an oxygen, a carbonyl, or a quaternary carbon. The triplet in the spectrum indicates that there must be two hydrogens on the adjacent carbon(s), likely an adjacent CH_2 group. The quartet indicates that there must be three hydrogens on the adjacent carbon(s), likely a CH_3 group. The groups from the triplet and the quartet could go together to make an ethyl group.

Splitting

Step 4. Use chemical shift data to complete the structure. Put the structure together in a manner that preserves the splitting data and is consistent with the reported chemical shifts. There are two possible arrangements: one with the oxygen directly attached to the CH_2, or one with a carbonyl attached to the CH_2. If the carbonyl were directly attached to the CH_2, then the CH_3 singlet would be attached to the oxygen, making that CH_3 signal absorb furthest downfield. If the oxygen were directly attached to the CH_2, then the CH_2 would absorb furthest downfield. Because the CH_2 is furthest downfield, the oxygen is directly attached to the CH_2. All chemical shifts match up with a structure where an ethyl group is attached to an oxygen that is attached to a carbonyl that is attached to a methyl group, giving us the structure of ethyl acetate.

Chemical shift

B. Sample of practice problems for the spectrum above:

What is the structure of the compound represented by the spectrum above?

All four spectral features

How many types of nonequivalent hydrogens are present in the compound represented by the spectrum above?

Number of signals

Figure 2.2. Example of spectral feature coding with sample worked example and practice problems.

Results

We coded 68 worked examples and 316 practice problems across our four selected textbooks (the four textbooks with the most worked examples and different pattern of spectral feature introduction). The ^{1}H NMR spectral feature most frequently identified in either worked examples or practice problems was the number of signals (62% and 69%, respectively); the least frequently identified feature was integration (36% and 55%, respectively).

Coverage of spectral features

After coding all textbook problems for the spectral features represented in each, we found that three of the four sampled textbooks included worked examples covering all four spectral features of ^{1}H NMR spectroscopy (Table 2.5). The number of signals was the most frequent spectral feature included in worked examples in three of the four textbooks (Brown, et al., 2008; Carey and Giuliano, 2011; Smith, 2011). The most common spectral feature in the other textbook (Jones and Fleming, 2014) was chemical shift, while the least frequently included spectral feature in the worked examples varied with each book. For Carey and Giuliano, and Smith, integration was the least frequently included spectral feature of the worked examples.

Table 2.5. Frequency of worked examples focusing on each ^{1}H NMR spectral feature by textbook. Numbers in parentheses are the number of problems focusing on each respective feature.

	Spectral Feature			
Textbook	**Number of Signals**	**Chemical Shift**	**Splitting**	**Integration**
Brown, et al.	**93% (14)**	20% (3)	33% (5)	53% (8)
Carey, Giuliano	**77% (24)**	16% (5)	39% (12)	0% (0)
Jones, Fleming	14% (2)	**93% (13)**	57% (8)	64% (9)
Smith	**63% (5)**	38% (3)	38% (3)	25% (2)
Average (± St Dev)	62% ± 34%	42% ± 35%	42% ± 11%	36% ± 29%

Note: Percentages can add to more than 100 as some worked examples include multiple spectral features of ^{1}H NMR.

All four examined spectral features were featured in the practice problems in all textbooks, both in the in-text and end-of-chapter practice problems (Table 2.6). The number of signals and chemical shift were the most frequent spectral features among the textbook problems. Among the practice problems, integration was featured the least, comprising of 55% of the problems on average across the textbooks.

Table 2.6. Frequency of practice problems focusing on each ^{1}H NMR spectral feature by textbook. Numbers in parentheses are the number of problems focusing on each respective feature.

	Spectral Feature			
Textbook	**Number of Signals**	**Chemical Shift**	**Splitting**	**Integration**
Brown, et al.	**95% (40)**	76% (32)	74% (31)	81% (34)
Carey and Giuliano	70% (28)	**85% (34)**	50% (20)	55% (22)
Jones and Fleming	40% (29)	**82% (60)**	66% (48)	42% (31)
Smith	**71% (97)**	50% (68)	60% (82)	41% (56)
Average (± St Dev)	69% ± 23%	73% ± 16%	62% ± 10%	55% ± 19%

We also explored the number of problems targeting single or multiple spectral features (Table 2.7). We found that, in general, worked examples were more likely to focus on a single spectral feature at a time, while practice problems focused on all four spectral features together.

Table 2.7. Percent of problems targeting ^{1}H NMR spectral features alone or in concert with multiple features. Numbers reflect the average percent (± St Dev).

Textbook	One Feature	Two Features	Three Features	All Four Features
Worked Examples	**51.3% ± 20.8%**	23.1% ± 11.4%	19.2% ± 24.1%	6.5% ± 7.5%
Practice Problems	29.2% ± 13.2%	22.4% ± 9.7%	8.3% ± 8.4%	**40.2% ± 19.0%**

Ordering of spectral features

We utilized a case-study approach to describe the ordering of spectral features within a textbook, examining each book individually. Modified sunburst diagrams allowed us to visualize the spatial ordering or chronology of the spectral features used in worked examples and practice problems; in addition, these diagrams allowed us to identify instances of blocking and interleaving within the problems.

A sunburst diagram is read in a clockwise manner, starting at the topmost notch in the circle. The gray ring indicates the page on which a particular problem was found. Each colored ring conveys the chronology of a different spectral feature within the textbook. For example, pink denotes number of signals, and the light pink signifies the spectral feature was observed in a worked example and dark pink in a practice problem. This convention is used for each spectral feature: blue denotes chemical shift, green denotes integration, and purple denotes splitting. If no color is present in a portion of the ring, the spectral feature for that respective ring was not exercised by the problem in question. Pages without any colored rings indicate a page with no problems.

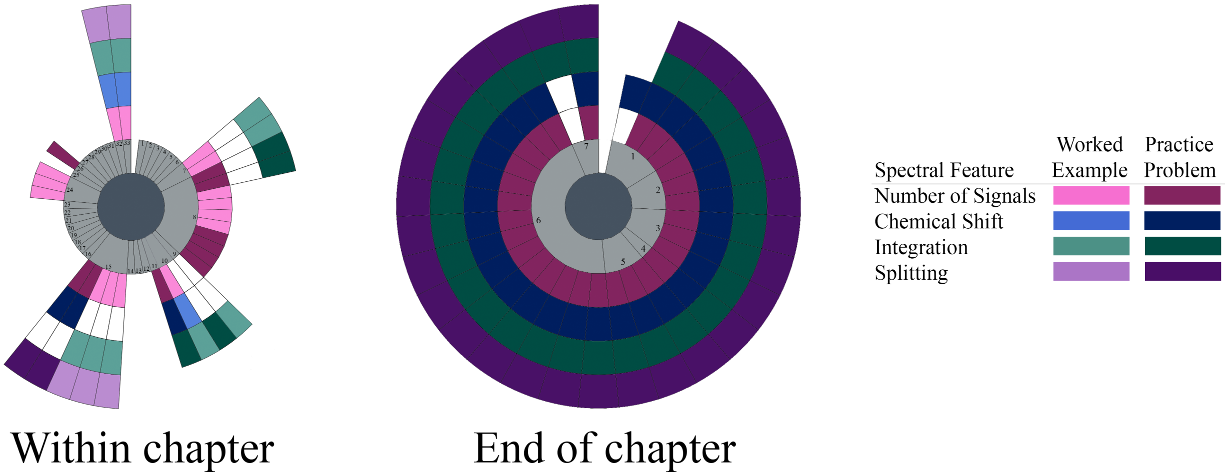
Sunburst diagrams support our exploration of blocking and interleaving of spectral features within worked examples and practice problems in both within-chapter and end-of-chapter problems. Given our definition of interleaving as the deliberate intermixing of spectral features, we would not expect to see solid rings of color in our sunburst diagrams, but we would see different colors mixed across the problems. With interleaving, we would not see multiple problems of a spectral feature in a row, as that would signal to a student that that is the feature to use. In contrast, if blocking provides a set of problems grouped together that exercise the same spectral feature(s), we would expect to see solid rings of color as evidence of blocking of spectral features.

Brown, et al. (2008)

In Brown, et al. (Figure 2.3), the ordering of spectral features in within-chapter problems mirrors the chapter narrative (Table 2.4). The text and problems start with number of signals, moving on to integration and chemical shift, and finally splitting. Within chapter problems appearing earlier in the chapter focus on just one or two spectral features, in particular number of signals and integration. Later problems add a third and fourth spectral feature. In contrast, worked examples alternate between targeting a single spectral feature or multiple spectral features.

We see little evidence of blocking or interleaving in the Brown, et al. within-chapter problems. Rather, we see some evidence of an additive approach, where the problems introduce one spectral feature and add subsequent spectral features in turn.

The end-of-chapter problems in Brown, et al. almost exclusively focus on the use of all four spectral features. There is no evidence of interleaving, and the use of all four spectral features in the bulk of problems shows evidence of poor scaffolding.



Within chapter

End of chapter

Figure 2.3. Spectral features targeted by each worked example and practice problem within the chapter and at the end of the chapter for Brown, et al. (2008). Pages are conveyed in light gray to show the order of the problems and highlight pages without any problems.

Carey and Giuliano (2011)

In Carey and Giuliano (Figure 2.4), the ordering of spectral features in the within-chapter problems also mirrors the narrative (Table 2.4). Carey and Giuliano begins by focusing worked examples and practice problems on chemical shift, adding a practice problem with chemical shift and integration, and then shifts the focus to the number of signals, adding splitting at the end. The worked examples target one or two spectral features at a time.

We see evidence of blocking in the within-chapter problems of Carey and Giuliano, with sets of problems devoted to chemical shift, then the number of signals, and later with the number of signals and splitting together. Again, the focus is primarily on one spectral feature at a time and no worked examples or practice problems target all four spectral features together.

The end-of-chapter problems begin with two spectral features, the chemical shift and number of signals, but expand to focus on all four spectral features at a time. Several problems then focus on chemical shift and integration, followed by a single problem on only splitting, and then a set of problems on all four spectral features again. At the end of the chapter narrative, the problems focus on random spectral features and combinations of spectral features before going back to all four spectral features together. We see little evidence of interleaving in the end-of-chapter problems, but there is evidence of blocking, followed by a set of problems with all four spectral features. While the ordering of the spectral features becomes more random toward the end of the problem set, most problems are focused on using three or four spectral features simultaneously.

Within chapter

End of chapter

Figure 2.4. Spectral features targeted by each worked example and practice problem within the chapter and at the end of the chapter for Carey and Giuliano (2011). Pages are conveyed in light gray to show the order of the problems and highlight pages without any problems.

Jones and Fleming (2014)

In Jones and Fleming (Figure 2.5), the narrative begins with integration, then moves to chemical shift, and ends with splitting; however, the within-chapter problems begin with chemical shift and integration together and then move to the number of signals, a spectral feature not described in the narrative. This is the only textbook where the within-chapter practice problems and worked examples do not align with the order of the spectral features as they are presented in the chapter narrative (Table 2.4). The worked examples target one or two spectral features simultaneously in the beginning, then add in a third spectral feature to the fold.

With the few within-chapter problems it is difficult to make claims about blocking or interleaving. There is some blocking toward the end of the section. One practice problem in the middle of the chapter targets all four spectral features, while no worked examples target all four spectral features together.

We see evidence of an additive approach to the spectral features in the end-of-chapter practice problems for Jones and Fleming, starting with the number of signals, then moving to chemical shift, and then chemical shift and integration before focusing on all four spectral features together. These problems show evidence of blocking. The ordering of the spectral features gets more unpredictable in the last two-thirds of the problems, focusing several problems on chemical shift then all spectral features together except the number of signals. More random combinations of spectral features are targeted before focusing primarily on all four spectral features together at the end. These random combinations could be possible evidence of interleaving, but with blocking throughout the problem set, the evidence for interleaving is not strong.

Within chapter

End of chapter

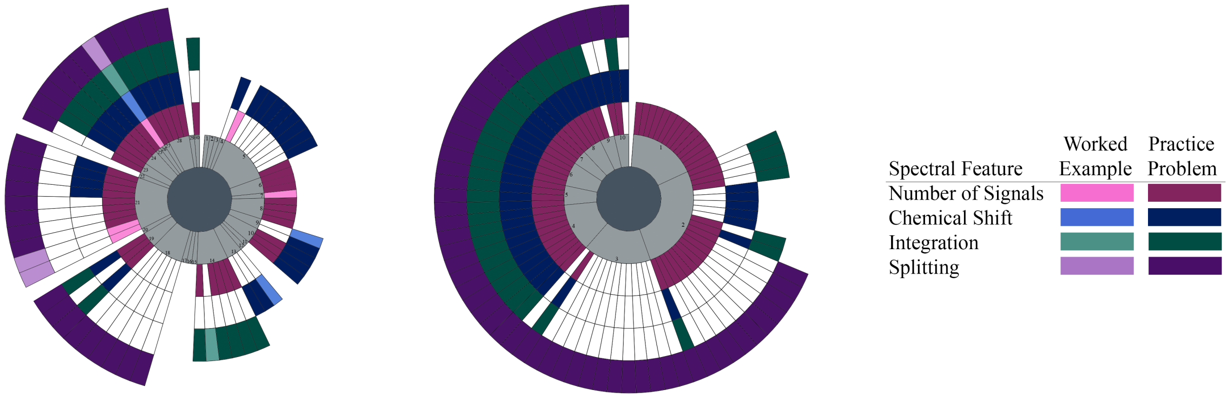
Figure 2.5. Spectral features targeted by each worked example and practice problem within the chapter and at the end of the chapter for Jones and Fleming (2014). Pages are conveyed in light gray to show the order of the problems and highlight pages without any problems.

Smith (2011)

In Smith (Figure 2.6), the within-chapter problems and worked examples reflect the order of the spectral features as presented in the chapter narrative (Table 2.4). Smith begins by focusing the worked examples and practice problems within the chapter with problems on chemical shift, then a series of problems on the number of signals. Problems targeting both the chemical shift and number of signals together are given before adding in a number of problems with integration, and then splitting. Problems with all four spectral features are provided for the last set of within-chapter problems. The worked examples focus on one spectral feature at a time, then two, and end with one example of all four spectral features together.

We see evidence of blocking with Smith's within-chapter problems. Overall, the within-chapter problems focus on a single spectral feature at a time throughout much of the chapter; some of the later problems incorporate three or four spectral features, but the spectral features are built up. This additive approach to the spectral features is shown as Smith focuses on the first two spectral features independently and then together. This building is repeated for a fourth spectral feature with a set of problems using only splitting, then using splitting with the three other spectral features. There is no evidence of interleaving.

We see evidence of blocking in the end-of-chapter problems, where a series of problems on the number of signals are given, followed by the number of signals with integration. Chemical shift problems are then provided, followed by problems with the number of signals and splitting. A series of problems on splitting are provided before problems are given on all four spectral features together. Each spectral feature is handled independently before all four spectral features are used together. There is no evidence of interleaving with the Smith end-of-chapter problems.



Within chapter

End of chapter

Figure 2.6. Spectral features targeted by each worked example and practice problem within the chapter and at the end of the chapter for Smith (2011). Pages are conveyed in light gray to show the order of the problems and highlight pages without any problems.

Across all four sampled textbooks, the ordering and combinations of within-chapter problems varied. Where Brown, et al. (2008) utilized an additive approach, beginning with one spectral feature then adding another spectral feature to that previous spectral feature, Carey and Giuliano (2011) focused on each spectral feature independently. Jones and Fleming (2014) moved back and forth from combinations of spectral features, and Smith (2011) was additive with spectral features, but also provided multiple practice problems and worked examples with all four spectral features together. In the end-of-chapter problems it is evident that all four spectral features together are utilized in all the textbooks, but the textbooks' approaches still differ. Brown, et al. (2008) almost exclusively focuses on all four spectral features together, Carey and Giuliano (2011) offer a few problems with all four spectral features in the middle of the problem set and then follows with problems with fewer spectral features and repeating this process. Jones and Fleming (2014) starts out with an additive approach and then gets more random in the combinations of spectral features, while Smith (2011) covers each spectral feature alone before combining multiple features and ending with all four spectral features together. In a full comparison, all four textbooks continue to vary in their approaches. Between all the worked examples and practice problems (within-chapter and end-of-chapter), three of the textbooks showed evidence of blocking (Carey and Giuliano, Jones and Fleming, and Smith). Three textbooks showed some additive approaches with the spectral features (Brown, et al., Jones and Fleming, and Smith). Only one textbook showed potential for interleaving (Jones and Fleming).

Discussion

Textbooks serve as reliable resources for students, supplementing and supporting classroom instruction (Knight, 2015). In order to identify how textbooks support learners in developing ^{1}H NMR spectroscopy problem-solving approaches, we analyzed four textbooks to describe how worked examples and practice problems ordered and combined four baseline spectral features. Practice problems in all four textbooks included all four spectral features, with number of signals and chemical shift the most common features observed. The ordering and combinations of within-chapter problems varied across all four of our sampled textbooks, but three textbooks showed evidence of blocking in within- and end-of-chapter problems, with little to no interleaving of the spectral features.

Individual spectral features

^{1}H NMR spectra are made up of four distinct features that function to guide problem solving. These spectral features include the number of signals, chemical shift, integration, and splitting, and make up the foundation of cognitive structuring the textbooks can address. We found that worked examples and practice problems in textbooks do not place equal emphasis on each ^{1}H NMR spectral feature, which results in an excess of problems for one feature and a dearth for other features. For example, in Carey and Giuliano's (2011) 31 total worked examples, 24 covered the number of signals, while zero discussed integration. By extension, this may send an implicit signal to students of what is important in the problem-solving process. Understanding how to interpret these spectral features is essential to successful problem solving; Cartrette and Bodner (2010) found that more successful solvers better mined the spectral data. Those successful solvers were guided by their understanding of the features of ^{1}H NMR spectroscopy. We know that understanding and attending to all four spectral features when solving is crucial, but without sufficient assessment, instructors cannot diagnose student difficulty with each spectral feature. If there are many problems on the number of signals and fewer on splitting, a student might assume erroneously that one is more important than the other. In the case of the textbooks we examined, the number of signals was most common across the textbooks, while integration was the least common. This may signal to students to focus on the number of signals while ignoring integration, thus limiting the development of their problem-solving abilities.

Without adequate practice with each individual spectral feature, textbooks could be shortchanging the learning process for students. As in many of the textbooks we chose not to include in this study, when there are few worked examples or practice problems on specific spectral features, it can impact the development of fluency in problem solving. Students working with a limited number of problems for a particular spectral feature will not see the diversity in problems and gain the fluency and flexibility necessary in using the spectral features together. As Stowe and Cooper (2019) observed, students do not build evidence-based arguments to support the answers they arrived at. We would argue that textbook coverage of spectral features could build problem solving fluency and by extension, improve students' argumentation. Furthermore, a lack of worked examples and practice problems could lead students to adhere to heuristics like generalization and rigidity, and students could make assumptions that spectral data should be absolute (Connor, et al., 2019). The more problems students have access to, the more ways they can observe spectral features being used, which could help them build fluency in using those spectral features.

In our analyses, we found that integration comprised 55% of the practice problems on average across the textbooks, the least of all the spectral features. Students may implicitly rely on those spectral features that are overrepresented, mistakenly believing those are key spectral features for solving problems. By extension, students do not develop a robust problem-solving approach. Without adequate practice on integration, a student could be uncertain in interpreting the number of hydrogens represented by individual signals sets and could therefore fail to see how to connect the structural pieces together. Each ^{1}H NMR spectral feature is important to the solution pathway. With some spectral features overrepresented in worked examples and practice problems, a student may develop an understanding that those lesser assessed spectral features are not as important to the problem-solving process. While it could be argued that some spectral features may be more foundational than others and therefore deem more practice, it is not necessarily the role of a textbook to determine what is needed most by students and a textbook should not signal what could be arguably more foundational—this is a role of the instructor. In their use of textbooks, instructors make decisions on what to use, supplement, and alter from a textbook (Mesa and Griffiths, 2012). Likewise, students search out examples in their use of textbooks (Weinberg, et al., 2012; Lee, et al., 2013). As sufficient support for scaffolded instruction, textbooks could instead include bountiful examples and problems of all types that an instructor can refer their students to.

Support for instructional scaffolding by combining spectral features

Overall, the worked examples and in-text practice problems we analyzed were geared toward helping students master interpretations with each spectral feature individually, with few of these problems integrating all four spectral features together. Only two textbooks (Brown, et al., 2008; Smith, 2011) incorporated worked examples with all four spectral features together, and there were only three in total of these examples. Worked examples that integrate all four spectral features fulfill the 'expert solver' role. These problems summarize and synthesize all four spectral features and provide the learner with an evidence-based pathway for problem solving. If the goal of spectroscopy instruction is to equip students with the knowledge and skills necessary to interpret and characterize spectra, it is essential that they learn to incorporate all four spectral features into a solution pathway.

Worked examples and practice problems support instructional scaffolding by giving learners many problems and examples involving each individual spectral feature prior to encountering a problem involving all the spectral features. If textbooks are to support instructional scaffolding in the learning process, we would expect to find worked examples and practice problems that examine each spectral feature in isolation as well as in combination to assess students' ability to interpret and use multiple spectral features. Students could benefit from seeing additional worked examples that combine spectral features to better learn how the four spectral features work in concert to solve a ^{1}H NMR spectroscopy problem. The novices in Topczewski, et al. (2017) spent time looking at all resonances in the spectra and did not discern the most critical areas of interest. Thus, organic chemistry students may require more practice using all spectral features together and models on expert approaches to interpreting the features all together. Students need to see how the features work together to be able to discern how to connect resonances with the structures and effectively perform checking procedures like experts and successful solvers (Cartrette and Bodner, 2010). Worked examples that combine multiple spectral features could work well toward the end of the chapter, after the introduction of each spectral feature, and ideally after the students have had opportunities to use and master each spectral feature. Instructors could then point students towards additional models of expert-like solving through worked examples as well as problems to practice their understanding.

