JOURNAL OF RESEARCH IN SCIENCE TEACHING VOL. 47, NO. 6, PP. 643–660 (2010)

Non-Mathematical Problem Solving in Organic Chemistry

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Received 30 November 2005; Accepted 18 March 2009

Abstract: Differences in problem-solving ability among organic chemistry graduate students and faculty were studied within the domain of problems that involved the determination of the structure of a molecule from the molecular formula of the compound and a combination of IR and ^{1}H NMR spectra. The participants' performance on these tasks was compared across variables that included amount of research experience, year of graduate study, and level of problem-solving confidence. Thirteen of the 15 participants could be classified as either "more successful" or "less successful." The participants in this study who were "more successful" adopted consistent approaches to solving the problems; were more likely to draw molecular fragments obtained during intermediate stages in the problem-solving process; were better at mining the spectral data; and were more likely to check their final answer against the spectra upon which the answer was based. Experience from research, teaching, and course work were found to be important factors influencing the level of participants' success. © 2009 Wiley Periodicals, Inc. J Res Sci Teach 47: 643–660, 2010

Keywords:chemistry; problem-solving; college/university

The cognitive processes involved in problem solving have been of interest for more than 100 years (Dewey, 1910; Helmholtz, 1894). The literature is therefore rich with studies that attempt to describe differences between the problem-solving behaviors of experts and novices in such diverse fields as biology (Simmons & Lunetta, 1993; Smith, 1988; Smith & Good, 1984), chemistry (Bodner, 1991; Bodner & Herron, 2002; Camacho & Good, 1989; Sumfleth, 1988), chess (Chase & Simon, 1973), computer programming (Adelson, 1981; Weiser & Shertz, 1983), mathematics (Schoenfeld & Herrmann, 1982), physics (Chi, Feltovich, & Glaser, 1981; Finegold & Mass, 1985; Larkin, McDermott, Simon, & Simon, 1980), and the social sciences (Voss et al., 1983).

The research community has studied many facets of problem solving, including: memory and its organization (Chase & Simon, 1973; Greeno, 1973; Niaz, 1989; Staver & Jacks, 1988); describing the problem space (Ernst & Newell, 1969; Mayer, 1975); categorizing problems (Bunce, Gabel, & Samuel, 1991; Chi, Feltovich, & Glaser, 1981; Middlecamp & Kean, 1987; Smith, 1992); testing conceptual understanding as it relates to problem solving ability (Gabel, 1981; Gabel & Bunce, 1994; Gabel, Sherwood, & Enochs, 1984; Herron & Greenbowe, 1986; Nurrenbern, 1979; Nurrenbern & Pickering, 1987; Sawrey, 1990); and teaching problem solving skills to students by a variety of methods (Bodner, 1987; Bunce & Heikkinen, 1986; Dods, 1996; Frank, Baker, & Herron, 1987; Friedel, Gabel, & Samuel, 1990; Phelps, 1996; Smith, Powell, & Wood, 1995; Towns & Grant, 1998). The outcomes of these studies have given science educators a better understanding of the numerous factors involved with solving a problem. Based on these reports, we have learned that: problem solving success and conceptual understanding are not always coupled; memory structure and organization are constructed in a more sophisticated manner among those problem solvers with more experience in a domain; that our efforts to explicitly teach problem solving strategies do not always meet success; and that problem solving is often accomplished by heavy reliance on algorithms or weak heuristics.

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DOI 10.1002/tea.20306

While much of the work cited above involved some facet of solving mathematical problems, there are studies which have focused on solving problems that require no mathematical manipulation. For instance, Chase and Simon (1973) tested master and novice chess players' abilities to recreate game set-ups. The authors concluded that master players were better able to recreate positions of pieces based on greater experience with playing the game. Greater experience gave the master players the ability to recognize positions based on possible moves, which in turn allowed for easier reconstruction of the board. Medical diagnoses studies have demonstrated that categorization of symptoms led to more successful initial diagnoses (Pople, 1977; Wortman, 1972). Collectively, the chess players study and the medical diagnoses studies concluded that success with a task depends upon memory organization and categorization of certain cues from the problem. Problem categorization, an important initial step in devising a solution pathway, depended upon long term memory stores, the organization of those memory stores, and a recognition of cues in the problem statement.

Non-mathematical problem solving research has also been reported in the sciences, especially genetics (Smith, 1988, 1992; Smith & Good, 1984). Smith and Good (1984) reported a list of 32 problem solving behaviors of successful problem solvers who solved an array of genetics problems. Smith continued work in the area of genetic pedigree analysis (Smith, 1988), concluding that less successful problem solvers approached complex problems with single-step solution strategies, were unable to explain the genetic principles underpinning the problem, and lacked organization in their problem solving approaches. Studies in chemistry have also examined non-mathematical problem solving, particularly in the areas of problem categorization (Bunce, Gabel, & Samuel, 1991), conceptual understanding (Herron & Greenbowe, 1986), and using analogies to enhance problem solving ability and conceptual understanding (Hesse & Anderson, 1992).