As we consider the framework on scaffolding from van de Pol, et al. (2010), this additive approach of spectral features within the worked examples and practice problems addresses the intent of scaffolding to reduce the degrees of freedom, allowing students to focus on and master interpretations with one spectral feature before introducing another degree of freedom in the form of another spectral feature. Building a student's fluency using spectral features from one to multiple moves from one degree of freedom to many. Increasing the degrees of freedom functions to fade support in scaffolded instruction. While we pointed out three textbooks that used an additive approach with the spectral features, our textbook analysis does not find any clear evidence of the textbooks helping establish mastery with additive scaffolding, where each spectral feature is first exercised alone and then in combination, in either the worked examples or practice problems. If we were to see evidence of scaffolding by adding in spectral features, we would expect the worked examples and practice problems within the chapter to block a number of problems on one spectral feature, before adding another spectral feature, before moving onto all four spectral features together. The Carey and Giuliano, and Smith textbooks both focus on mastering individual spectral features before moving onto additional spectral features. However, we note that there is not a clear signal for additive scaffolding in these books, as some spectral features are combined with others before covering the new feature on its own. A purposeful additive approach in scaffolding would cover one spectral feature on its own, then another on its own, and then combine the two features. A third spectral feature could then be introduced with practice problems of its own, and then either combined with the other two features or with one of the other features. Additive scaffolding in this sense then offers mastery of a single concept before adding another concept and increasing the degrees of freedom.

Support for instructional scaffolding by ordering spectral features

Beyond the use of individual spectral features and combinations of multiple spectral features in problems, the ordering of spectral features through interleaving and blocking can aid in instructional scaffolding. Blocking spectral features acts to reduce the degrees of freedom when scaffolding instruction. In the textbooks we sampled, we saw little evidence of systematic blocking and interleaving, although we note that end-of-chapter problems tended to block spectral features individually or examined all four spectral features simultaneously. Students may need substantial practice using a single spectral feature to fully understand how the spectral feature is interpreted. Once students have some proficiency with interpreting a spectral feature, they can then begin combining spectral features to develop a problem-solving pathway. Textbook ordering of practice problems can systematically support instructional scaffolding by initially removing degrees of freedom to focus on single spectral features (blocking) and then reintroduce degrees of freedom by interleaving problems, to help learners build fluency.

The lack of interleaving found in our sampled textbooks shines a light on an area in need of addressing. If textbooks utilized systematic blocking and interleaving it could be possible to mitigate the difficulties students have shown in problem solving with ^{1}H NMR spectra. Topczewski, et al. (2017) showed that students spent time focusing on all resonances in the spectra, struggling to recognize or understand the connections needed to be made. Too much blocking could exacerbate issues such as these, where students could be led to believe that they must focus on and analyze all areas in the spectrum, using more of their working memory capacity in the process. Scaffolding could also aid in helping students see how the spectral data works together. Connor, et al. (2019) found that students made assumptions that the N+1 rule should hold true and that spectral data like typical chemical shift values should be absolute. In these cases, scaffolding and more blocking with each of the spectral features could help in picking out patterns within each of the spectral features alone, before having to use all spectral features together. Stowe and Cooper (2019) observed that students possessed procedural knowledge, but could not make well-supported arguments for the answers they found. In this situation, too much blocking could promote issues in knowing how to use all the information together.

Topczewski, et al. (2017) also found in their study that students did not spend time connecting specific resonances with the structures. Here, interleaving could help students gain mastery in finding and connecting the relevant spectral support for a structure. Connor, et al. (2019) also found that students used heuristics like rigidity and one-reason decision making, using only some or one of the spectral features to make their decisions. The use of such heuristics could be mitigated through interleaving, so students can understand how to use all spectral features together and see patterns across problems incorporating all spectral features. Since the students in Stowe and Copper's (2019) study possessed adequate procedural knowledge and were able to arrive at the answers just fine, they needed help in using all the information. Interleaving could help students gain flexibility in using procedural knowledge and help students discern not only how to apply a strategy, but when to use that strategy (Rohrer, 2012). Practice with interleaved problems would help students see how general rules in interpreting spectral features are not absolute and would provide students with opportunities to see the shortcomings of specific heuristics.

Our suggestion to block spectral features before interleaving contrasts with existing research conducted primarily in mathematics education. In math, substantial research supports the efficacy of interleaving in helping students develop robust problem-solving approaches (Mayfield and Chase, 2002; Rohrer and Taylor, 2007; Rohrer, et al., 2014). Success in mathematics requires that students learn to choose appropriate strategies when solving problems. However, we believe blocking may be important in solving spectroscopy problems as students need to master interpretations with each spectral feature independently, before combining spectral features to solve a problem. Certainly, further research is warranted that explores the effects of interleaving and blocking on students' ability to solve spectroscopy problems.

Conclusions

As instructors and researchers, we know the importance of scaffolding the learning experience. Textbooks can be a tool to support scaffolding, especially when they are designed and written using evidence-based practices like interleaving. In the present research, we identified several practices that could be more fully used by textbooks. For example, textbooks could deliberately structure the narrative, worked examples, and practice problems to focus on each spectral feature independently and then together. Moreover, practice problems could begin by blocking each spectral feature and then move towards interleaving the spectral features.

Although we focused on just one textbook chapter, we believe these results underscore a greater need to use the research from the learning and cognitive sciences and discipline-based education research to design textbooks. Much is known about problem solving and the importance of scaffolding and this research can inform textbook design, including the ordering and combination of worked examples and practice problems. A systematic approach to textbook design, including deliberate decisions about the order spectral features are introduced, using blocking and interleaving with practice problems, supports instructional scaffolding and by extension, student learning.

Limitations and Future Directions

Instructors have discretion in structuring their instruction which may temper or limit the effects of textbooks on student learning. Textbooks, however, influence course design, as instructors use textbooks to help structure courses (Mesa and Griffiths, 2012). As a result, the impact of textbooks on student learning is likely substantial. Textbooks have the potential to support scaffolded instruction, but based on this research, they do not have the worked examples and practice problems designed and ordered to achieve this. Instructors may take the brunt of scaffolding, but more research is needed in this area to figure out if scaffolding is happening in the classroom and if it is, to what extent it promotes learning.

Given the lack of worked examples throughout all four textbooks we analyzed, robust conclusions are limited. Examining the chapter narrative could provide further insight into the nuances of how the spectral features of ^{1}H NMR are described and taught. This research focuses on four baseline spectral features, but there are additional spectral features that become pertinent to chemists beyond the undergraduate level.

While we can use principles from the learning sciences to design textbooks, i.e. how we might order problems, further insights from students solving problems would help to refine and systematically shape textbook problems and worked examples. We know from Topczewski, et al. (2017) that novice solvers pay attention to all four spectral features, but we do not know how students may struggle in discriminating between the spectral features and if they know when one spectral feature versus another provides them with the information necessary to solve for the structure of the problem. More research is needed that focuses on how students use and integrate the four spectral features of ^{1}H NMR spectroscopy presented here.

Some spectral features involve an understanding of others to be properly applied. For example, splitting and integration involve an understanding of proton equivalence. In our study, we only went as far as the prompts explicitly told students to solve for or reason with. The only problems that had an absence of specific features to solve for were the problems that asked for a whole structure, and those problems were coded for all four spectral features. Textbook analysis therefore contributes to this limitation, as we would not know if students are drawing on interrelated spectral features in that way or not. Stowe and Cooper's (2019) findings showed that as students displayed adequate procedural knowledge, they did not support their reasoning with spectral evidence. Likewise, the findings from Topczewski, et al. (2017), where novices did not connect spectral features with the provided structure answer choices, also shows that students are not drawing back to specific spectral features. We would not be sure if students were truly reasoning with the other features or not. Making such determinations turns into an examination of the problem-solving process and is therefore a facet of the individual human that cannot be determined from the textbook analysis itself.

Moreover, one spectral feature in a ^{1}H NMR spectrum can often be more critical than other features in determining the structure of the compound represented. On this level, blocking and interleaving could actually underly problems that would otherwise seem to assess all spectral features, such as the end-of-chapter problems for Brown, et al. (2008). It is possible that critical spectral features could be deliberately intermixed within a set of problems that, on the surface, cover all four spectral features. Future research should examine the nature of such critical spectral features and provide an intersection between the difficulties in solving students exhibit, as this involves aspects of the individual problem-solving process and characteristics of novice and expert solvers.

Implications

Implications for instruction

We described different areas in which an instructor might rely on a textbook to support scaffolded instruction. As our study examined the ways in which textbook worked examples and practice problems focused on the spectral features of ^{1}H NMR, we can address how an instructor could use textbooks in the stages of providing students with practice and using problems for different assessments. Findings from this study suggest that textbooks may not provide students with enough practice with interpreting each individual ^{1}H NMR spectral feature. Limited practice could impede the development of problem-solving fluency and may, in fact, support student use of inappropriate heuristics. As we carefully consider the nature of the four ^{1}H NMR spectral features we focused on, the number of signals and chemical shift allow the solver to hypothesize what structural and functional pieces could be present, but splitting and integration allow the solver to connect these structural pieces together. If the practice students get with interpreting the spectral features aligns with our findings from the textbooks, students may be able to find the structural and functional pieces from a ^{1}H NMR spectrum, but may lack adequate practice with putting those pieces together into a whole structure. We encourage instructors to take a closer look into how these spectral features are presented to students and how these spectral features are assessed. If an instructor chooses to incorporate textbook problems in their own assessments, we would encourage them to examine the spectral features focused on by each question to ensure alignment with their unit objectives. Reflective instruction that deliberately introduces and assesses each of the four spectral features could support students as they master the spectroscopy solving process. Likewise, deliberate use of blocking and interleaving with the spectral features could help students develop solving fluency.

Implications for research

Using principles from the learning sciences with scaffolding, blocking, and interleaving, our research systematically explores how textbooks introduce and reinforce spectral features when teaching students to solve ^{1}H NMR spectroscopy problems. While textbooks generally introduce students to all spectral features, we find that the approach does not reflect practices of scaffolding, interleaving, or blocking. We recognize that textbooks do not directly reflect classroom practice; thus, we believe there is a need to further study how spectral features of spectroscopy are introduced to students in the natural setting of an organic chemistry classroom.

In addition, the ordering of spectral features may impact how students use the spectral features to solve spectroscopy problems. To date, we know of few studies investigating students' reasoning when solving spectroscopy problems; more work is warranted in this area. To our knowledge, no study has investigated how the spectral features behind ^{1}H NMR spectroscopy are presented to students. This approach with spectral features provides a new way to frame what is seen in student reasoning when solving ^{1}H NMR spectroscopy problems. Studies should explore how students use and reason with each specific spectral feature. Finally, there is a need for research that explores how blocking might help or hinder the ^{1}H NMR spectroscopy solving process. Blocking is generally viewed unfavorably in the learning sciences community, but we posit that blocking may be beneficial when learning to solve complex, multistep spectroscopy problems.

CHAPTER 3. OPERATOR ERROR: THE IDENTIFICATION AND TESTING OF OPERATORS IN ^{1}H NMR SPECTROSCOPY PROBLEM SOLVING

Introduction

Organic chemistry involves extensive problem solving, from devising synthetic pathways to interpreting visual representations. Nuclear magnetic resonance (NMR) spectroscopy is a vital technique for synthetic chemists to characterize and analyze chemical compounds (Thomas, 1991) and because of NMR spectroscopy's importance to chemists and organic synthesis, interpreting ^{1}H NMR spectra serves as a unit of instruction in organic chemistry.

Students solving ^{1}H NMR spectroscopy problems may be impacted by assumptions and the steps they take

Problem solving with NMR spectroscopy is noted as being hard for students, but there is limited research describing that difficulty. Of the limited studies on student learning and problem solving with NMR spectroscopy, we know that novice solvers may hold to invalid chemical assumptions, such as over applying the N+1 rule or holding to general chemical shift values as being absolute, and enact heuristic reasoning like representativeness and one-reason decision making while solving (Connor, et al., 2019). Learners may not utilize problem-solving steps like drawing molecular fragments from the data or checking their answers (Cartrette and Bodner, 2010; Topczewski, et al., 2017). While students have the procedural knowledge to propose reasonable structures from ^{1}H NMR spectra, they struggle to support their answers from spectroscopic evidence (Stowe and Cooper, 2019). Moreover, without proper scaffolding, students may not develop equitable mastery and fluency of problem solving with each spectral feature of ^{1}H NMR spectroscopy (Anderson, et al., 2020). From these studies, we have an idea of some areas where students are prone to errors and how they may have learned how to problem solve with these spectral features, but what does the overall problem-solving process look like? While all these assertions can be further examined through students' problem-solving pathways, we need to first establish what that problem-solving pathway is and then discern possible sources of difficulty.

Theoretical Framework

Operationalizing the problem-solving pathway can give insight into students' problem-solving processes

While problem solving is essential to chemistry, the act of problem solving has been defined broadly and examined in a variety of ways. Problem solving is required when there is a goal to reach; it is the construction of a path to achieving that goal. An often-cited definition of problem solving in chemistry education research states that problem solving is what you do when you don't know what to do (Wheatley, 1984). While this definition promotes a lively exploration into the juxtaposition of algorithmic and conceptual solving, expert/novice and successful/unsuccessful problem solving, there is more to the problem-solving path that is unexplored. These approaches to and broad definitions of problem solving do not lend themselves to an investigation of students' stepwise problem-solving processes. We therefore need a theoretical framework that can provide insight into students' problem-solving processes.

The problem-solving process is achieved through searching the problem space

Newell and Simon's (1972) problem space theory suggests that problems are solved through a search and evaluation of different pathways to a solution. A problem consists of an initial situation (problem state), a set of operators (the actions taken to move from one state to another) that can be used to change the situation (transforming the current state into a different state that may or may not be the goal state), and a goal state (Newell and Simon, 1972; Greeno and Simon, 1988). The construction of that path is the problem-solving process. In the problem-solving process, the solver first extracts the given and goal information and attempts to understand the problem, then searches for a way to solve the problem, and finally, implements that solution path. If the solution path is not successful, they must go back to an earlier stage in their solution path to redefine the problem or revise the path (Greeno, 1978; Gick, 1986). With any given problem, solvers can try and apply multiple solutions before they find a solution path that ultimately solves the problem and gets them to their desired goal state. Likewise, in any solution path, the solver may encounter multiple intermediate states along the way. There may be many possible states and paths through this space, and only a subset may lead to the goal state. The solver may not know all the steps involved and may utilize strategies like working forward or backward to reduce the differences between their current state and the goal state. Due to the high cognitive load involved with searching the problem space, problem solving may be limited by working memory capacity (Beilock and DeCaro, 2007; Wiley and Jarosz, 2012). The problem space theory provides tangible units, i.e. operators and states, to examine student problem solving, allowing us to establish what those units are in terms of problem solving with ^{1}H NMR spectroscopy problems.

Can ^{1}H NMR spectroscopy problem solving be characterized through elements of Newell and Simon's problem space theory?

Within the context of ^{1}H NMR spectroscopy problems, students begin with a clearly defined goal state (i.e. determine a chemical structure) and a starting state (the spectrum and a provided molecular formula). Students must then identify the actions, referred to as operators, necessary to getting to the goal state. While the problem space theory posits these ideas of states and operators, we do not know what these operators are, specifically, in the context of ^{1}H NMR spectroscopy.

Despite limited research on the steps of the problem-solving paths undergraduate students take as they solve ^{1}H NMR spectroscopy problems, there are some ideas we can apply from Cartrette and Bodner's (2010) interviews with graduate students as they solved spectroscopy problems. Cartrette and Bodner's analyses indicated that a key difference between successful and unsuccessful solvers was that successful solvers drew out fragments of compounds as they solved. This action of drawing fragments could be one operator among many. Other operators involved in the problem-solving process with ^{1}H NMR spectroscopy problems need explication. In addition, if we are to understand students' problem-solving processes, we must investigate how students select and use operators. If students cannot successfully use operators, they are unlikely to complete the problem-solving process. While operators could be identified from either the expert or student perspective, we have an idea of the identity of common operators from the expert-like solving in Cartrette and Bodner's study, but we do not have a similar detailed depiction of the solving process of undergraduates in prior research. Ultimately, we desired to examine the operators emergent from the student perspective; we wanted to articulate what this solving process is for students. In particular, the following studies sought to (1) identify and describe the operators or actions students apply when solving ^{1}H NMR spectroscopy problems, and (2) identify those operators, if any, that are problematic for students to complete.

Study A

In the first study, we examined students' reasoning in think-aloud interviews as they solved ^{1}H NMR spectroscopy problems to identify the operators they used while solving. We interviewed twenty students from two different universities as they solved for the structures of two compounds from ^{1}H NMR spectra. Using thematic analysis of interview transcripts, we identified the operators students used when solving ^{1}H NMR spectroscopy problems. Specifically, we asked:

What operators do students use in their problem-solving processes with ^{1}H NMR spectroscopy problems?

Methods

Context

This study was conducted with students from two public universities in the upper Midwest. University A is a master's degree granting university with approximately 6,000 total students. University B is a doctoral degree granting university with high research activity and enrolls over 14,000 students (Indiana University Center for Postsecondary Research, 2018). The chemistry departments at both universities offer Organic Chemistry II during the spring semester. Organic Chemistry II at both universities serves students of diverse majors including chemistry, biology, engineering, and pre-professional health majors.

During the spring semester of 2012, we recruited 20 undergraduate students enrolled in the second-semester sequence of organic chemistry, which is when NMR spectroscopy is first taught at both universities. We solicited students for the interviews after the spectroscopy unit was complete. To ensure representation from both institutions, we accepted the first ten students that volunteered from each university. Student participation was completely voluntary and they received neither monetary compensation nor extra credit course points for their participation. Recruited students were primarily female, in their sophomore year, and from a variety of majors (Table 3.1).

Table 3.1. Interview participant demographics (n=20).

Gender	**Participants**
Male	35% (7)
Female	65% (13)
Academic Year	
Sophomore	60% (12)
Junior	25% (5)
Senior	10% (2)
Transfer/Non-traditional	5% (1)
Academic Major/Minor	
Biochemistry	15% (3)
Zoology/Biology	40% (8)
Pre-pharmacy	35% (7)
Biotechnology	5% (1)
Microbiology	5% (1)
Chemistry Minor	35% (7)
Cumulative GPA	
4.00-3.50	65% (13)
3.49-3.00	30% (6)
2.99-2.50	0% (0)
2.49-2.00	5% (1)

Interview Protocol

Students were interviewed individually as they used ^{1}H NMR spectra and molecular formulae to solve the structures of two organic compounds. The interviews were constructed as think-aloud and semi-structured, and were adapted from Schönborn and Anderson's (2009) 3-Phase Single Interview Technique (3P-SIT). We chose the 3P-SIT to guide our interview protocol development because it was designed to uncover students' thinking as they interpreted external representations (ERs) in biochemistry and ^{1}H NMR spectra are ERs commonly used in organic chemistry. A 3P-SIT interview probes the interviewee's reasoning during interpretation of the ER while also eliciting the interviewee's conceptual understanding in absence of the ER and controlling for the mode of representation itself.

Schönborn and Anderson (2009) designed and validated a model that depicted the factors that influence the interpretation of an ER (Figure 3.1). Their data support the interplay of three factors involved in the interpretation of representations: conceptual understanding (C), reasoning strategies (R), and the mode of representation (M). Though tested within the context of biochemistry, we believed their model would be fruitful for examining student problem solving in organic chemistry. Specifically, we applied their model to understand how students solve organic structures from spectral data. The first phase of Schönborn and Anderson's 3P-SIT was used to probe students' conceptual and prior knowledge, which is depicted in the yellow part of the model shown in Figure 3.1. More specifically, in Phase 1, the interviewee was asked to describe their understanding of the concepts related to the ER, prior to seeing the ER. The second phase was used to probe a student's reasoning abilities with the ER and the concepts related to the ER, as shown in the blue part of the model in Figure 3.1. In that second phase, the interviewee was given an ER and asked to interpret it. The third phase was used to probe the effects of the mode of representation, as shown in the red part of the model in Figure 3.1. In the third phase, the interviewee was asked to evaluate and critique the ER.

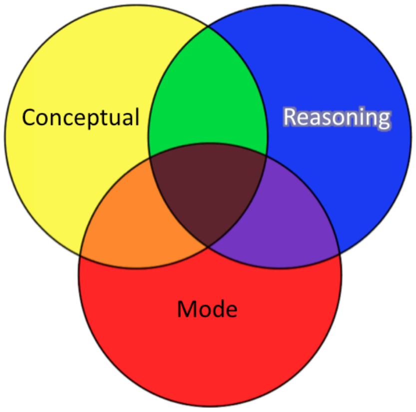


Figure 3.1. Schönborn and Anderson's model of factors affecting the interpretation of ERs.

Upon review of pilot interviews, we revised our interview protocol (shown in Table 3.2) to solicit students' conceptual understanding and reasoning for specifically solving ^{1}H NMR spectroscopy problems. From the original 3P-SIT, we kept Phase 1 the same and sought responses that would help to characterize the interviewees' knowledge of conceptual and procedural principles behind spectroscopy—before they were presented with any spectra. Phase 2 focused only on solving with ^{1}H NMR spectra. From the pilot interviews, we observed that interviewees discussed more features of the spectra with the more complex structures than with the simple structures. Therefore, in an effort to more fully capture students' reasoning, we split Phase 2 into Phases 2A and 2B, where 2A was added to build the interviewees' confidence and establish a baseline of their solving abilities. The student was asked to solve the structure of isopropyl alcohol (Figure 3.2) from its ^{1}H NMR spectrum and describe their thoughts as they were solving. Phase 2B was where the interviewee was provided with a more complex ^{1}H NMR spectrum to reveal the extent of reasoning with and interpretations of the ^{1}H NMR spectral features. In Phase 2B, the student was given the second representation and asked to solve for the structure of 5,6,7,8-tetrahydronapth-2-ol (Figure 3.2).

Table 3.2. Adaptation of the 3P-SIT.

	3P-SIT	**Revised Protocol**
Phase 1	The interviewee is asked to describe conceptual knowledge underlying a particular visual representation before being presented any representations.	The interviewee is asked to describe the conceptual and procedural principles behind spectroscopy before being presented any spectra.
Phase 2	The interviewee is given a representation and asked to interpret it.	**Phase 2A** This phase was added to prime the interviewee and be sure they could solve a simple spectrum. **Phase 2B** The interviewee is provided with a spectrum of sufficient complexity to reveal the extent of student reasoning and interpretation of the ^{1}H NMR spectral features.
Phase 3	The interviewee is asked to evaluate and critique the representation.	To isolate student reasoning independent of the mode of representation, the interviewee is given a data gallery of other types of spectra that could be used to support their structure from Phase 2B.

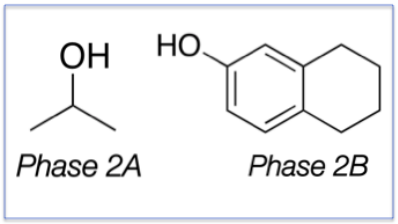


Figure 3.2. The structures of the compounds students solved for in the interviews.

As authentic solving and characterization utilizes other types of spectra, additional spectra were introduced in Phase 3. Phase 3 focused on what may have been confusing to the interviewee while solving the original ^{1}H NMR spectra. The interviewee was then given the opportunity to utilize a data gallery of other spectra (IR, ^{13}C NMR, MS) of the same compound to support their structure from Phase 2B. These additional spectra also provided the possibility of isolating student reasoning independent of the mode of representation. As the 3P-SIT model shows, reasoning with a single representation is denoted in the purple part of Figure 3.1, but with more modes of representation for the same compound, reasoning in general (in the blue part of the model) and independent of the mode of representation can be isolated.

In deciding the structure to give the interviewees, consideration went into the difficulty of the problem, keeping in mind the basic spectral knowledge students typically acquire in an undergraduate organic chemistry course. We wanted the problem to be solvable by undergraduate students, given what is covered during the unit. We also wanted the problem to be difficult enough where they were not able to simply glance at the spectrum and know the answer immediately—we needed to have the opportunity to see and hear their solving process. However, we did not want to overwhelm interviewees with a more difficult problem alone, so we revised the protocol to include spectra from a simple organic compound to build the interviewees' confidence and establish a baseline of solving ability. The interview protocol can be found in Appendix A of this dissertation.

Coding

Interviews were both audio and video recorded. Video recordings captured students' writing while they solved the problems. Audio recordings were transcribed verbatim and coded (see below for coding methodology). Videos were time stamped with codes where visual verification was needed. Structures students drew were also time-stamped and later redrawn by the research team and incorporated into the interview transcripts.

Interviews were coded in Nvivo version 10 (QSR International Pty Ltd, 2012) and we used a mixture of inductive and deductive approaches. We began with elements of thematic analysis (Braun and Clarke, 2006). During the first phase of analysis, interviews were transcribed and we familiarized ourselves with the data, jotting down initial ideas of solving. We focused on what actions students were taking as they solved, the areas of the spectrum they were paying attention to, and their understanding of the concepts of NMR spectroscopy. In the second phase of analysis, we generated initial codes based on what the interviewees mentioned as they solved the problems or did with their drawings. These descriptive codes developed from interview to interview as one researcher coded the entire data set. In the third phase of analysis, the final descriptive codes that emerged from coding all the interviews were reviewed and used to check and recode all of the interviews to ensure that coding was consistent among all interviews. In the fourth phase of analysis, codes were collapsed into themes: the spectral features interviewees mentioned, the reasoning or interpretations made with the spectra, and the strategies applied. These themes and codes were then revisited in accordance with our theoretical frame of problem space theory as we considered what operators could emerge from the coding scheme. We defined students' operators as the moments when interviewees wrote or drew anything. All moments when interviewees were writing were compiled and compared. We had a couple codes to describe students' actions, but more emerged as we focused on just the actions the interviewees had exhibited. These operator codes were reviewed and used to check and recode all videos to ensure the coding was consistent among all interviews.

Results and discussion

From our analysis of interviews with 20 students from two different universities as they solved for the structures of two ^{1}H NMR spectroscopy problems, we identified four types of operators (Table 3.3). The operators were calculating the elements of unsaturation, proposing bonds from the elements of unsaturation, proposing fragments of a structure, and constructing a whole structure. At some point in their solving processes, multiple interviewees exhibited these operators described above. Table 3.4 shows the number of interviewees using each operator. All interviewees proposed fragments and constructed structures at some point in their problem-solving processes. Not all interviewees calculated or used the elements of unsaturation.

Table 3.3. Descriptions of the four types of operators identified from the interviews.

Operator	**Description**
Calculate elements of unsaturation	Interviewee attempts to calculate the elements of unsaturation from the provided molecular formula. Whether they arrive at a correct answer or not, the act is still coded for this operator.
Propose bonds from the elements of unsaturation	Interviewee draws the types of bonds they believe would account for the elements of unsaturation. These drawings are coupled with language on the elements of unsaturation.
Propose fragments	Interviewee draws part of a structure. This is purposeful for the interviewee to note ideas of the specific components of a structure, and not a result of attempting to draw a whole structure.
Construct structure	Interviewee attempts to draw a complete structure from scratch or by putting fragments together. An unfinished structure would still count as constructing a structure and not a fragment, as the intent was to draw a complete structure.

Table 3.4. Number of interviewees using each operator while solving.

Operator	**Number of interviewees using the operator (Total N=20)**	
Calculate the elements of unsaturation	13	65%
Propose bonds from the elements of unsaturation	8	40%
Propose fragments	20	100%
Construct structure	20	100%

Calculating the elements of unsaturation

With the elements of unsaturation, 65% of the interviewees attempted calculating the value at some point in their solving whether it was with one of the problems from Phase 2 or with both problems. Here we see Makenzie explain the calculation aloud:

"So right now, right off the bat we can do something I forgot to do on the other one is calculate the elements of unsaturation. This lets us see if we have any alkenes. So it is 2C+2 minus the amount of hydrogen divided by 2. That would be 22 minus 12 divided by 2, which is 5. That is our elements of unsaturation."

Makenzie began the second problem with calculating the elements of unsaturation and remarks on forgetting to do so with the first problem from Phase 2A. Makenzie calculated the value correctly, but we still accounted for the use of this operator even if a student did not correctly calculate the elements of unsaturation. Here we see Addison calculate the elements of unsaturation incorrectly and still propose an aromatic ring from it:

"I'm not super confident with elements of unsaturation right now, but… elements of unsaturation. 10 times 2, twenty, minus 12 hydrogens equals 8, minus 2 for oxygen, gives me six EU. Which looks like a high number, but if I look at the chemical shift here is in the aromatic region. Aromatic region, so that would explain like four elements of unsaturation. EU doesn't really help me at the moment."

Addison admitted a lack of certainty, but still attempted to calculate the number, used the value to make a structural prediction and verified their prediction, but ultimately did not find the practice useful. Again, even though the number was not calculated correctly or used later on, we still counted any moment the interviewees calculated the elements of unsaturation.

Although Cartrette and Bodner (2010) examined graduate students as they solved spectroscopy problems, they too observed their more successful participants calculate the elements of unsaturation. Their findings coupled with our findings make a good case for this action as an operator. This operator of calculating the elements of unsaturation can only emerge when students are presented with a molecular formula; other studies (Topczewski, et al., 2017; Connor, et al., 2019; Stowe and Cooper, 2019) did not identify students calculating the elements of unsaturation in their solving processes because students did not have a molecular formula. Cartrette and Bodner showed how their successful solvers utilized this operator, so while this operator could be useful it has not yet been determined if it is imperative to the solving process.

Proposing bonds from the elements of unsaturation

Forty percent of interviewees proposed bonds from the elements of unsaturation, and 62% of those that calculated the elements of unsaturation used the number they calculated to consider the presence of unsaturation like double bonds or aromatic rings. For example, Jamie calculated the elements of unsaturation correctly and proposed reasonable types of bonds from that value:

"We know we have five elements of unsaturation and a ring would give us four elements of unsaturation. Four elements of unsaturation, so we have one more element of unsaturation.

Which may lead us toward a carbonyl group, since that has a double bond in it which counts as an element of unsaturation.”

Jamie suggests that there could be an aromatic ring and carbonyl double bond to account for the elements of unsaturation calculated, so we see how using the elements of unsaturation is another operator students can perform beyond calculating the mere value attributed to the elements of unsaturation. As noted earlier, Cartrette and Bodner (2010) found that their more successful participants calculated the elements of unsaturation. However, it is unclear how their participants used the elements of unsaturation. Nearly half of our participants used the elements of unsaturation to propose bonds and we believe that it is worthwhile to separate as an operator outside of calculating the elements of unsaturation as 38% of our participants that calculated the elements of unsaturation did not use the value further. For example, Parker calculated the elements of unsaturation correctly, but then immediately moved on to another part of their solving without proposing anything from the number they had calculated:

“The first thing that came to mind was that I should probably do is find how many EUs there are. Elements of unsaturation. So I’m trying to remember how to do that exactly. I think it’s ten times two. It’s not terribly important. I can probably do it without finding EU. [continues calculating the value] Five, which I feel like is probably wrong. We will come back to that later maybe.”

Parker never came back to use the elements of unsaturation they had calculated. This demonstrates that there is a difference between simply calculating and actually using the elements of unsaturation. Calculating the elements of unsaturation is a completely algorithmic operator; proposing bonds from the elements of unsaturation goes beyond the algorithmic aspect of the task as a whole. Stowe and Cooper (2019) found that students can deploy algorithms well and possess the procedural knowledge to do so, but what is less clear is how students use that information to make structural predictions. By identifying a second operator, we begin to parse out when and how students use the elements of unsaturation to make structural predictions.

Proposing molecular fragments

All interviewees proposed molecular fragments at some point in their problem-solving processes, making a decision that certain groups could be part of the final proposed structure. Interviewees paid attention to different information to make assertions about what fragments could be present. From the excerpt below, we see that Lane proposed an aromatic ring due to the chemical shift of the signal set they were pointing at:

"I think this would probably be an aromatic ring somehow because it is kind of close to the seven range and the aromatic ring is in that seven area. And I think there are three hydrogens on that, so if we draw that…"

Lane may have gotten the three hydrogens from the integration on that same signal set they were pointing at, but a different interviewee, Kendall, points to the integration specifically and draws fragments from that data alone:

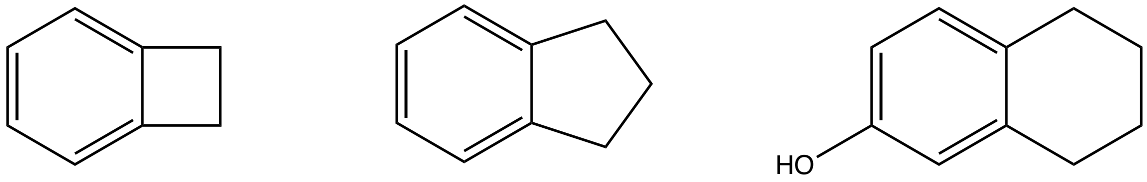
"It's got six hydrogens, so I'm going to say it is two CH_3 groups. If it is not I can change it later."

These students utilize the fragments operator in their solving process, but use different information to develop these molecular fragments. Cartrette and Bodner (2010) found that their more successful participants deduced fragments first and then used that information to draw a whole structure. All of our interviewees happened to deduce fragments from the spectral or molecular information first, but most were unsuccessful in solving the final structure. Overall, the identification of the operator proposing fragments is consistent with Cartrette and Bodner's findings, but how the operator is arrived at or used may influence success in solving. Proposing molecular fragments is a broad operator where students may use it in different ways and to different ends, but the identity of an operator is not tied to where the action specifically resulted from—the operator is that students draw a fragment, not that students draw a fragment from the chemical shift versus the elements of unsaturation. Additional studies could distinguish the process behind operator selection and interpretation.

Constructing whole structures

In constructing whole structures, interviewees attempted to draw a complete structure, not just single fragments. The interviewees constructed many different structures, some correct, many incorrect, but all structures represent different states of problem solving. While the structures themselves represent different states in problem solving, the action of drawing a whole structure represents the operator to get to those states. Unsurprisingly, all of our interviewees attempted to construct whole structures, aligning with the intent of the problem-solving task given. For example, Sydney talks through drawing a series of structures that leads to the correct final structure:

“I want to make a second ring, but that would leave another element of unsaturation. Now I’m going to try two rings combined [draws Structure A in Figure 3.3, erases the alkyl ring then draws Structure B]. [Draws Structure C] Two six carbon rings to see if my Hs work out because that would give two CH_2 groups that overlap.”



Structure A Structure B Structure C

Figure 3.3. The last three structures drawn by Sydney while solving the spectrum from Phase 2B.

Sydney constructed three structures during this time, and no fragments. While constructing a structure is the goal of the overall task in our study and in Cartrette and Bodner's study, even when structures were present as answer choices in the task as in Topczewski, et al. (2017), experts showed evidence of spending time considering how to construct the structure, but novices spent time focusing on the features of all the structures present rather than using the spectral information to come up with the correct structure. These results confirm that constructing a structure is an operator that is useful independent of the task's goal.

The interviews provided insight into the operators students used during the ^{1}H NMR problem-solving process. These operators included calculating and using the elements of unsaturation, proposing molecular fragments, and constructing a structure. Our data confirm and extend prior work by Cartrette and Bodner (2010) and Topczewski, et al. (2017). From this research, we have an understanding of potential operators students use in their problem-solving processes; however, it is not clear from this study which operators, if any, students struggle to use.

Study B

Using the operators we identified from the student interviews, we developed a problem set that targeted each of the operators independently. Problem sets were completed by 558 students from three different universities. Our goal was to determine whether any individual operator posed a significant challenge to students in the problem-solving process. Specifically, we asked:

To what extent do students correctly perform each operator in solving ^{1}H NMR spectroscopy problems?

Methods

Context

This study was done with students from three different public universities. All three universities are land-grant institutions, all with very high research activity. As described in Study A above, University B is located in the upper Midwest, enrolls over 14,000 students, and as a doctoral degree granting university, holds the high research activity classification in the Carnegie classifications (Indiana University Center for Postsecondary Research, 2018). University C is located in the upper Midwest and enrolls about 25,000 students. University C holds the very high research activity classification. University D is located in the southwestern United States and enrolls over 42,000 students. University D also holds the very high research activity classification. All three universities begin their spectroscopy instruction in the second-semester sequence of organic chemistry. The students from University D consisted of non-chemistry majors, while the students from Universities B and C both had a mix of chemistry majors and non-chemistry majors.

The face validity of the operators identified in Study A was verified with three expert organic chemists and then targeted using problem sets. A series of questions were designed to target a specific operator and spectral features that would need to be reasoned with for that operator. The problem sets were piloted in two rounds during the spring and summer semesters of 2014 at University B, with 156 then 57 students, respectively. Upon revision after each semester, three expert organic chemists validated the problem sets. The final version of the problem set was administered to students in the second semester sequence of organic chemistry during the spectroscopy unit at three different universities.

Problem set design

The problem sets were given as a take-home extra credit assignment, with one week allotted for completion. Five points of extra credit were awarded to students that completed the assignment, regardless of the correctness of answers. Table 3.5 below shows the number of participants from each university.

Table 3.5. Total problem set participants from each university.

School	Number of problem set participants	Total students enrolled in the course	Response rate
University B	123	156	79%
University C	231	236	98%
University D	204	326	63%

Each problem set consisted of eight problems, with each item targeting a specific operator. Some questions targeted the same operator, but differed in the task features given to the students to be able to complete that operator (i.e. a student would need to construct a structure from a spectrum and molecular formula in one question, and then construct a structure from a spectrum with given fragments of the whole structure). The questions were designed to be at a level similar to what would be included in class at the institutions and were examined for face validity by three expert organic chemists, two of whom are routine instructors for the course.

From the interviews featured in Study A above, four general operators were identified and the problem set questions were designed to target each of those operators (further details on the operators found is presented below in the results section):

- Calculating the elements of unsaturation
- Proposing bonds from the elements of unsaturation
- Proposing fragments of structures
- Constructing whole structures

Two questions in the problem set were given on the elements of unsaturation. Students needed to calculate the elements of unsaturation (EU) from a given molecular formula and then propose the possible ways to satisfy the calculated EU. One question was given for the proposing fragments operator. Multiple questions on the problem set targeted the operator of constructing a structure, given the many task features available for reasoning with when constructing a structure. We varied the combinations of information available to the students with regard to the spectrum, molecular formula, and fragments. Because the proposing of fragments can be a separate operator, fragments were provided to students in some questions to disentangle the different effects the two operators could have. Likewise, the elements of unsaturation operators are obtained from the molecular formula, and we made the molecular formula available to some questions to separate the effects those operators could have on the task of constructing a structure. When students solve ^1H NMR spectroscopy problems, they are typically given a molecular formula with the spectrum. One question targeted this typical case of solving. One question was given when the students had to solve for a structure from the given spectrum, molecular formula, and fragments for each signal set. Another question was given to solve for a structure from the given spectrum and fragments for each signal set, but no molecular formula was provided. Students were asked to construct a structure that satisfied a given molecular formula and fragments, but no spectrum. Finally, one question was given where students had to construct all possible structures from a given molecular formula, where fragments and a spectrum were both not provided. An annotated problem set with the answers and details on scoring are provided in Appendix B of this dissertation.

Results and discussion

Problem sets were designed around the operators found in the interviews featured in Study A above. Students at three different universities (n=558) completed the problem sets. The combined results for each of the operators is shown in Figure 3.4 below. While students overall could execute each operator, the results vary among the students at different universities and among the different types of questions targeting the same operator. Table 3.6 below shows detailed results for each question by the students at each university and all the students combined.

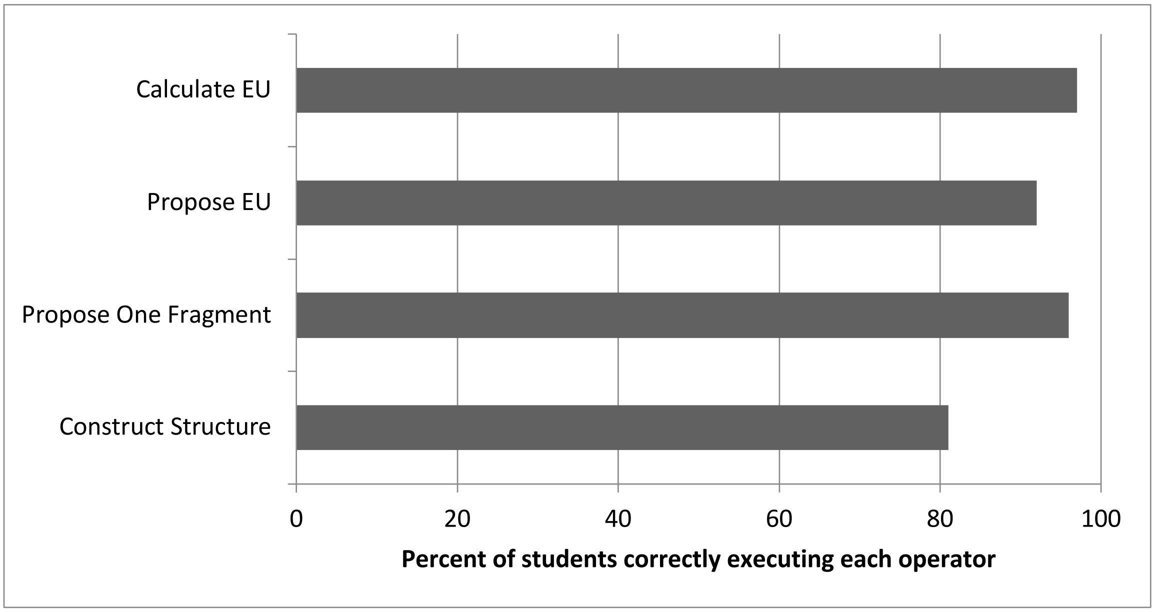


Figure 3.4. Combined results of all students correctly executing the different types of operators.

Table 3.6. Percent of students from each university correctly executing each operator question.

Operator	University B	University C	University D	Combined
Calculate EU	93	99*	96	97
Propose bonds from EU	87*	95	94	93
Propose fragment for each signal set	41***	77	73	68
• Propose one fragment	96	98	94	96
Construct structure—spectrum and molecular formula	92***	99	99	97
Construct structure—fragments, spectrum, molecular formula	65	80**	66	72
• Correct structure or close ester	76	96***	85	88
Construct structure—fragments and spectrum	76***	90	91	87
Construct structure—fragments and molecular formula	78*	87	92	87
Construct structure—All from molecular formula	37***	68	66	61
• Construct one structure	96*	99	100	99

Note: *p<.05, **p<.01, ***p<.001

As shown in Table 3.6, performance from the students at University B was significantly different than the performance of students at the other two universities. Students at University B did not perform as well as the other groups on nearly all problems. Students at University C, however, outperformed students at the other universities on most problems and were significantly better on two of the tasks. This difference in performance at universities similarly comprised of chemistry majors and nonmajors suggests that the instructor and instruction may influence student performance. As we discuss each operator, we will focus on the performance of all participants combined.

Elements of Unsaturation

The two elements of unsaturation questions required students to calculate the number and then propose the types of bonds that could make up that value for the elements of unsaturation. Because the second question relied on correctly answering the first question, both questions were incorrect if the first question was incorrect. As shown in Figure 3.4, the results indicate that the largest number of students executed the elements of unsaturation operators correctly.

One possible explanation of why more students correctly answered these problems is because calculating EU is algorithmic, in that there is an exact computation to use for finding that value and those same steps are applied each time when answering that type of question, with little necessity for reflecting on the conceptual theory behind the calculation itself. The other operator, proposing the bonds from the EU, has only three general types of bonds that are possible, a double bond, triple bond, and a ring, making the answer unambiguous.

Students often possess algorithmic knowledge in chemistry courses, but lack conceptual understanding (Nurrenbern and Pickering, 1987; Sawrey, 1990; Zoller, et al., 1995; Chiu, 2001), as an algorithmic understanding requires only a repetition of what they have seen to be able to execute an action. Algorithmic thinking alone, however, is insufficient for students because they may not be thinking about what they are doing, why they are doing it, or what it actually does for them (Niaz and Robinson, 1993; Pushkin, 1998; Cracolice, et al., 2008). Within the context of solving ^{1}H NMR spectroscopy problems, a potential problem could arise from students not utilizing these operators to their fullest extent—as a tool for narrowing down the possibilities for the compound represented by a spectrum or hypothesizing what could be present. This solely algorithmic use of the elements of unsaturation was observed in the interviews from Study A as well.

With 97% of all students correctly calculating the EU and 93% correctly proposing the types of bonds that would result in the calculated EU, these data suggest students can correctly complete the elements of unsaturation operators. These data do not indicate how students use the operators, and these operators still have the potential to be a source of difficulty in a student's problem-solving process. In the context of ^{1}H NMR spectroscopy problem solving, students can deploy algorithms to extract spectral information, but it is unclear if that information informs students' structural predictions (Stowe and Cooper, 2019). We conclude that students have the procedural knowledge to calculate and propose bonds with the EU, but we do not know if the students can reasonably use that information to inform their structural predictions.

Proposing Fragments

One question was given for the proposing fragments operator. In the proposing fragments question, students were given a spectrum with the number of signals, chemical shift, splitting, and integration all provided. The results show that students can correctly complete the operator of proposing fragments, as 96% of the students from all universities could correctly propose at least one fragment from a spectrum. However, it is important to remember that students were given a full spectrum from which they had four signal sets to make fragment predictions from and 68% were able to propose correct fragments for *each* signal set. While students were able to correctly complete the operators of proposing a fragment, the information they used to find the fragment could lead to incorrect predictions.

As noted in Study A, students can extract information from multiple sources to propose a fragment. For example, our interviewed students used chemical shift values or integration to determine a fragment. From Connor, et al. (2019), we know that students hold assumptions that spectral data should be absolute and believe that the chemical shift values should match the reference material. In our specific problem, the majority of students from each university struggled with the signal set at 3.7 ppm, which was a 2H triplet (a CH_2). This result suggests that students may have found the uncharacteristically downfield chemical shift of the CH_2 as confusing. In relying on the chemical shift alone, a student could think that there is an ether or an alcohol present. Because the effects on chemical shift are additive and students work off of a range of numbers that would be plausible, what they must reason with is unique to the compound and requires reconciling the uncertainties that are part of ^{1}H NMR spectroscopy. While our data suggest that students can propose correct fragments, there may be more that influences the process that leads to successful use of that operator.

Constructing Structures

Multiple questions in the problem set targeted the operator of constructing a structure, given the many possible task features that could be available for reasoning with when constructing a structure. The results from all these questions are shown combined in Figure 3.4 and separate in Table 3.6. With 81% of students constructing correct structures across all five problems, our data suggest that students can correctly complete the operator of constructing a structure.

While the majority of students overall can correctly execute the operator of constructing a structure, there is variation across the problems, which reflects the differences in task features provided. Consistent with Cartrette and Bodner (2010) who found that more successful solvers deduced fragments prior to constructing whole structures, we hypothesized that more students should correctly construct a structure when given fragments for each signal set in the spectrum. We hypothesized that students would be more successful when given the fragments, molecular formula, and spectrum in contrast to getting just the formula and spectrum. The fragments reduced the operators students had to employ prior to constructing a structure, and therefore should have reduced the degrees of freedom of the problem. However, our results do not support this hypothesis. This could be due to the nature of the questions themselves, where the answer to the question with fragments included an ester and the location of the alkyl groups required verification with the chemical shift observed. Those task features made it possible for two answers that would work with the splitting, integration, and number of signals, that only differed in nuances in the chemical shift. Again, Connor, et al. (2019) found that students held incorrect assumptions with the chemical shift. However, if we ignored that potential influence of using chemical shift and counted the close ester as correct, 88% of students constructed a structure when given the molecular formula, spectrum, and fragments. This result with the molecular formula, fragments, and structure is still less than when students were provided with just the molecular formula and spectrum and suggests that there is more at play than the completion of the operators themselves.

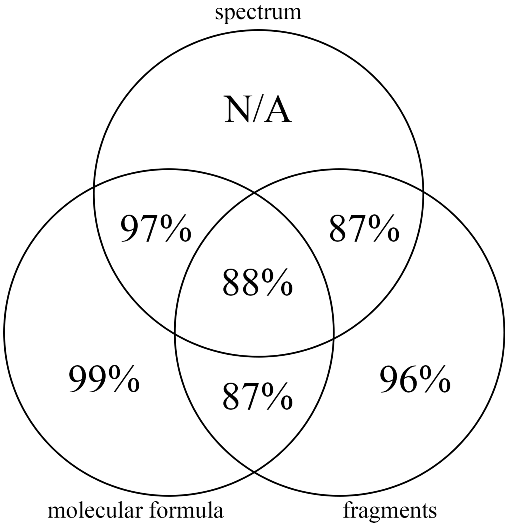


Figure 3.5. Relationship between degrees of freedom involved with the provided task features and student success in constructing structures.

If we explore the relationship between the degrees of freedom and student performance, we would expect to see an inverse relationship: student success increases as degrees of freedom decreases. However, we instead see the opposite: as degrees of freedom increases, students are more successful (Figure 3.5). The degrees of freedom we refer to are the task features students have to interpret and the subsequent steps left in the problem-solving process. When provided with fragments, students no longer have to deduce what those fragments are; those fragments are a certainty. As we move toward the center of Figure 3.5, the degrees of freedom are reduced, where students had more problem-solving features available to them. By having the fragments already determined in the center problem, students did not have to make that interpretation in part of their problem-solving process. When students were given the spectrum and the fragments, but no molecular formula, the percentage of students correctly answering the question was 87%. Again, there are fewer students correctly answering this question than the 97% students correctly answering the question with only the molecular formula and spectrum, and students performed slightly better with constructing a structure when provided with the molecular formula, spectrum, and fragments (88%). Because the performance was comparable on the fragments and spectrum question as with the molecular formula, fragments, and spectrum question, it supports the hypothesis that the presence of the fragments were not necessarily responsible for the difference in performance. Students performed similarly with the fragments and molecular formula question (87%). When given only a molecular formula, 61% of students could construct all possible structures and 99% could construct at least one structure consistent with the molecular formula. Overall, students can correctly execute the operator of constructing structures, but because of the differences in constructing a correct structure among all of the questions and the inconsistency in performance when provided with fragments, these data suggest that there is additional information pertinent to the solving process beyond the successful completion of operators.

General Discussion

Knowing how or when to use an operator

In these two studies, we identified the operators for problem solving with ^{1}H NMR spectra (Study A) and found that most students can successfully perform the operators (Study B). Cartrette and Bodner (2010) found that their successful solvers calculated the elements of unsaturation, and drew fragments in their problem-solving processes. Similarly, a majority of our participants, whether in the interviews of Study A or with the problem sets of Study B, were able to successfully perform these operators. The coupling of our results with Cartrette and Bodner's suggests that the characteristics of less successful solvers may be in knowing *how* or *when* to use the operators.

While we seem to have evidence that students can perform operators, we do not know if they understand why they are using these operators. We have some sense that students are being algorithmic, and not systematic in using the operators. In Stowe and Cooper's study (2019), students possessed the procedural knowledge to extract spectral information. Operators could be functioning similarly to the procedures students were able to perform in Stowe and Cooper's study, where just because students are able to perform a procedure or operator does not mean they know how to use those actions. Moreover, in Topczewski, et al. (2017), their novices looked at all areas of interest in a spectrum instead of making purposeful connections between the answer choices and the spectral features, but the experts came to an answer and then checked their answer. The experts exuded more focus in solving. It is possible that the focus their novices lacked could be explained by not knowing how or when to use operators in solving. Moreover, Connor, et al. (2019) found that students solving processes contained the use of many heuristics. Heuristics like one-reason decision making and generalizations could influence the operators students use instead of using the provided information in meaningful ways to inform operator selection.

Understanding the spectral features behind operators

Inconsistencies in student performance with the same operators, but different spectra suggest that other task features and how students interpret those task features in using an operator are where student difficulties exist. In our interviews, students were found drawing fragments from different spectral features, such as the chemical shift and integration. With the presence of a molecular formula, students were found to even propose fragments from that non-spectral data. How students use these task features to select operators needs to be explored, as the ways in which student interpret spectral features could impact their overall solving abilities.

The presence of fragments should have simplified the solving by reducing the degrees of freedom in the solving process, but our results show that they did not: 97% of students were able to correctly solve the problem with the molecular formula and spectrum while only 88% of students were able to correctly solve or get structurally close to solving the problem with the molecular formula, spectrum, and fragments. If all that is left in the problem-solving process is determining the connectivity of the fragments, do students have adequate practice with splitting, integration, and other spectral features to see the connectivity?

More successful solvers typically perform a final check of their solution after mining the spectral data (Cartrette and Bodner, 2010; Topczewski, et al., 2017), and can directly connect their answers to relevant spectral data. Novices struggle to articulate these connections (Topczewski, et al., 2017), and in fact, students are unable to use their procedural knowledge flexibly enough to form claims supported with the spectral information (Stowe and Cooper, 2019). These arguments and final checks in solving require adequate knowledge of the principles underlying each spectral feature.

Students may not be getting adequate practice with connectivity spectral features, like integration. Textbook practice problems do not provide students with practice on all spectral features equally (Anderson, et al., 2020). Moreover, students hold incorrect assumptions that spectral data should be absolute and that the N+1 rule should hold (Connor, et al., 2019). Students also showed further incorrect assumptions with splitting, the number of signals, and shielding. We conclude that students may know enough to solve simple ^{1}H NMR spectroscopy problems and perform operators, but they may lack the knowledge with specific spectral features that could impact their overall solving abilities.

Conclusions

Operators are the actions students use to move from one state to another. From student interviews, we identified four types of operators that students typically use: calculating the elements of unsaturation, proposing bonds from the elements of unsaturation, proposing fragments, and constructing structures. Further, a majority of students can correctly execute the operators in isolation; however, there is inconsistency in student performance with these same operators, which suggests that something beyond the operators alone is affecting student performance.

The operators we found expand on the characteristics of successful solvers found by Cartrette and Bodner (2010), where successful solvers calculated the elements of unsaturation and drew fragments. Because our undergraduate students were able to perform the operators, we contend that knowing how and when to use these operators more specifically contribute to success in solving. Understanding how students reason with the spectral features, and therefore how they select each operator within their problem-solving processes may provide further insight into student problem solving within the context of spectroscopy.

Limitations and Future Directions

The performance of operators was examined in one question each for calculating the elements of unsaturation, using the elements of unsaturation, and proposing fragments. While we examined over 558 students, our results are constrained to the single questions provided for those operators and discrepancies in performance could be found in other questions of the same type as was found with the constructing structure questions.

Student performance was significantly different on the problems based on the university. While the difference in performance seems to be instructor dependent, we did not examine instruction in this study. Previous studies on ^{1}H NMR spectroscopy solving has focused on the characteristics of solvers (Cartrette and Bodner, 2010; Topczewski, et al., 2017; Connor, et al., 2019; and Stowe and Cooper, 2019), the pedagogical content knowledge of teaching assistants (Connor and Schultz, 2018), and the support of scaffolding in organic chemistry textbook practice problems (Anderson, et al., 2020). Studies have not yet explored instruction of ^{1}H NMR spectroscopy which may have a profound impact on students' solving.

When selecting spectra, we consulted with content experts and course instructors to ensure the problems were at an appropriate level of difficulty for the students. With the different spectra used for each question, we potentially introduced varying levels of difficulty among the questions on the same operator, and student performance could be a reflection of the level of difficulty with the problem. Nevertheless, the difficulty of a problem could be due to the different spectral features in the question, not just on the level of fragments and the molecular formula, but also with the level of the chemical shift, integration, etc. It is necessary to look specifically at the spectral features and inferences to verify if constructing a structure is challenging due to the those provided features. While we did not want structures to be too simple or complex, there is no research indicating what characteristics of spectra and structures lead to the level of difficulty in solving from ^{1}H NMR spectra. Likewise, when different problems have different critical spectral features that can get students the answer, students may be able to solve a problem because they understand the specific critical spectral feature for the problem and lack the flexibility in solving with other spectral features. Future research needs to examine how students reason with the spectral features while solving and how students do or do not use the critical spectral features in their solving.

Implications

Implications for instruction

We showed how student performance may be instructor dependent due to the differences in performance we saw across the three different universities. Instructors should take care in applying what is known from the research on student problem solving with ^{1}H NMR spectroscopy. Likewise, we now know that there are more skills to be developed beyond the characteristics that successful solvers have exhibited before. Students know how to do the basic actions, but may require more instruction and practice to know how to use the operators. Instructors should model for the students how and when to use operators, and how to use the spectral information to influence how the operators are selected.

Implications for research

In our interviews, we found that adapting and using the 3P-SIT for problem solving provided valuable structure to think-aloud interviews. Schönborn and Anderson's (2009) 3P-SIT could be applied to any context in interviewing. In our second study, we saw how different instruction impacted student performance and that shows a greater need to explore how students are taught ^1H NMR spectroscopy. As a majority of our students were able to perform the operators, and therefore the tasks behind some characteristics of successful solvers from Cartrette and Bodner (2010), there is more behind student solving processes. Student performance on different constructing structure problems was inconsistent, suggesting that another area in the solving process, such as the spectral features may be where student difficulties arise. We know students have some incorrect assumptions and they may struggle with connectivity, but further research should examine how students use and interpret the spectral features.

CHAPTER 4. STUDENT REASONING WITH ^{1}H NMR SPECTRAL FEATURES

Introduction

Nuclear magnetic resonance (NMR) spectroscopy is an indispensable tool for chemists in characterizing and analyzing chemical compounds, and this practice of spectral analysis is a routine process in learning organic chemistry (Thomas, 1991). Spectroscopy provides fundamental information on atomic and molecular levels, molecular geometry, chemical bonding, and the mechanisms of chemical reactions (Parker, 1988). Expert chemists are proficient at transforming spectral representations into their respective structural representations (Kozma and Russell, 1997). As a result of NMR spectroscopy's importance to chemists and its vital role in synthesis, interpreting these spectra and identifying unknown compounds with spectra serve as an essential component of organic chemistry education.

Studies on problem solving with ^{1}H NMR spectroscopy all underscore a need to elucidate students' use of spectral features. In interviewing graduate students as they solved ^{1}H NMR spectroscopy problems, Cartrette and Bodner (2010) found that their successful solvers mined the spectral data more thoroughly than their unsuccessful solvers, for example, utilizing coupling constants while deciphering splitting patterns. While Stowe and Cooper's (2019) students were able to mine the spectral data sufficiently enough to correctly match proton environments in their structural predictions with peaks in the ^{1}H NMR spectra when prompted, they found that their students struggled in forming evidence-based claims in their reasoning arguments and did not cite spectral data in those arguments. These studies show that purposeful mining of the spectral data is necessary to the solving process, but students lack fluency with the spectral features.

Successful solvers also check their answers against the spectral data. Topczewski, et al. (2017) observed experts and novices as they solved ^{1}H NMR spectroscopy problems with eye-tracking instrumentation and found that experts performed checks connecting the spectral data with the answer, while novices did not make these connections back to the spectral data. Cartrette and Bodner (2010) also found that successful solvers confirmed their answers with the spectral data, showing that successful solvers could both interpret the spectral data and use it to confirm their answers. From these characteristics of successful solvers we see the actions that set them apart from the unsuccessful solvers, but that does not mean that the unsuccessful solvers do not know how to perform these actions. In fact, from our previous study with the operators students perform in solving ^{1}H NMR spectroscopy problems (see Chapter 3 in this dissertation), we found that undergraduate students could perform the actions of problem solving. The inconsistencies we found in student performance with the same actions, but with different spectra suggested that a disconnect was happening when students were interpreting the spectral features.

There is precedence for why students may struggle to interpret spectral features in ^{1}H NMR spectroscopy. From our previous study, we know that students may not have adequate practice interpreting all spectral features (Anderson, et al., 2020). For example, in the textbooks we sampled, integration was least represented in worked examples and practice problems. Students in the study by Connor, et al. (2019) were also found to hold assumptions that spectral data should be absolute. Some students believed that the N+1 rule should hold at all times. They also found that students held incorrect assumptions on what to observe with splitting, the number of signals, and shielding. Taken as a whole, these studies find that students can do the actions and procedures of making structural predictions from ^{1}H NMR spectra, but there is limited information about how students interpret the spectral features. We do not know whether students know how to use and interpret the spectral features or if they know just enough to ‘get by’. Our goal in the present study is to understand how invalid assumptions impact a student’s solving process and how students interpret spectral features when solving ^{1}H NMR spectroscopy problems.

Research questions

1. What are the task features and inferences students utilize in their problem-solving processes with ^{1}H NMR spectroscopy problems and how well do these task features align with the inferences students made?
2. To what extent do students pay attention to the critical spectral features necessary to solve the problem?
3. What is the relationship between problem solving success and students' use of task features and inferences? How does the presence of correct and/or incorrect inferences impact solving?

Theoretical Framework

Problem solving is fundamental to science and chemistry. "Problem solving is what chemists do, regardless of whether they work in the area of synthesis, spectroscopy, theory, analysis, or the characterization of compounds" (Bodner and Herron, 2002). While problem solving is essential to chemistry, it has been defined broadly and examined in a variety of ways. An often-cited definition of problem solving in chemistry education research states that problem solving is what you do when you don't know what to do (Wheatley, 1984), yet depicting and exploring problem solving is intricate. Problem solving is a complex process, driven by a number of cognitive elements that shape the decisions made by a solver. Consequently, a study of ^{1}H NMR spectroscopy problem solving requires a lens where the researcher can investigate how areas of cognition function in problem solving. Our research is guided by the synthesis of two cognitive theories: problem space theory and the heuristic-analytic theory of reasoning.

Problem space theory provides observable components in the problem-solving process: states and operators

Problem space theory suggests that problems are solved through the search of different paths to a solution (Newell and Simon, 1972). A problem is described as having many states, where one begins at the initial state and seeks to get to the goal state, possibly encountering intermediate states along the way (Figure 4.1). The actions used to move from one state to another are referred to as *operators*. In any given state many different operators can be applied and each of those operators will give rise to other possible states. There may be many possible states and paths in this space, but only a subset may lead to the goal state. People use their knowledge to find a path to the goal state.

Figure 4.1. Model of problem solving, where any number of intermediate states can occur along with the individual operators that lead to those individual intermediate states.

Within the context of solving spectroscopy problems, students begin with a clearly defined goal state (i.e. interpret spectral information to determine a chemical structure) and search the problem space to determine the steps to necessary in getting to that goal state. Problem space theory has the potential to describe the variability in the pathways students take as they navigate towards a solution. In prior research (see Chapter 3 from this dissertation), we identified the operators students used. We also found that students were able to perform the operators, but our research did not discern whether students struggled knowing when or how to use a particular operator.

The heuristic-analytic theory of reasoning depicts the cognitive process underlying the selection of operators in problem solving

While problem space theory describes the more observable states and operators one may go through in encountering a problem, it does not describe why an individual uses any particular operator. Dual-process theories of reasoning attempt to explain the cognitive actions involved in endeavors like problem solving (Evans, 2003, 2008; Stanovich, 2010), and thereby explain why or how an operator is selected. Evans proposed and refined a specific model, the heuristic-analytic theory of reasoning (Evans, 1984, 1989, 2006, 2008; Evans, et al., 2003), to operationalize dual process theories in reasoning tasks. In the heuristic-analytic theory of reasoning, heuristic processes (also called Type 1 processes) begin when the problem solver notices task features that seem relevant (Figure 2). These heuristic processes supply the hypotheses on ways to interpret the problem; analytic processes (also called Type 2 processes) function to critically evaluate these heuristics and modify or replace them if necessary. Analytic processes, however, may or may not be employed due to factors such as cognitive ability and time (Kyllonen and Christal, 1990; Schroyens, et al., 2003; Evans and Curtis-Holmes, 2005; De Neys, 2006, Evans, 2006).

Based on the heuristic-analytic theory of reasoning, a student can examine a ^{1}H NMR spectrum and notice the task feature of a broad singlet and make an inference that the signal means there is an alcohol group. This processing would all be considered heuristic processes if they made the inference automatically. If instead the student began to think hypothetically about that broad singlet and confirm that the peak integrates for one proton and has an appropriate chemical shift, they are evaluating their idea with their analytic processes prior to making their inference. Thus, the heuristic-analytic theory provides a means to describe the ways in which students think about a problem.

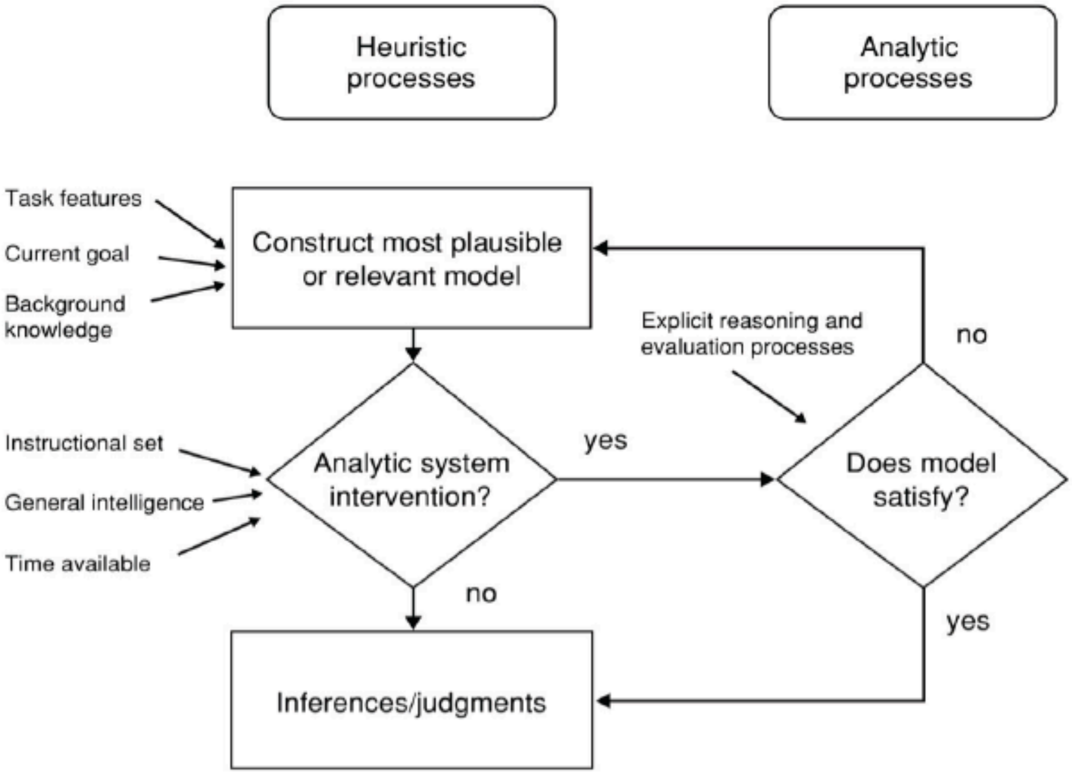


Figure 4.2. Model of heuristic-analytic reasoning (Evans, 2006).

Insight into how students solve spectroscopy problems through merging the problem space theory and the heuristic-analytic theory of reasoning

The heuristic-analytic theory of reasoning helps to explain the cognitive aspect of selecting an operator. When a student begins solving a problem, they start at an initial state, where they must use the given information to make inferences. Heuristic processes interpret the information at that initial state and propose information to become inferences that the analytic processes can evaluate prior to becoming the inference that is carried out. The inferences inform the operators a student chooses. Based on the type of problem given, they may know exactly what the goal state might be (see the Tower of Hanoi problem, where they must get all the rings on a specific side in as little movements as possible) or they may only know some small characteristics that the goal state may have (such as needing to draw some structure from an NMR spectrum that matches the number of atoms indicated in the molecular formula). In order to proceed from that initial state to another state, they must use an operator (the action to move from one state to another). In selecting an operator, reasoning works where something about the initial state (i.e. the features of the task itself, the current goal of the solver, or any available background knowledge) will cue some first impression or idea of what to do—this happens quickly and unconsciously in the heuristic processes.

To better explain the problem-solving process and the selection of an operator through reasoning, the ideas behind the two theories were combined into a model of reasoning and problem solving (Figure 3). Beginning with the initial state, encapsulated by the current state in the model, a solver uses the task features to make a hypothesis toward a solution for the problem. With each task feature, solvers form their hypotheses through their heuristic processes in solving the problem, and may or may not evaluate how those hypotheses play out with their analytic processes before drawing an inference. If they start consciously considering a hypothesis, that hypothesis undergoes analytic evaluation and the solver may determine that the hypothesis would be fruitful and draw their inference, or they may decide their hypothesis will not work and return to the task features or their prior knowledge. They use that new information in adjusting their current goal in forming another hypothesis. Inferences may be carried out as operators, then resulting in the altering of the current state. Not all inferences necessarily lead to an operator; in some cases inferences can further inform the task features or adjust the current goal of the problem, and be reasoned through the heuristic and analytic processes. Likewise, to end the problem-solving process with the goal or final state, one may draw the inference that they are done and analytically check to make sure, or simply have the response that they are done and carry that out as an inference by deciding to make that their endpoint. While we could investigate many components of this framework, we are interested in how students interact with specific task features. The goal of this research therefore focuses on the task features that problem solvers pay attention to and the inferences that they subsequently make.

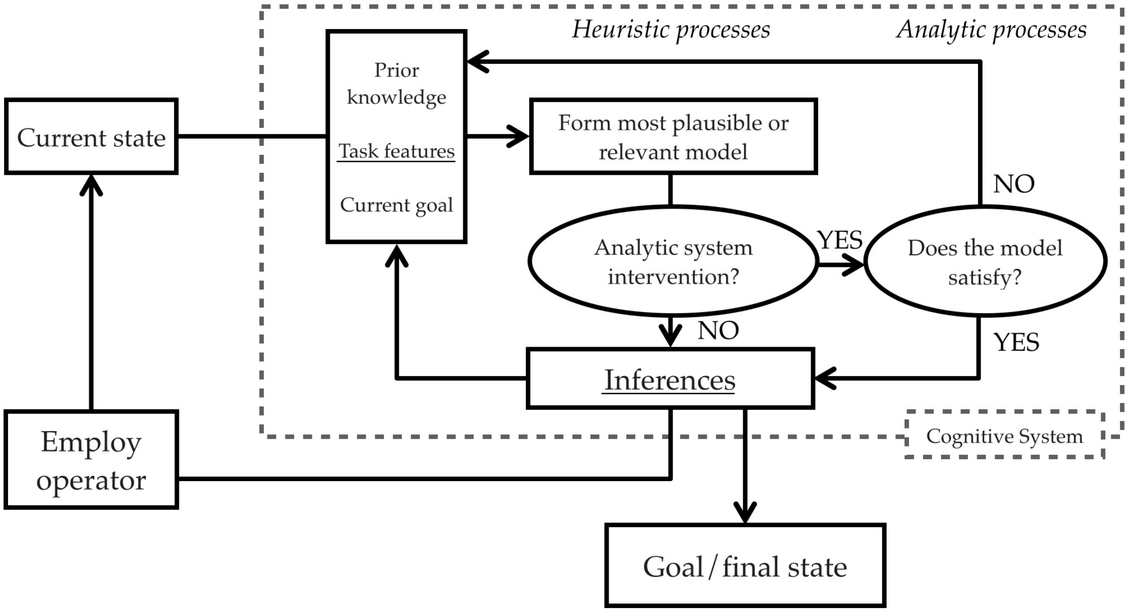


Figure 4.3. Model of the reasoning and problem-solving process. In this study, our focus is on the task features and inferences, underlined in the figure.

Methods

Context

This study was done with students from three different public universities. All three universities are land-grant institutions, all with very high research activity. University B is located in the upper Midwest, enrolls over 14,000 students, and as a doctoral degree granting university, holds the high research activity classification in the Carnegie classifications (Indiana University Center for Postsecondary Research, 2018). University C is located in the upper

Midwest and enrolls about 25,000 students. University C holds the very high research activity classification. University D is located in the southwestern United States and enrolls over 42,000 students. University D also holds the very high research activity classification. All three universities begin their spectroscopy instruction in the second-semester sequence of organic chemistry. The students from University D consisted of non-chemistry majors, while the students from Universities B and C both had a mix of chemistry majors and non-chemistry majors.

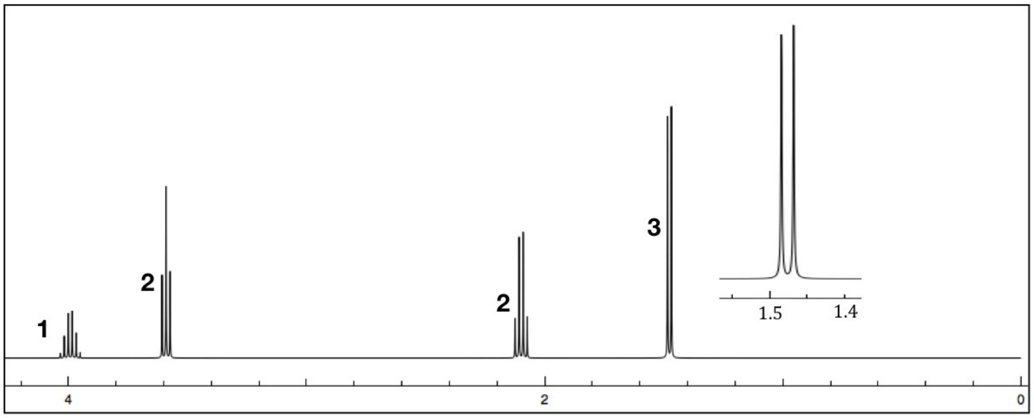
Data collection

Four ^{1}H NMR spectroscopy questions were designed and administered on spectroscopy unit assessments. Two questions were embedded on the unit quiz (Figures 4.4 and 4.5), and two questions were embedded on the unit exam (Figures 4.6 and 4.7). University D did not have any quizzes during that unit and therefore only administered the two exam questions. Students from universities B and C were administered all four questions. Table 4.1 below shows the number of participants from each university who completed each question.

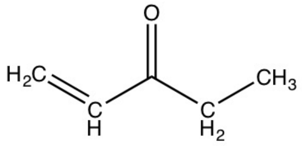
Table 4.1. Number of participants from each university who completed each question.

University	Question 1 (quiz)	Question 2 (quiz)	Question 3 (exam)	Question 4 (exam)
B	156	156	116	116
C	223	223	236	236
D	0	0	323	323

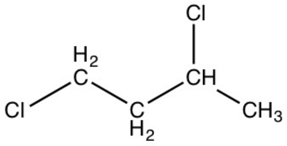
What is the structure of the compound in the ^{1}H NMR spectrum below?



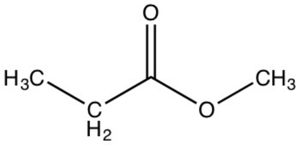
A.



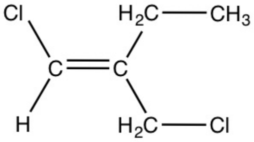
B.



C.

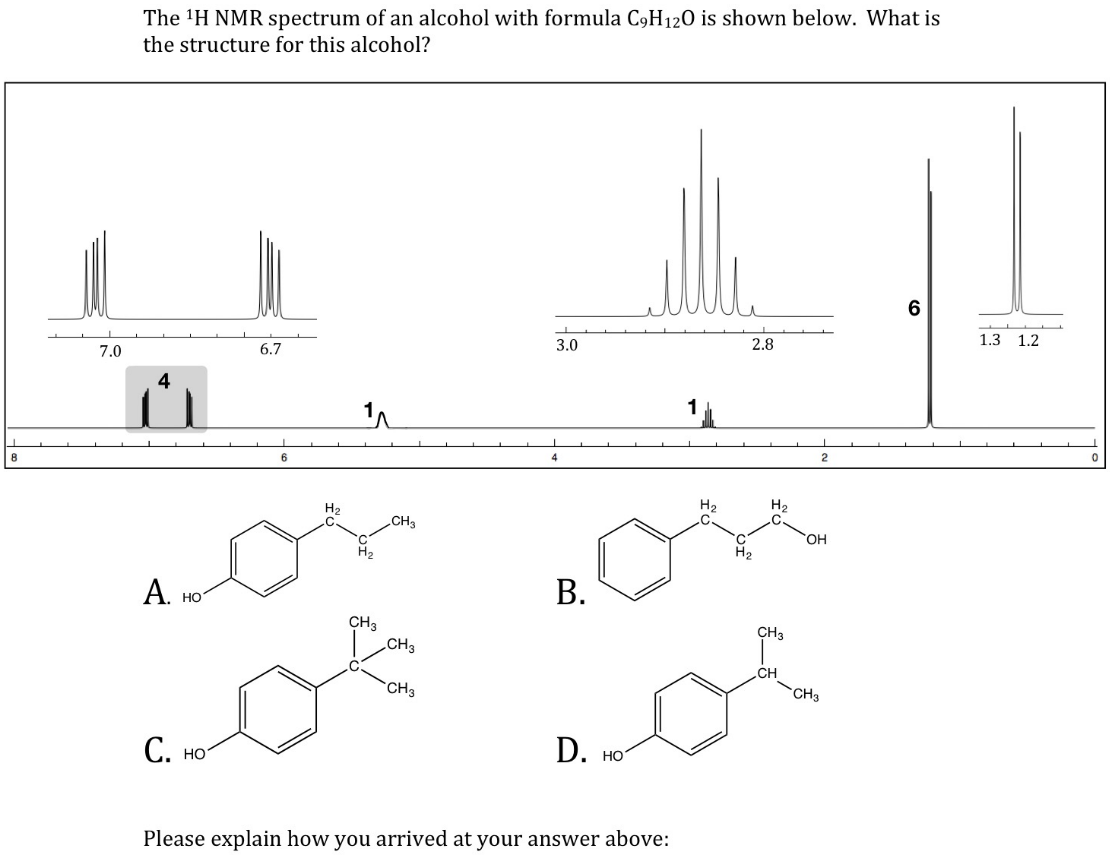


D.



Please explain how you arrived at your answer above:

Figure 4.4. One of the quiz questions given to students at Universities B and C, referred to as "Question 1," where the correct answer is B.

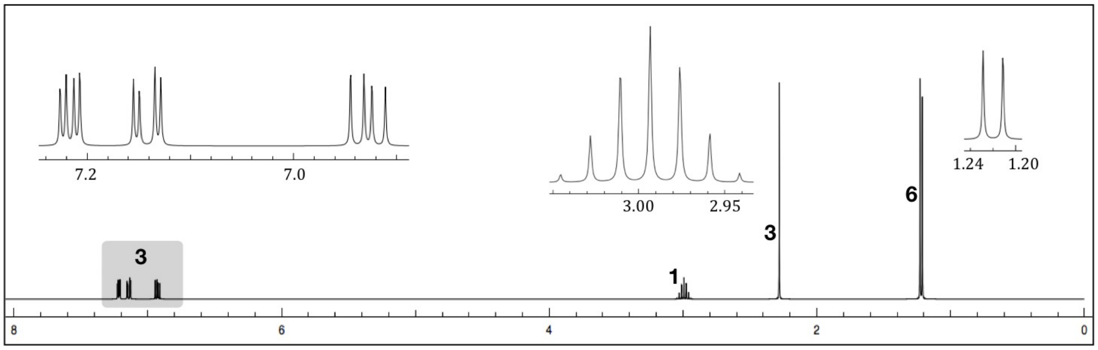


The ^{1}H NMR spectrum of an alcohol with formula $C_9H_{12}O$ is shown below. What is the structure for this alcohol?

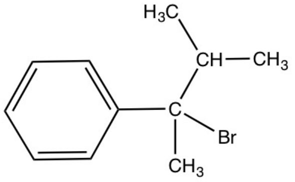
Please explain how you arrived at your answer above:

Figure 4.5. One of the quiz questions given to students at Universities B and C, referred to as "Question 2," where the correct answer is D.

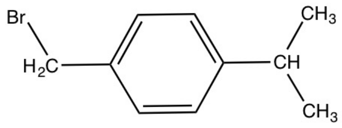
What is the structure of the compound in the ^{1}H NMR spectrum below?



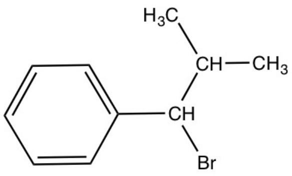
A.



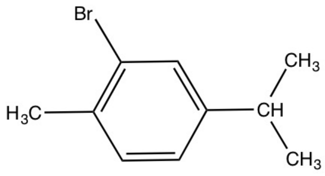
B.



C.

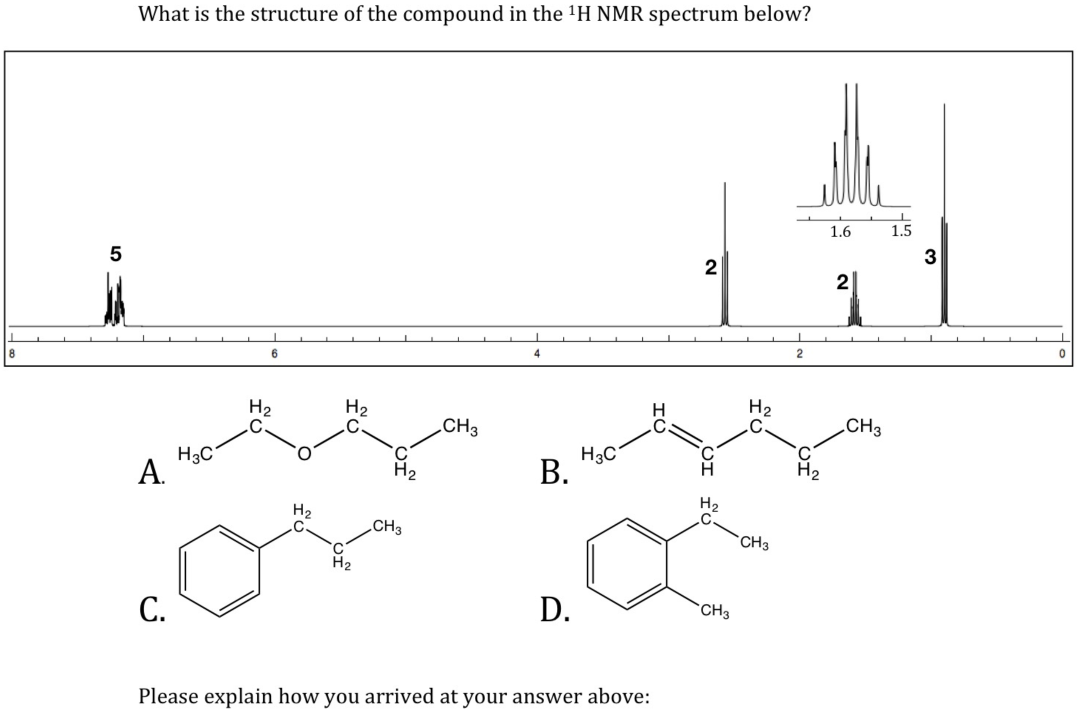


D.



Please explain how you arrived at your answer above:

Figure 4.6. One of the exam questions given to students at each university, referred to as "Question 3," where the correct answer is D.



What is the structure of the compound in the ^1H NMR spectrum below?

Please explain how you arrived at your answer above:

Figure 4.7. One of the exam questions given to students at each university, referred to as "Question 4," where the correct answer is C.

Assessment design

The administered questions were designed as multiple-choice with four options from which students were to select one. Only one option was correct for each question. Students were given a ^1H NMR spectrum, the structures of four possible compounds, and were prompted to explain how they arrived at their answer. The annotated questions can be found in the Appendices C and D in this dissertation.

Interviews with experts were designed retrospectively to further probe the spectral features to which students can pay attention. Three expert organic chemists were interviewed individually to identify if a critical set of spectral features existed that students should pay attention to in correctly answering the problems. The experts were provided with each question in the same format as the students (spectrum and answer choices) and were asked to identify what one would need to pay attention to at a minimum in order to answer the problem correctly. All three experts arrived at the same critical spectral features for each question (Table 4.2). These critical spectral features were used in comparison with the student results, to explore the aspects of solving with the spectral features.

Table 4.2. Critical spectral features determined by experts.

Problem	**Critical set of spectral features**
Question 1 (quiz)	Splitting and Integration
Question 2 (quiz)	Splitting and Integration
Question 3 (exam)	Integration
Question 4 (exam)	Integration and Chemical Shift

Coding

Students' answer choices were recorded and their explanations were inductively analyzed using thematic analysis (Braun and Clarke, 2006). In the first phase of analysis, one researcher became familiarized with the responses, noting ideas on what students paid attention to and what they were inferring. In the second phase of analysis, two initial coding schemes were generated based on the task features students stated they paid attention to and the inferences students made in their explanations. In the third phase of analysis, the coding schemes were developed and refined iteratively among three coders, where a series of response samples were coded independently by the three coders and then discussed. The coding schemes were both revised when consensus was not reached in coding discussions, prompting another sample of responses to be coded under the emerging coding scheme. This process accounted for methods, as prescribed by Krippendorff (2004), to achieve reliable data and improve confidence in the data beyond measured reliability. Krippendorff suggested using three or more independent coders, and for those coders to discuss discrepancies in post-coding deliberations and reach consensus. Once the coding schemes were agreed upon and themes were defined, a sample of 150 responses was used to establish inter-rater reliability in the fourth phase of analysis. Following the calculations as suggested by Lacy and Riffe (1996), shown in Equation 4.1 below, due to their inclusion of the standard error possible with regard to the percent chance agreement that could occur (while others assume that ideally no agreements are made by chance), 97 samples would be the minimum sample size necessary for establishing a coding scheme with a 90% confidence interval. Our sample size was increased to 150 responses to reduce any potential sampling error and strengthen the reliability of the application of the coding scheme to the subset of data. We had 92% agreement and upon reaching consensus in the coding discussions, the remaining responses were coded by a single member of the coding team. Lacy and Riffe's equation calculates the minimum sample size necessary for a reliability check, where n is the sample size for the reliability check, N is the total subjects in the study, SE is standard error (found by dividing the confidence interval at the researcher's acceptable level of probability by the Z score associated with that interval), P is the minimal level of percent agreement acceptable by the research, and Q is 1-P (taking into account the disagreement).

$$n = \frac{(N-1)(SE)^2 + PQN}{(N-1)(SE)^2 + PQ} \qquad \text{(Equation 4.1)}$$

We identified thirteen task features that students identified, including spectral features ("I noticed the integration") (Table 4.3), spectroscopy concepts ("the electronegative atom made me believe…") (Table 4.4), and provided structures (Table 4.5). Tables 4.3-4.5 further describes the codes for each task feature. We did observe instances (n=38) where a student was paying attention to something that was not clearly evident or able to be encapsulated by any task feature codes; we coded these as 'other' (OTH) and did not include them in any analyses.

Table 4.3. The task features coding scheme of the spectral features and descriptions of individual codes. These codes describe the areas of the spectrum students pay attention to.

Code	Description
Chemical Shift (CS)	Students note the location of peaks and/or hydrogens on the scale. In their explanations, students may state the exact numbers (e.g. 6.0 ppm) or general trends (e.g. upfield/downfield).
Chemical Shift Table (CST)	Instances when the chemical shift table is explicitly referenced.
Number of Signals (#S)	Students identify the number of signals in the NMR spectrum, referring to the peak sets, not to splitting. Often these responses describe the different proton groups that these different signals arise from. "Sets of peaks" and "groups of peaks" may also be other ways students describe the number of signals. More than one signal should be mentioned in this case, being sure not to include the times when a student is just using the term "signal" and not drawing on the concept of the number of different signals that appear on the spectrum.
Signals—Other (#O)	Student refers to a number of signals or peaks and it is not clear if they are referring to the splitting or the number of signals.
Integration Number (INT)	Explicit reference of the integration numbers from the spectrum using terms like the "integral" or "integration" when describing the hydrogens to which they are referring. This does NOT include articulating their use of the N+1 rule.
Splitting (SPL)	Students identify the number of peaks within a signal set or reference the multiplicity (e.g. quartet) and/or number of lines.
Number of Hydrogens (#H)	Students identify some number of hydrogens, whether from the spectrum or the structures. They may pay attention to the total number of hydrogens in the structures, or the hydrogens from part of a structure.

Table 4.4. The task features coding scheme on the concepts involved with spectroscopy and descriptions of individual codes. These codes describe the task features that students pay attention to over the concepts and theory involved with ^{1}H NMR spectroscopy.

Code	**Description**
Equivalent Groups (EQ)	Students identify the number of equivalent (or unequivalent) groups in a structure or predict equivalence from the NMR spectrum. Students may also use terminology such as, “different” groups or hydrogens in explaining this concept.
Symmetry (SYM)	Student describes the symmetry within a structure.
Electronegativity (EN)	Students identify parts of the compound or atoms as being electronegative or electron withdrawing.
Shielding (SHL)	Students explicitly identify the shielding effect on groups.

Table 4.5. The task features coding scheme on the provided structures or molecular formula and descriptions of individual codes. These codes describe when student pay attention to the structures that were provided as answer choices or the provided molecular formula.

Code	**Description**
Focus on Non-hydrogen Atom (HET)	Students identify atoms other than hydrogen. Includes instances when students may falsely describe hydrogens in the spectrum as carbons. Students may also identify the number of these non-hydrogen atoms in a structure.
Structure (STR)	The student is paying attention to the structure(s) in the answer options and not the NMR spectrum. Students can match up the spectrum with the structure, but must identify the specific features of the structure to be considered under this code (giving evidence beyond, “this means this”), taking it a step further by identifying that characteristic in the structure(s). Students may mention parts of the structure or defining characteristics of all the given structures from the answer choices. If they notice a specific heteroatom only identified by the given structures, then they had to have looked at the structures. If they cross out answer choices or draw on answer choices, then this code applies as well. **This does not include when students are making inferences about the structure from the spectral information.**

The inferences describe the moments students mention an interpretation of the material, which goes beyond noticing some part of the problem to describe how they are interpreting that portion of the problem. We identified fourteen areas students made inferences on, and they included when students interpreted areas of the spectrum ("the integration at the peak is six, *so there must be six equivalent hydrogens*") (Table 4.6), the concepts on ^{1}H NMR spectroscopy ("this weak signal should be more shielded") (Table 4.7) or thoughts on what they believed should be in the compound (Table 4.8), as fragments or as neighboring groups or atoms ("there should be 2CH_3s next to that group"). Tables 4.6-4.8 below summarize the inferences that emerged from students' written responses. Each inference was also coded on the basis of that inference being correct or incorrect (Table 4.9). Many of the task features and inferences codes can deal with the same concept but they differ in how the student used that information, i.e. a student could pay attention to the splitting in the spectrum by noticing a doublet (splitting spectral feature) and then infer that one of the structures should have a triplet (splitting inference). We did observe instances (n=16) where a student was making an inference on something that was not clearly evident or able to be encapsulated by any inference codes; we coded these as 'other' (OTH) and did not include them in any analyses.

Table 4.6. The inferences coding scheme for the inferences on the areas of the spectrum and descriptions of individual codes. These codes describe the areas of the spectrum that students make inferences on. These inferences predict specific characteristics on what should be present on the spectrum.

Code	Description
Chemical Shift (CS)	Students make the inference that the chemical shift is stronger/further left/further right—or should be somewhere on the scale (upfield/downfield).
Integration (INT)	Students infer that there should be a specific integration. They may describe how something should integrate to a certain number of hydrogens.
Number of Signals (#S)	Students infer the number of peaks that the structures should show in the NMR spectrum. Students may discuss that the spectrum should have some specific number of sets of peaks.
Number of Other (#O)	This code applies when it is not clear whether or not the student is making an inference on the number of signals or the number of peaks in a splitting pattern. Students often vaguely referred to a number of peaks that should be there.
Splitting (SPL)	Students make an inference of what the multiplicities of peaks should be. They may say that there should be a triplet, or quartet, etc.

Table 4.7. The inferences coding scheme for the inferences on the concepts underlying ^{1}H NMR spectroscopy and descriptions of individual codes. These codes describe the inferences made on the areas of the spectrum or provided structures with regard to specific concepts involved in the greater theory behind ^{1}H NMR spectroscopy.

Code	Description
Equivalent Groups (EQ)	Students infer the number of equivalent (or unequivalent) groups that should be in a structure or predict equivalence from the NMR spectrum. Students may also use terminology such as, “different” groups or hydrogens in explaining this concept.
Symmetry (SYM)	A student makes an inference on the symmetry that should be within a structure.
Electronegativity (EN)	Students infer that there should be parts of the compound or atoms that are electronegative or electron withdrawing.
Shielding (SHL)	Students explicitly make an inference on the shielding effect that should be present with groups.

Table 4.8. The inferences coding scheme for the inferences on the structure of the compound represented and descriptions of individual codes. These codes describe any inferences made on certain parts of the goal structure, where students predict atoms, neighboring groups, fragments, or hydrogens that should be present.

Code	**Description**
Non-hydrogen Atom (HET)	Students make inferences that there should be specific kinds of atoms other than hydrogen. Students may also make inferences on the number of these non-hydrogen atoms that should be in a structure.
Structural—Fragment (FRA)	The student makes the inference that a functional group, atom, or an incomplete part of a compound should be present. This is not from just looking at the structures in the answer choices. They may explain how certain types of bonds should be present as well (i.e. there should be a double bond).
Structural—General Neighbors (GNEI)	Students infer that there should be a general number of hydrogens neighboring.
Structural—Specific Neighbors (SNEI)	Students make an inference that there should be specific groups neighboring (CH_2, instead of 2 hydrogens).
Hydrogens (non-neighboring) (HY)	Students make an inference on a number of hydrogens that does not reference that they are neighboring hydrogens. If the student talks about hydrogens that should be there, but does not mention where or what they are next to, then this code applies—but this code is not to be used every time.

Table 4.9. The inferences coding scheme for the correctness of individual inferences and descriptions of individual codes. These codes describe the results of the students' reasoning.

Code	**Description**
Correct Inference	The inference made is consistent with the correct answer to the question.
Incorrect Inference	The inference made is not consistent with the correct answer to the question or is made with the incorrect use of the spectral feature.

Data analysis

For the third research question, SAS version 9.4 (SAS Institute Inc, 2013) was used to run logistic regression analyses to determine how each task feature and inference impacted the outcome of answering the question correctly. Logistic regression is used to predict the outcome of a binary dependent variable based on multiple independent variables (Menard, 2002). These independent variables can be continuous or binary, but in the case of this study the independent variables are binary. Correctly or not correctly answering the question is the dependent variable, Y, with the value of 1 representing the desired outcome of correctly answering the question and 0 representing the outcome of not answering the question correctly. The following equation shows the probability of occurrence of the outcome event as a function of the independent variables: $Y=\beta_0 + \beta_1X_1 + \beta_2X_2 + \ldots + \beta_KX_K$, where β_0 is constant and X_K are the independent variables. The β_K coefficients describe the relationship between each independent variable and the student's outcome of correctly answering the question. A positive coefficient shows the independent variable is linked to an increase in the odds of success, while a negative coefficient shows the independent variable is linked to a decrease in the odds of success (Hosmer and Lemeshow, 2000). Odds ratios are also generated for each independent variable, where the odds of an event is the probability of an outcome event occurring divided by the probability of the event not occurring. Odds ratios greater than 1.0 show an increase in odds and odds ratios less than 1.0 show describe a decrease in odds (the inverse relationship). In predicting the outcome of a certain dependent variable based on a series of independent variables, a model (based on the equation described above) is generated from the results of the analysis. The goodness of fit of the model describes how accurately the model classifies the data, while the R^2 in the case of logistic regression describes to what extent the model predicts the outcome (not just in the context of fitting the data). In the case of this study, Hosmer and Lemeshow's (1980) goodness of fit was used to determine the accuracy of each model, and Cox and Snell's (1989) R^2 was used to describe the predictive power of the models. Acceptable p-values from Hosmer and Lemeshow's goodness of fit should be greater than 0.05 to support the null hypothesis that the model has a good fit.

Results and Discussion

What are the task features and inferences students utilize in their problem-solving processes with ^{1}H NMR spectroscopy problems and how well do these task features align with the inferences made?

The percent of students denoting they paid attention to the task features in solving ^{1}H NMR spectroscopy problems were compared with the inferences students made on each question (Figure 4.8). Students seemed to pay attention to all spectral features and make inferences from all spectral features. This is consistent with Topczewski, et al. (2017), where novices paid attention to all points of interest. Students pay attention to the chemical shift and splitting spectral features most, regardless of the question. However, students do not always indicate that they made an inference from chemical shift. Chemical shift was one of the critical spectral features for Q4 and it appeared as a task feature identified by students most in that question, but the percent of inferences for chemical shift in that question were similar to the other questions. Spectral features like chemical shift function well in checking procedures, but students may not engage in checking procedures (Cartrette and Bodner, 2010; Topczewski, et al., 2017). Students could also be using the chemical shift to make inferences on fragments.

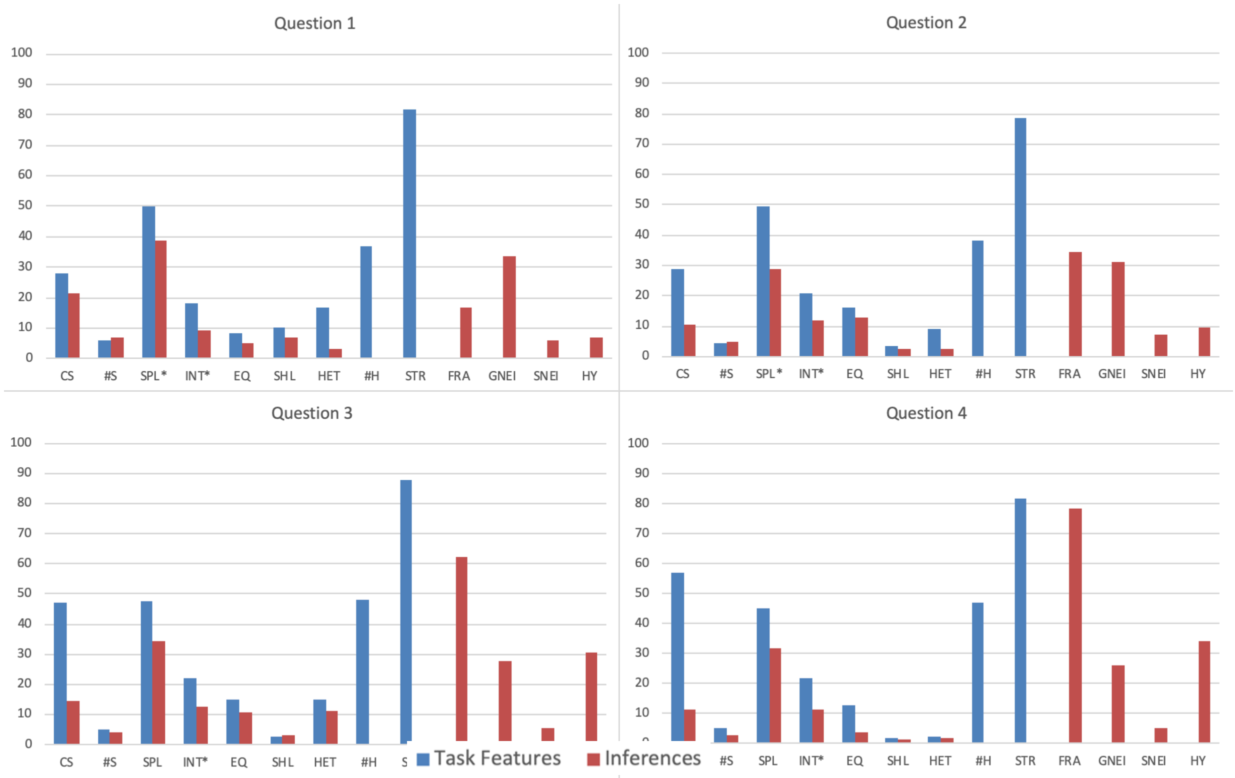


Figure 4.8. Comparing the percent of students paying attention to the specified task features with the percent of students making the corresponding inference on each question. Critical features are denoted with an asterisk. Codes appearing in less than 5% of the responses and codes classified ‘other’ were omitted from this figure.

The task features and inferences were generally aligned, with students making less inferences from those task features, but there are a number of other inferences that could be made that are not necessarily tied to one task feature. Students not making as many inferences on the spectral features as they notice is consistent with Stowe and Cooper (2019), where their students were able to complete the procedures in solving, but did not reference spectral data in their reasoning. Likewise, because splitting is tied to a procedural process, the N+1 rule, students may know how to use this information more than other spectral features and this could be why students notice splitting the most of the spectral features. Additionally, similar to Topczewski, et al. (2017), where their novices paid attention to the structures, most of our students (>70% on each question) mentioned the answer structures in their reasoning. Because so many students look to the structures in their reasoning, it seems that providing structures could prevent students from reasoning with the spectral information as much as we as researchers and instructors would hope for.

To what extent do students pay attention to the critical spectral features necessary to solve the problem?

The results from the task features coding were examined to determine how much the students paid attention to the critical features and how they subsequently performed on each question. Table 4.10 below shows how many students pay attention to the critical features for each question. A majority of students (41.9%-71.7%) did not indicate they paid attention to the critical features identified by experts, and they still answered the question correctly. Perhaps students were guessing. This could be similar to Stowe and Cooper (2019), where students could perform the problems, but did not include spectral evidence in their arguments. Students may not think to cite that spectral information and may not recognize that the information is critical.

Table 4.10. Comparison of the frequency of students identifying the critical features with their performance on the questions. The percent of total students under for each category are noted in italicized font below the frequencies.

Critical set of spectral features identified	Question answered incorrectly	Question answered correctly	Total
Panel A. Identification of critical features on Question 1			
No	74	253	327
	19.5%	*66.8%*	
Yes	1	51	52
	0.20%	*13.5%*	
Total	75	304	379

Critical set of spectral features identified	Question answered incorrectly	Question answered correctly	Total
Panel B. Identification of critical features on Question 2			
No	67	253	320
	17.7%	*66.8%*	
Yes	1	58	59
	0.20%	*15.3%*	
Total	68	311	379

Critical set of spectral features identified	Question answered incorrectly	Question answered correctly	Total
Panel C. Identification of critical features on Question 3			
No	242	283	525
	35.9%	*41.9%*	
Yes	35	115	150
	5.2%	*17.0%*	
Total	277	398	675

Critical set of spectral features identified	Question answered incorrectly	Question answered correctly	Total
Panel D. Identification of critical features on Question 4			
No	88	485	573
	13.0%	*71.7%*	
Yes	4	99	103
	0.60%	*14.7%*	
Total	92	584	676

How do we get students to notice what is critical and why? If they don't notice the critical feature, then according to our model and consistent with the results in the first research question, they do not make inferences on those features. Nearly all students that indicated that they paid attention to the critical features answered the questions correctly. On Question 3, 35 (5.2%) of the students indicated that they noticed the critical feature (integration) but did not answer the question correctly. Noticing features is a start, but it is not enough to make a structural prediction—that requires an inference. Students may not be making inferences, or they may not be making correct inferences. Question 3 could also be more challenging because it relies on only one critical feature. It is possible that students may not fully understand what is fruitful from the integration or they may not understand how to interpret the integration. Compared with Figure 4.8, about 20% of students noticed the integration regardless of the question.

If we couple our results with the eye tracking study by Topczewski, et al. (2017), novices notice all points of interest in a spectrum, so there likely is not a problem in noticing the critical features. The problem is in evaluating the spectral features to determine which are critical to the problem-solving process. Students need to learn how to discern what is critical in a spectrum, so they can later make inferences from that information.

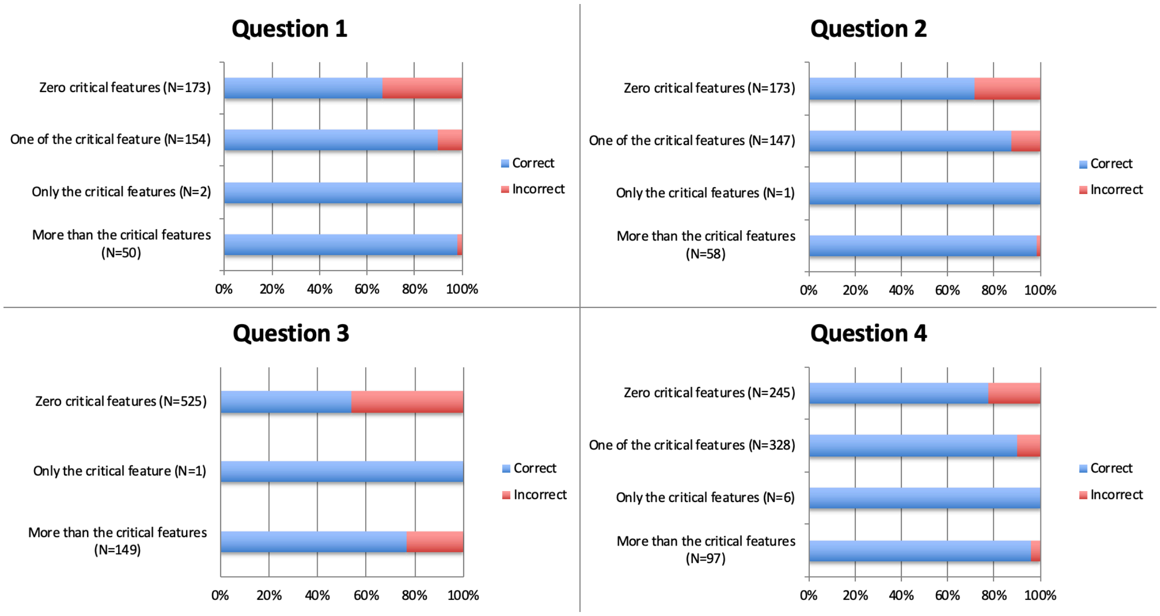


Figure 4.9. Comparison of the amount of critical features students indicated they noticed with question performance.

On all of our questions, most students identified no critical features in their reasoning (Figure 4.9). Of those students that failed to indicate any of the critical features, 20-40% answered the questions incorrectly. A higher percentage, 85-90%, of students that indicated that they paid attention to one critical feature answered the questions correctly than those that indicated none of the critical features. Helping students notice critical features would be beneficial.

In only ten instances, students identified only the critical feature(s). All those students were able to answer the questions correctly. There are not enough cases to definitively say that this is the best route, but if we consider those that noticed more than the critical features and the results from Topczewski, et al. (2017), where novices noticed everything, students need a more focused solving path. It is not necessarily better to notice more. If students processed all the things they noticed, it could lead to a high load on working memory capacity. It seems that students would benefit from more practice with the spectral features to build fluency in noticing what is critical to solving the problem and why. This is consistent with the recommendations from Anderson, et al. (2020, see Chapter 2 in this dissertation).

What is the relationship between problem solving success and students' use of task features and inferences? How does the presence of correct and/or incorrect inferences impact solving?

Binary logistic regression analysis was conducted to examine what task features and inferences predicted success. Tables 4.11-4.14 show the results from the logistic models for each question.

Table 4.11. Estimated regression coefficients and odds ratios from binary logistic regression for Question 1. The Hosmer and Lemeshow's goodness of fit test showed the model had a p-value of 0.5296, showing the accuracy of the model is acceptable and in a test on the data the model was able to correctly predict the outcome for Question 1 82.84% of the time. The R^2 for the model's predictability was 0.2426, indicating that 24.26% of the variation in the dependent variable is explained by the model.

Coefficient	**Estimate**	**SE**	***p* Value**	**Odds Ratio Estimate**
Intercept (β_0)	-0.55	0.23	0.0186	NA
University C (β_1)	1.40	0.33	<0.0001	4.0
Splitting Task Feature (β_2)	0.97	0.36	0.0078	2.6
Integration Task Feature (β_3)	1.33	0.59	0.0256	3.8
Splitting Inference (β_4)	2.30	0.47	<0.0001	10.0
General Neighbors Inference (β_5)	1.04	0.39	0.0092	2.8

In Question 1, university was a significant predictor of success, as students in the organic chemistry course at University C were four times more likely to answer correctly than students in the organic chemistry course at University B (only Universities B and C did the first two questions). This result suggests that instruction impacts success on this quiz question. Students that identified paying attention to the splitting were 2.6 times more likely to answer the problem correctly than those that did not, and students that identified paying attention to the integration were 3.8 times more likely. Students that made inferences on the splitting were ten times more likely to answer the question correctly, and students that made inferences about general neighbors were 2.8 times more likely to answer the question correctly than those that did not. These task features present, integration and splitting, are the critical features identified by experts for this question.

Table 4.12. Estimated regression coefficients and odd ratios from binary logistic regression for Question 2. The Hosmer and Lemeshow's goodness of fit test showed the model had a p-value of 0.7719, showing the accuracy of the model is acceptable and in a test on the data the model was able to correctly predict the outcome for Question 2 82.85% of the time. The R^2 for the model's predictability was 0.1928, indicating that 19.28% of the variation in the dependent variable is explained by the model.

Coefficient	**Estimate**	**SE**	***p* Value**	**Odds Ratio Estimate**
Intercept (β_0)	-0.25	0.24	0.2976	NA
University C (β_1)	0.82	0.31	0.0099	2.3
Splitting Task Feature (β_2)	1.17	0.34	0.0007	3.2
Number of Hydrogens Task Feature (β_3)	1.42	0.38	0.0003	4.1
Splitting Inference (β_4)	1.30	0.47	0.0059	3.7
General Neighbors Inference (β_5)	1.46	0.51	0.0040	4.3

In Question 2, university was still a significant predictor of success, with students from University C 2.3 times more likely to correctly answer the question. Splitting and the number of hydrogens task features were both significant predictors of success, and both align with the critical features as the number of hydrogens can be an indirect reference to the integration, but this claim is limited, as the students do not explicitly mention the term integration. Students that made inferences on splitting were 3.7 times more likely to answer the question correctly and students that made inferences on the general neighboring groups were 4.3 times more likely to answer the question correctly.

Table 4.13. Estimated regression coefficients and odd ratios from binary logistic regression for Question 3. The Hosmer and Lemeshow's goodness of fit test showed the model had a p-value of 0.5653, showing the accuracy of the model is acceptable and in a test on the data the model was able to correctly predict the outcome for Question 3 70.66% of the time. The R^2 for the model's predictability was 0.2393, indicating that 23.93% of the variation in the dependent variable is explained by the model.

Coefficient	**Estimate**	**SE**	***p* Value**	**Odds Ratio Estimate**
Intercept (β_0)	-0.49	0.16	0.0027	NA
Splitting Task Feature (β_1)	-0.42	0.19	0.0259	0.7
Integration Task Feature (β_2)	1.05	0.24	<.0001	2.9
Fragment Inference (β_3)	0.47	0.18	0.0111	1.6
Non-neighboring Hydrogens Inference (β_4)	2.62	0.29	<.0001	13.8

In Question 3, an exam question, university was not a significant predictor of success. Splitting was a negative significant predictor of success in this question, with students paying attention to the splitting being slightly less likely to answer the question correctly. Splitting as a negative predictor makes sense as the doublet, septet splitting pattern applies to three out of the four answer choices. These results suggest that while critical features seem to aid in solving, paying attention to other task features that are not essential to answering the problem correctly could lead to selecting an incorrect answer. When considering cognitive load, focusing on one task feature that is not in the critical set could distract students and increase that cognitive load when they realize that the information they are focusing on may not eliminate answers, taking up their time and impeding their solving process. This is consistent with the suggestions from Topczewski, et al. (2017). Students could also be making inferences that are not correct from the splitting, or they may not have any other definitive evidence to go off of in their answer choice. Except for the aromatic region, splitting patterns for all signal sets would have been the same in three of the answer choices.

Integration was a significant predictor of success, as students paying attention to that task feature were 2.9 times more likely to answer the question correctly than those that did not pay attention to the integration. Inferences on fragments and non-neighboring hydrogens were both significant predictors of success. Fragments as a predictor of success is consistent with the results from Cartrette and Bodner (2010), as they found that their successful solvers wrote out fragments in their solving processes. Inferences on non-neighboring hydrogens refer to the number of hydrogens represented by the peaks, which could be an indirect inference on the integration, but again is limited by the lack of a direct reference. Both the task feature and inference related to integration as predictors align with the single critical feature for the question, the integration.

Table 4.14. Estimated regression coefficients and odd ratios from binary logistic regression for Question 4. The Hosmer and Lemeshow's goodness of fit test showed the model had a p-value of 0.9256, showing the accuracy of the model is acceptable and in a test on the data the model was able to correctly predict the outcome for Question 4 88.61% of the time. The R^2 for the model's predictability was 0.2771, indicating that 27.71% of the variation in the dependent variable is explained by the model.

Coefficient	**Estimate**	**SE**	***p* Value**	**Odds Ratio Estimate**
Intercept (β_0)	-0.02	0.35	0.9463	NA
Integration Task Feature (β_1)	2.10	0.63	0.0009	8.2
Splitting Inference (β_2)	1.87	0.41	<.0001	6.5
Non-neighboring Hydrogens Inference (β_3)	2.58	0.76	0.0007	13.2

In Question 4, university again was not a significant predictor of success, which means for the quiz questions university was a predictor for success, but was not for the exam questions. This could suggest that instruction and the instructional activities matter for formative assessments like quizzes, but we also had a difference in population with the students between the quiz and exam. University D was added for the quizzes. If we look back at performance on our operators problem sets (see Chapter 3 in this dissertation) with the students at Universities B, C, and D, students at University B performed significantly worse on multiple problems in the problem set, while students at University C performed significantly better on two of the problems. Students at University D performed in between the other two universities on all but two problems in the problem set. Performance from students at University D could have lessened a disparity between Universities B and C.

The integration task feature and non-neighboring hydrogens inference were again significant predictors of success, aligning with one of the critical features. Making an inference on splitting also showed to be a predictor of success, with students being 6.5 times more likely in answering the question correctly if they made an inference on splitting. Chemical shift was a critical feature, but was not a significant task feature as a predictor of success. As we saw in Figure 4.8, 57% students identified chemical shift as a task feature they noticed, but only 11% made an inference on chemical shift in their explanations. Students may not know what fruitful inferences can be made with chemical shift, and they may not know what makes the chemical shift a critical feature.

While most critical features are predictive of success on each question, the independent variables that have the highest odds ratio estimates for each question is an inference. As discussed earlier, the critical features are significant predictors of success in problem solving, but the inferences play a larger role. Students need to use the information. When considering our theoretical model of problem solving and reasoning, these results suggest that the task features could be important to the solving process as they dictate what inferences are possible, but the nature of those inferences and perhaps how they are used later on determine one's success in solving spectroscopy problems.

The overall results from the regression modeling suggest that the critical features alone are not sufficient for successful solving. Students must interpret the information on the spectrum, and as with Stowe and Cooper (2019), students need to build fluency with the spectral features to make these interpretations. The inferences seem to result from the critical features as well. When considering the theoretical model of problem solving and reasoning with spectroscopy, the task features are important because they dictate the inferences that are made (especially if they are not analyzed by the solver's explicit processes), as those inferences have the highest odds ratios found in the regression modeling. The nature of those inferences could play a role as well.

Even if students make inferences on the critical set of spectral features, those inferences may not be correct. Incorrect inferences could also impede or negatively impact students' solving processes. Tables 4.15-4.18 below show the correct and incorrect inferences made, and whether or not students answered the questions correctly.

Table 4.15. Frequencies for correct and incorrect inferences and answers for Question 1.

Presence of correct and incorrect inferences	**Question answered incorrectly**	**Question answered correctly**	**Total**
No Inferences	18 *4.82%*	35 *9.38%*	53
Only Correct Inference(s)	15 *4.02%*	257 *68.9%*	272
Only Incorrect Inference(s)	18 *4.83%*	2 *0.54%*	20
Correct and Incorrect Inferences	23 *6.17%*	5 *1.34%*	28
Total	74	299	373

Table 4.16. Frequencies for correct and incorrect inferences and answers for Question 2.

Presence of correct and incorrect inferences	**Question answered incorrectly**	**Question answered correctly**	**Total**
No Inferences	22 *5.93%*	34 *9.16%*	56
Only Correct Inference(s)	3 *0.81%*	266 *71.7%*	269
Only Incorrect Inference(s)	25 *6.74%*	1 *0.27%*	26
Correct and Incorrect Inferences	14 *3.77%*	6 *1.62%*	20
Total	64	307	371

Table 4.17. Frequencies for correct and incorrect inferences and answers for Question 3.

Presence of correct and incorrect inferences	**Question answered incorrectly**	**Question answered correctly**	**Total**
No Inferences	34 *5.12%*	15 *2.26%*	49
Only Correct Inference(s)	37 *5.57%*	340 *51.2%*	377
Only Incorrect Inference(s)	53 *7.98%*	4 *0.60%*	57
Correct and Incorrect Inferences	152 *22.9%*	29 *4.37%*	181
Total	276	388	664

Table 4.18. Frequencies for correct and incorrect inferences and answers for Question 4.

Presence of correct and incorrect inferences	**Question answered incorrectly**	**Question answered correctly**	**Total**
No Inferences	17 *2.57%*	21 *3.16%*	38
Only Correct Inference(s)	7 *1.05%*	536 *80.7%*	543
Only Incorrect Inference(s)	29 *4.37%*	2 *0.30%*	31
Correct and Incorrect Inferences	35 *5.28%*	17 *2.57%*	52
Total	88	576	664

As would be expected, with the correct and incorrect inferences, greater than 90% of students that made only correct inferences answered each question correctly. Likewise, 90% or more of the students that made only incorrect inferences did not correctly answer each question. These results support the notion that the nature of the inference in terms of correctness plays a role in students' solving processes. A majority (67-84%) of the students making both correct and incorrect inferences also do not answer the questions correctly, suggesting that recovering from an incorrect inference could prove challenging. With regard to the theoretical model, incorrect inferences could potentially feed back into the model in many directions, leading to an incorrect fragment proposed, or an incorrect assumption feeding into the goals of the problem thereby cueing a student to ignore one vital area of information and set their attention elsewhere, or an incorrect inference could feed back into the model as a task feature from which further incorrect inferences are made. Nevertheless, 16-30% of the students making both correct and incorrect inferences still answered the questions correctly, suggesting that it is still possible to recover from an incorrect inference, though less likely. There is a possibility that some of these correct answers could have resulted from guessing, but they could also result from incorrect inferences being made on areas of the spectrum not in the critical set and not affecting the solver's final decision making. This shows how invalid assumptions, like those found in Connor, et al. (2019), can impact student solving.

Even though greater than 90% of the students that made only correct inferences answered the questions correctly, there were still 1-10% of the students answering those questions incorrectly. These results suggest that merely making inferences that are correct is not enough, especially if those task features do not aid the student in choosing their answer. Inferences need to further students' solving, covering more than general declarative information, and result from fruitful task features, such as the critical spectral features.

Conclusions

In our model, we proposed that inferences emerge from task features. Aptly, students did not make as many inferences as the number of spectral features they noticed. Similar amounts of students noticed the spectral features regardless of the question and different critical features. It is possible that when spectral features do not have clear procedures, like with the N+1 rule, students may not know how to interpret the information and thereby use it less. It could also be that because students notice and use the spectral features similarly across different questions, students know how to interpret the spectral features individually, but may not know how to use all the features together.

Overall, students need to develop fluency with spectral features and need to understand how experts prioritize critical features in solving. A majority of students identified none of the critical features in their reasoning explanations. Our previous study (Anderson, et al., 2020) provides suggestions on how to develop fluency with spectral features. Likewise, we found that integration was least practiced among spectral features in the practice problems in that previous study. In our present study, students struggled with Question 3 the most, a problem where integration is the sole critical feature. In the expert view of integration, do we neglect the notion that there could be challenges in interpreting this spectral feature and believe it is easy to interpret when compared with the other spectral features? It may be necessary for students to get more practice with all spectral features, including integration.

Our regression analyses showed that inferences had the highest odds ratios in predicting success. Instruction should model how to make inferences when solving. This takes solving a step further from noticing spectral features. Students may not have enough practice using the spectral information to make predictions or inferences. Even when students made a mixture of correct inferences with incorrect inferences, a majority still answered the questions incorrectly. Invalid assumptions like the ones identified in Connor, et al. (2019) matter and need to be addressed in the classroom.

Limitations and Future Directions

While we were able to examine 2108 different responses, some claims are limited because we do not know if students were guessing, due to the multiple-choice design. It is possible students could have chosen correct answers despite holding incorrect inferences because they made the right guess. Likewise, it is possible students guessed correctly even when they did not pay attention to the critical features. Future studies could study how students understand the critical features through categorization tasks with experts.

Although the questions we administered were different, we discovered post-administration that they had similar critical features. As a result, we did not ask questions that explored how students interpreted the number of signals, though some answer choices required using knowledge on the number of signals. The spectral features should be examined more, perhaps in an interview setting. There are some instances where we could not confidently code a response as referring to the integration when they indicated a number of hydrogens and from where students made their inferences on the fragments. Students could be using inferences more than can be conveyed in their written responses.

We observed that University C was a significant predictor of success, but we do not know much about the students themselves to be able to say if they were similar populations or not. Likewise, instruction at all three institutions was unable to be observed, limiting the ability to pinpoint the differences between the different groups in the overall population and instruction. Instruction of spectroscopy needs to be explored.

Implications

Implications for instruction

Students need support in noticing the critical features of ^{1}H NMR spectra and knowing how to interpret those features. Students need practice in making inferences so they can develop the fluency necessary to understanding the limitations with certain interpretations, such as knowing if the integration reflects the amount of hydrogens shown or is a ratio of what is shown on the spectrum. Because we observed how making incorrect inferences could impact student performance, students need opportunities for feedback on the inferences they are making, not just the results of finding a structure.

Implications for research

Based on this research, we have several suggestions for improving instruction, yet evidence-based instruction is needed. As a start, research should explore the current state of ^1H NMR spectroscopy instruction. Additionally, we developed a model of problem solving that provided insights into student problem solving of ^1H NMR spectroscopy. We believe this model could apply to other problem-solving contexts. The model offers ways to consider what students may be doing and thinking, and provides key areas that can be examined including operators, problem states, task features, and inferences.

CHAPTER 5. CONCLUSIONS

The goal of this dissertation research was to examine how students learn about and solve ^{1}H NMR spectroscopy problems. I accomplished this research goal by investigating how students could interact with the spectral features, what the operators were for a solver to move from one state to another in ^{1}H NMR spectroscopy problem solving, and the nature of inferences students made when reasoning with the task features in solving.

I investigated the ^{1}H NMR spectral features presented in worked examples and practice problems across four undergraduate organic chemistry textbooks, and examined the frequency and ordering of spectral features to explore how the textbooks could support scaffolded instruction. Spectral features like the number of signals and chemical shift were covered by problems more frequently, while integration was covered least. Our findings suggest that textbooks do not provide sufficient practice with all ^{1}H NMR spectral features. I observed no discernible pattern in how textbooks ordered spectral features of ^{1}H NMR spectroscopy in problems, indicating that there is little systematic method to the design of textbook chapters and limited support for scaffolded instruction.

From think-aloud interviews, the operators students use in solving ^{1}H NMR spectroscopy problems were identified: calculating the elements of unsaturation, proposing bonds from the elements of unsaturation, proposing fragments, and constructing structures. From the results of those interviews, problem sets were developed to investigate how well students could use the operators. I observed that students can perform operators, but it remains to be seen if students know how and when to use the operators. Student performance was different with the same operators, but different spectra, indicating that these inconsistencies could be attributed to students' interpretations of the spectral features. Our findings suggest that students may know enough to solve simple ^{1}H NMR spectroscopy problems and perform operators in isolation, but they may lack the knowledge with specific spectral features that could impact their overall solving abilities.

A series of ^{1}H NMR spectroscopy problems were designed and administered to investigate the task features identified and the inferences made by organic chemistry students while solving. I found that a majority of students identified zero of the expert-identified critical spectral features in their reasoning explanations. Regression analyses revealed that the inferences students made contributed most to success in structural predictions, and a majority of students made solely correct inferences in their reasoning explanations. When a mixture of correct and incorrect inferences were made, a majority of those students were unable to answer the questions correctly. Our findings indicate that students will require considerable support in deciphering the critical features in ^{1}H NMR spectroscopy problems and developing robust, correct inferences across diverse examples with all spectral features.

Implications for Instruction

Instruction matters in learning spectroscopy and I showed how student performance was instructor dependent in this dissertation research (see Chapters 3 and 4). Based on prior studies (Connor, et al., 2019; Stowe and Cooper, 2019) and the results of this dissertation research, I recommend organic chemistry instructors place focus on the four main spectral features involved in undergraduate problem solving (the number of signals, chemical shift, splitting, and integration). Students need help building appropriate interpretations of the spectral features and this could be accomplished through scaffolded instruction, where instructors take special efforts to model their expert reasoning to students. Instructors should help students recognize and identify the critical spectral features, allowing students to develop problem-solving processes that offload aimless procedural approaches, in favor of developing expert-like focus (see Topczewski, et al., 2017). Moreover, instructors should consider what spectral features are being measured in their formative and summative assessments. Based on the textbooks I examined, the onus of scaffolded instruction with the spectral features relies on the instructor. Problems may not be designed well enough to know how students are doing, as a student with poor interpretation skills with most spectral features could get by if questions primarily focus on the spectral feature they can interpret. If an expert such as an instructor does not notice when students cannot develop robust interpretations from the problems they assign, how then can we expect a student to have the metacognition to recognize what they are missing?

Instructors should also contemplate their goals in spectroscopy education. If the desire is for students to develop their interpretations of the spectral features, then task features like chemical shift tables and molecular formulae may not be appropriate at all times. Furthermore, problems should challenge the typical interpretations students make. Our students struggled with an integration of three hydrogens in the aromatic region. Some students had not considered an aromatic ring to be tri-substituted because any example they were accustomed to involved mono-substituted aromatic rings. Invalid assumptions like believing the N+1 rule should always hold (as seen in Connor, et al., 2019), such as with alcohol protons or in pi-bonded systems, can also be addressed by exposing students to those spectra. Assessments and instructional activities should also directly examine student inferences of spectral features. For example, ask students what the splitting of a specific signal set indicates to them.

My research has provided a bigger picture of the reasonable recommendations that can be made from education research on teaching ^{1}H NMR problem solving. While Cartrette and Bodner (2010) suggested instructors teach students consistent problem-solving approaches, where they should draw molecular fragments, there is more to the story. Our research with operators showed that students could propose molecular fragments from ^{1}H NMR spectra, but when given the fragments ahead of time, students did not perform better than without the fragments (with different spectra). While there are individual spectral features attributed to the problems, students' abilities with connecting fragments could be an issue. Students can accomplish the procedures (Stowe and Cooper, 2019) and may have the pieces of the puzzle, but can they put it together? When ^{1}H NMR spectroscopy is explained and assessed according to the individual spectral feature (as I found in the textbooks), students may not build the skills necessary to putting a whole compound together. In the textbooks I examined, only a couple of books provided even a single worked example that put all the spectral features together to show how to make structural determinations from start to finish. Instructors should use scaffolding techniques to show students how to build connections across the spectral features, and provide students with problems that interleave the critical features.

Implications for Research

Even though I examined an aspect of instruction through the presentation of ^{1}H NMR spectroscopy in organic chemistry textbooks, and Connor and Shultz (2018) examined the pedagogical content knowledge of teaching assistants on teaching NMR spectroscopy, research remains to explore how NMR spectroscopy is taught. From my studies, we know that spectroscopy instruction varies across instructors. What does spectroscopy instruction look like? There is theoretical basis for the instructional strategies I suggest, in terms of scaffolding, blocking, and interleaving, but the impact of these strategies on ^{1}H NMR spectroscopy problem solving is yet to be explored.

As an example, going into my first interviews, I had ideas of what made a harder ^{1}H NMR spectroscopy problem. Researchers have some idea of what spectra and compounds are challenging or easy (Cartrette and Bodner, 2010; Topczewski, et al., 2017; Stowe and Cooper, 2019), but no one has explored the characteristics of ^{1}H NMR spectra that make problems more difficult. When students were to construct structures with varied task features in our operators study, student performance declined with spectra that contained more signal sets. Do more signal sets contribute to problem difficulty, as there is more to interpret and connect? I discussed the irregularities in spectral features earlier: how do irregularities in spectral features or unfamiliar types of structures impact student performance?

Finally, the idea of critical spectral features appeared in our studies (Anderson, et al., 2020; Chapters 1 and 3 in this dissertation), and while the extent to which students mention those features in their reasoning arguments was observed, it is not known how students view the utility of these critical spectral features. Researchers should provide an intersection between the difficulties in solving students exhibit with the critical features, and should utilize categorization tasks to examine characteristics of novice and expert solvers in distinguishing critical features in ^{1}H NMR spectra.

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APPENDIX A. INTERVIEW PROTOCOL FOR STUDY 2

1. Phase 1(20-30 minutes, without any spectra):
    a. Think about organic spectroscopy and chemistry. Take your time and tell me what you are thinking about.
    b. What do you know about organic spectroscopy? Be as specific as you can be.
    c. Describe what you know about NMR spectroscopy?
    d. *Meanwhile, they will be asked to clarify and define terms in their own words.
    e. Are you satisfied with your explanations? (If no, why not? If yes, move on)
2. Phase 2 (30-40 minutes, with NMR spectrum they must solve the structure for): What are you thinking about as you solve for the structure? What are you focusing on?
    a. PART A (Give the NMR for isopropyl alcohol)
        i. Let's see if you can show me what you've just explained.
        ii. Looking at this spectrum, talk me through all the concepts you've explained as you solve for the structure.
        iii. Typical questions in this phase tend to be: what are you thinking now, why are you doing that, explain to me what you get out of that spectral feature you are focusing on now, etc. I'll ask questions to make sure they're still verbalizing their thoughts as they solve and then I'll have them clarify what they mean and why they do the things they do. The goal is to see if they change any conceptual ideas they mentioned earlier in Phase 1 before seeing the spectrum, and to see if they are focusing on surface features of the spectrum or if they have specific reasoning behind what they focus on. Once they've come to a

        structure, I will challenge them to see how certain they are and why they are or are not certain.

        iv. Once they are set on their structure, move to Part B.

    b. PART B (Give the NMR for 5,6,7,8-tetrahydro-2-napthol)

        i. Use same line of questioning as Part A.

        ii. Once they are set on their structure or decide to give up, move to Phase 3.

3. Phase 3 (15-20 minutes, after NMR interpretation): As you solved for the structures during the second phase, were you confused about anything on the spectra?

    a. Is there anything on the spectra in particular that you don't understand or find confusing?

    b. Consider yourself a diagram designer or textbook author. If you could change the spectra in any way, what would you do to improve it, if anything?

    c. Do you think this is a good and clear representation? Give reasons for your answer.

    d. I have other spectra for the same compound…

        i. Here's some additional data. Take a look at them and tell me if you are more or less confident with your solution.

        ii. Here's some additional data that may help you come to an answer. Take a look and see if you can get any further.

        iii. Comment on these types of spectra in general, and your feelings on interpreting them.

APPENDIX B. PROBLEM SET FOR STUDY 2

1. Calculate the degrees of unsaturation for the formula below, and list all the possible types of bonds you might expect for the degrees of unsaturation you calculated.

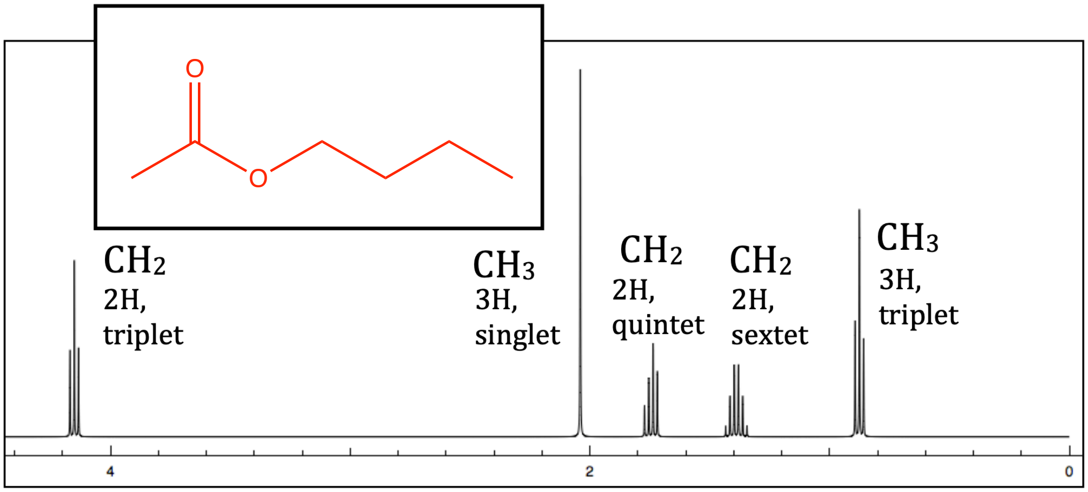
Molecular formula: $C_6H_{10}O_2$

Degrees of unsaturation: ________ *2EU, This question was scored as correct or not.*

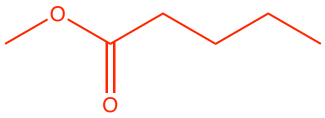
List the possible ways to satisfy your calculated degrees of unsaturation: *This question was open ended, so the answer was counted as correct if students drew structures containing two double bonds, one triple bond, two rings, and one ring and a double bond. Drawing those bond combinations in absence of a structure was also considered correct.*

2. In the designated box, draw the structure of the compound represented by the ^{1}H NMR spectrum below. Note the scale of the spectrum (in ppm) and the given molecular formula.

Molecular formula: $C_6H_{12}O_2$

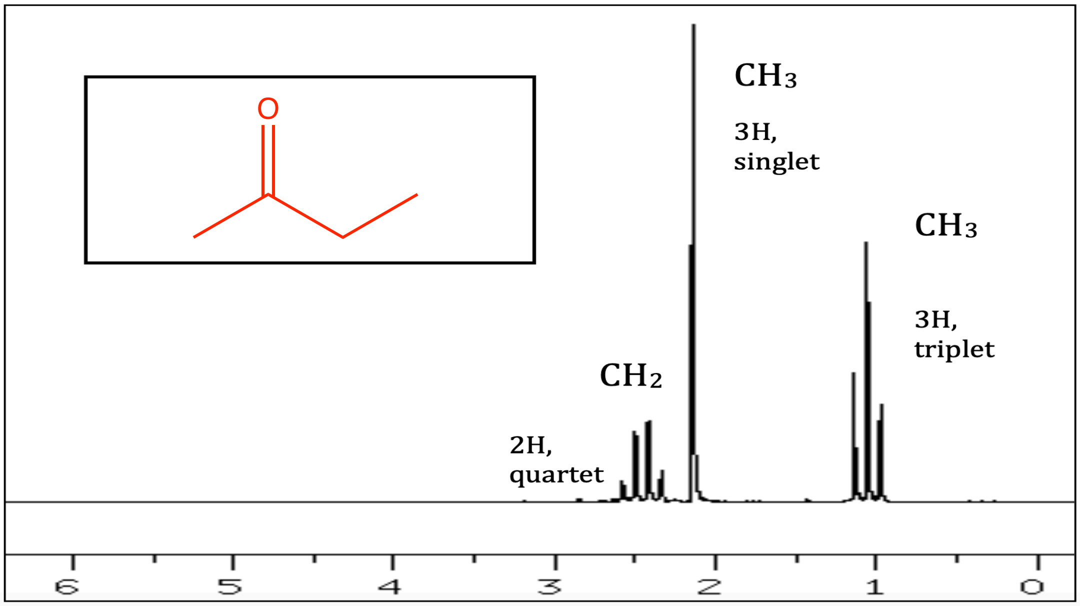


This question was scored as correct if the structure shown in the box was drawn. Students with the close ester shown below were also noted separately. We chose to count the close ester, as students showed that they were able to construct a structure that could satisfy the molecular *formula, fragments, and most of the spectrum, save the chemical shift of the atoms by the ester carbonyl and oxygen.*



Close ester

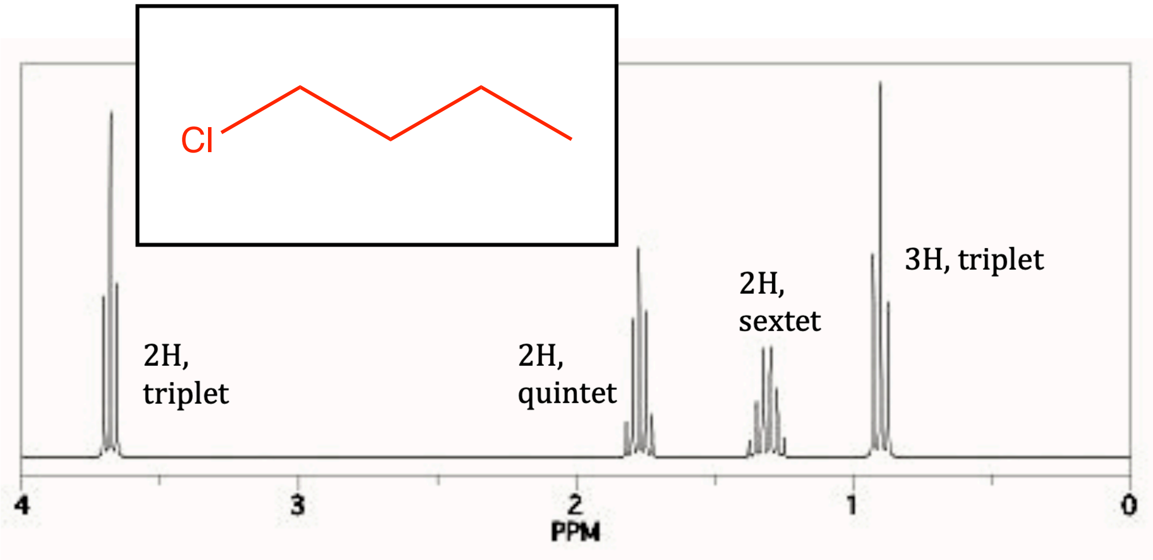
3. In the designated box, draw a whole structure from the provided molecular fragments and ^{1}H NMR spectrum. Note the scale of the spectrum (in ppm).



This question was scored as correct if the structure shown in the box was drawn.

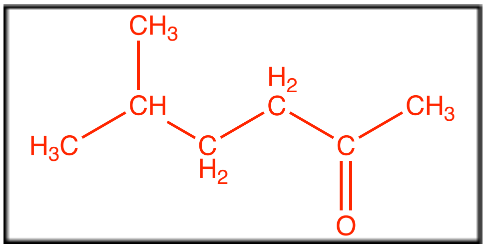
4. In the designated box, draw a whole structure from the ^{1}H NMR spectrum. Note the scale of the spectrum (in ppm) and the given molecular formula.

Molecular formula: C_4H_9Cl



This question was scored as correct if the structure shown in the box was drawn.

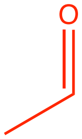
5. In the designated box, draw one possible whole structure from the following information: The molecular formula of the compound is $C_7H_{14}O$, and you know for certain that you have 3 CH_3 groups, 2 CH_2 groups, and 1 CH group in the compound.

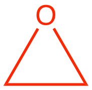


This question was scored as correct if any structure drawn satisfied the fragments and molecular formula. An example is shown in the box above.

6. In the space below, draw all the possible structures from the following molecular formula:

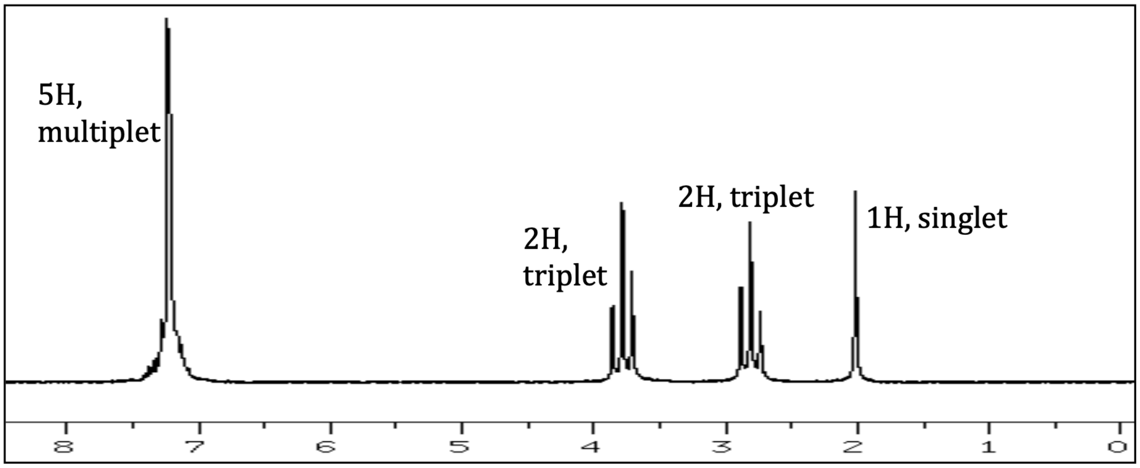
C_2H_4O





This question was scored as correct if all structure shown above were drawn. Because our intent was to see if students were able to just execute the operator, we counted students that had any of the above structures as well.

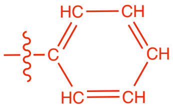
7. Given only the spectrum below, list **all possible** fragments for each set of peaks. Note the scale of the spectrum (in ppm).



1H, singlet at 2.1 ppm: OH, CH, O=C-H, NH

2H, triplet at 2.8 ppm: CH_2, 2CH

2H, triplet at 3.7 ppm: CH_2, 2CH

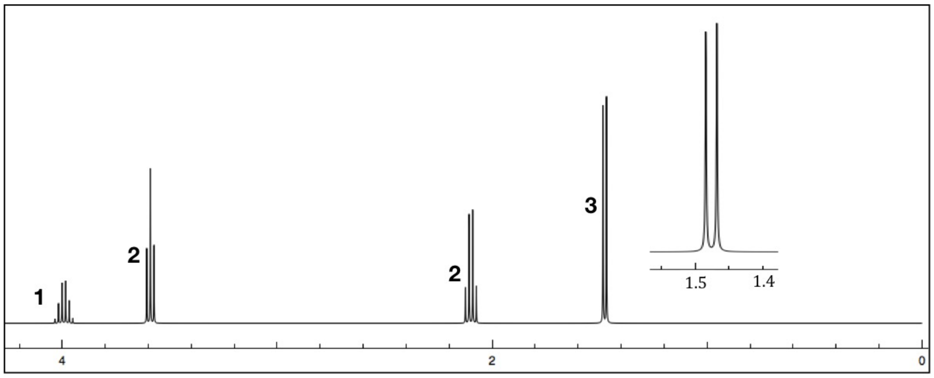
5H, multiplet at 7.2 ppm: 

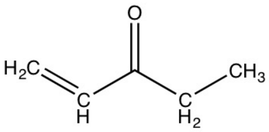
While the prompt asked for all possible fragments, we wanted to discern if students could execute the operator and propose any fragment. The question was counted as correct if any of the fragments above were proposed.

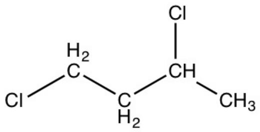
APPENDIX C. ANNOTATED QUIZ QUESTIONS FOR STUDY 3

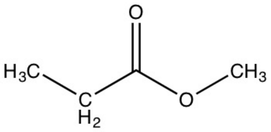
Question 1

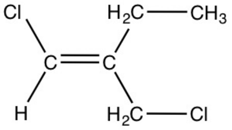
What is the structure of the compound in the ^{1}H NMR spectrum below?



A.


B.


C.


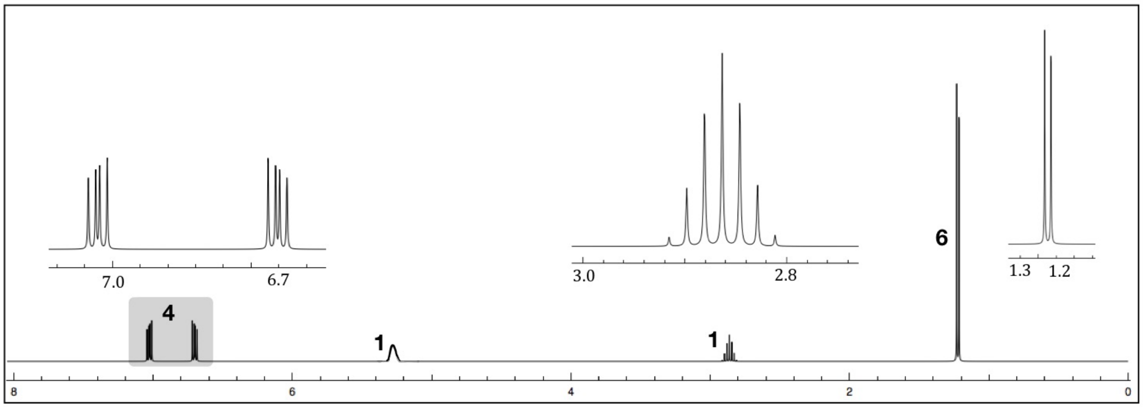
D.


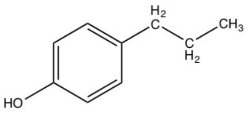
Please explain how you arrived at your answer above:

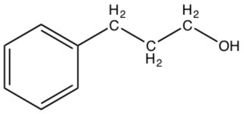
- *The correct answer is B, and the critical features were determined to be the splitting and integration.*
- *In answer A, the compound would exhibit different splitting patterns due to the ^2J coupling in the alkene protons.*
- *In answer C, the compound does not have the correct number of signals, and is therefore missing a signal set. Splitting would also not match the ester CH_3. Chemical shift would also differ.*
- *In answer D, the compound would not exhibit the correct splitting patterns.*

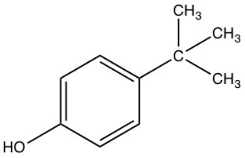
Question 2

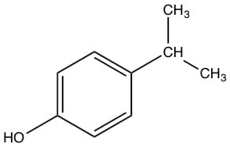
The ^{1}H NMR spectrum of an alcohol with formula $C_9H_{12}O$ is shown below. What is the structure for this alcohol?



A.


B.


C.


D.


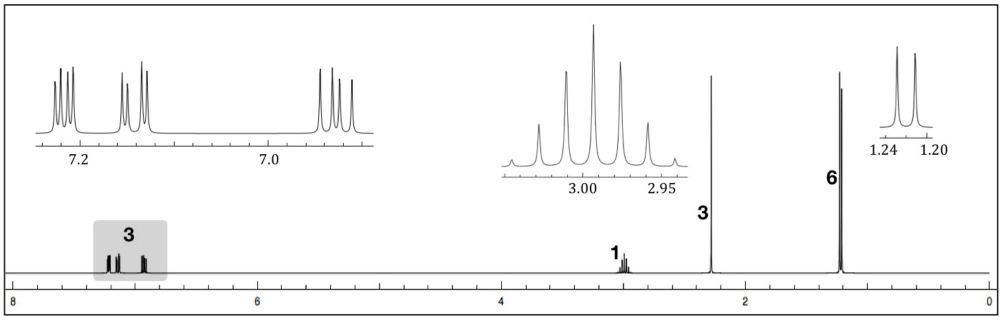
Please explain how you arrived at your answer above:

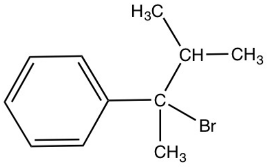
- *The correct answer is D, and the critical features are splitting and integration.*
- *In answer A, the compound would exhibit different splitting patterns for the alkyl protons and would exhibit a different number of signals.*
- *In answer B, the compound would not give rise to the integration of the aromatic ring, as well as the splitting. This compound would also have a different number of signals.*
- *In answer C, the compound would not exhibit the correct splitting patterns or number of signals, as well as the resulting integration.*

APPENDIX D. ANNOTATED EXAM QUESTIONS FOR STUDY 3

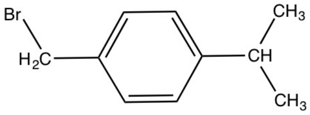
Question 3

What is the structure of the compound in the ^{1}H NMR spectrum below?

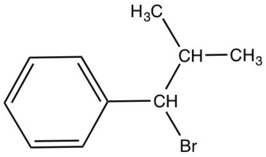




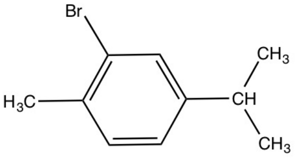
A.



B.



C.



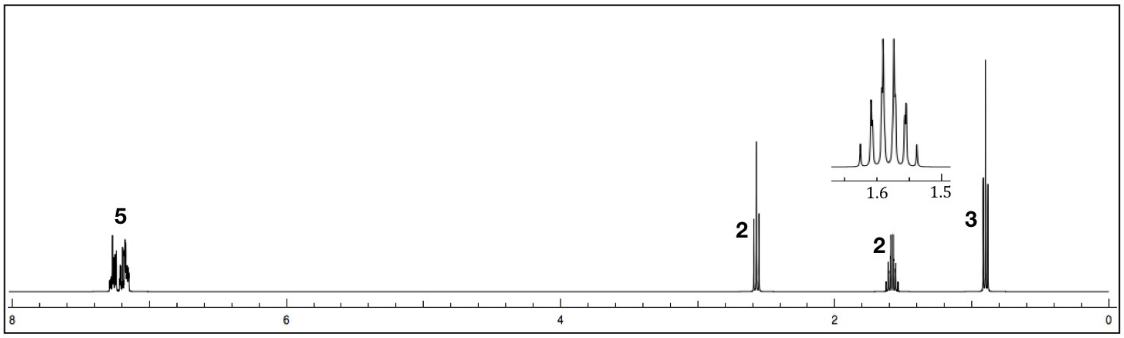
D.

Please explain how you arrived at your answer above:

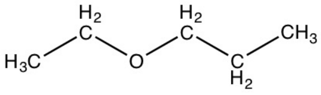
- *The correct answer is D, and the critical feature is the integration.*
- *In answer A, the compound would exhibit incorrect integration for the aromatic group. The chemical shift would also be slightly different.*
- *In answer B, the compound would not give rise to the integration of the aromatic ring. The integration of the* CH_2 *is not present, and that group would likely shift further downfield.*
- *In answer C, the compound would not exhibit the correct integration of the aromatic ring. The splitting would also be incorrect, as well of the chemical shift of the CH neighboring the bromine.*

Question 4

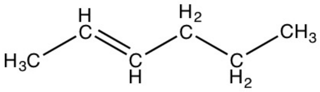
What is the structure of the compound in the ^{1}H NMR spectrum below?



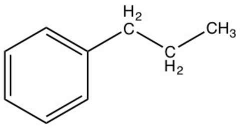
A.



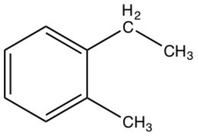
B.



C.



D.



Please explain how you arrived at your answer above:

- *The correct answer is C, and the critical features are the integration and chemical shift.*
- *In answer A, the compound would exhibit more signals than in the spectrum. The compound also would not have the same chemical shift. The integration is also incorrect.*
- *In answer B, the compound would not give rise to the chemical shift observed in the aromatic region (as with answer A). The splitting would also differ, as well as the integration and number of signals.*
- *In answer D, the compound would not exhibit the correct splitting patterns or number of signals, as well as the resulting integration. The integration is incorrect for the aromatic region, as are the splitting patterns for the alkyl groups.*