For the purposes of this article, we will focus on the research pertaining to the differences in expert and novice or between successful and unsuccessful problem-solving behaviors. The adjective *expert* is widely accepted as the characteristic of an individual with broad competence, experience, and knowledge of a given domain, such as faculty or graduate students in that domain (Chi, Feltovich, & Glaser, 1981; Heyworth, 1999; Smith, 1988). *Novice*, in contrast, has been used to characterize individuals with limited competence or experience in a domain. Research has shown that experts and novices show marked differences in several aspects of problem solving ability, including problem representations (Bodner & Domin, 2000; Bowen, 1990; Chi, Feltovich, & Glaser, 1981; Greenbowe, 1983; Heyworth, 1999; Larkin & Rainard, 1984), experience solving similar problems (Heyworth, 1999), and problem solving strategies (Niaz & Astudillo, 1996).

Larkin et al. (1980) noted two strategies in the process of constructing computer simulation of problem-solving behavior in physics: means-ends analysis and knowledge development. They noted that expert problem-solving behavior correlated strongly with the knowledge development, a working-forward strategy, whereas novices were more likely to use means-end analysis strategies. Priest and Lindsay (1992) found that both experts and novices used forward inference strategies when solving problems in physics, but experts tended to plan their attacks at the metacognitive level. Whereas novices focused their solutions on one or two pieces of information, experts were more holistic in their approach and examined more factors and variables in the problem statement.

Camacho and Good (1989) described marked differences in four problem-solving behaviors of experts and novices working on chemical equilibrium problems: perception of the task, strategic knowledge, content knowledge, and problem representation. They argued that experts tend to view a problem as a task that deserves careful analysis and reasoning, whereas novices viewed problems as tasks where importance was placed only on the solution of the problem.

Smith and Good (1984) utilized a different approach to dichotomizing their sample population in a study of genetics problem solving. They noted 32 separate behaviors that could be used to differentiate between *successful* and *unsuccessful* problem solvers, including the tendency to store knowledge in a hierarchical fashion; to seek patterns in problems rather than focus on individual parts of the problem; whether a qualitative analysis guides the problem-solvers plan of attack; the strength of the heuristics applied to the solution; and whether the problem-solver checked their answer to ascertain whether it made sense.

In their analysis of genetics problem-solving behavior, Smith and Good (1984) concluded that the terms *expert* and *novice* did not describe their participants accurately. These terms may be adequate when describing the individual's level of experience with content, but the terms *successful* and *unsuccessful* are more useful when discussing problem-solving processes or behaviors. Smith therefore applied the successful/unsuccessful continuum to pedigree analysis problems (Smith, 1988) and problem categorization tasks (Smith, 1992) in genetics. He noted that unsuccessful problem solvers try single-step solutions to complex problems, did not explain the scientific principles at work in the problem, showed inadequate background understanding, failed to read the problem completely, showed no planning phase in finding a solution, and generally lacked organization in their approach to solving the problem. We agree with Smith's opinion that *expert* and *novice* are inadequate terms for use in studies of problem solving behaviors. Exclusive use of these terms do not allow for experts who cannot solve problems, or for novices who can solve complex problems. As such, we adopted Smith's approach by classifying our participants as *successful* or *unsuccessful*.

More recently, Heyworth (1999) has examined three key factors that differ among successful and unsuccessful problem solvers: solution strategies, problem representations, and differences in conceptual knowledge. While successful problem solvers quickly identified the problem, worked in a forward direction, and reached a solution rapidly, "less successful" participants did not. "Less successful" problem solvers were also more likely to use erroneous formulae and had less confidence in their solutions. Both less and more successful participants based their initial representations on key phrases given within the problem statement. From there, the "more successful" problem solvers set up two further representations: a qualitative and a mathematical representation. The mathematical representation acted as a guide for formula choice. "Less successful" participants appeared to skip the qualitative representation and move directly into the mathematical one. For them, the process of solving problems was mathematically or formula driven, perhaps because of their weaker understanding of the chemical concept in question. This hypothesis was supported when Heyworth examined the conceptual understanding of both groups. He reported that, while conceptual understanding was roughly equivalent at the macroscopic level in both groups, at the microscopic level only about a third of "less successful" participants held the correct chemical conception.

Prior research suggests that "more successful" problem solvers have a better understanding of the content domain, are able to fragment and restructure problem statements to better devise a solution plan, have a more procedurally useful knowledge structure, and have more experience with various types of problems within the domain. Yet the majority of the work in chemistry was performed in subdomains that are fundamentally different from organic chemistry, a domain which includes such non-mathematical problem-solving tasks such as designing the step-by-step synthesis of an organic molecule (Bhattacharyya, Calmisiz, & Bodner, 2004: Bhattacharyya & Bodner, 2005; Bowen & Bodner, 1991), deducing mechanisms (Ferguson & Bodner, 2008), or deducing the molecular structure of a compound from its IR and NMR spectra. Organic chemistry is not steeped in mathematics, like analytical, inorganic, or physical chemistry. Successful organic chemistry problem solving relies on rationalizing trends in reactivity, determining spatial relationships, and devising coherent mechanisms to explain or predict chemical transformations. To probe structure elucidation problem solving in organic chemistry, we carried out a study based on the following guiding research questions:

- How do organic chemistry graduate students and faculty solve combined spectral problems?
- What problem solving characteristics differentiate successful and unsuccessful solvers?
- Can a continuum of problem solving ability be established for these participants?

Although this study was domain specific, the research questions which guided it may be applied to any field in which qualitative problem solving is used. A broader, fuller description of the problem solving behaviors of successful and unsuccessful participants will lead to a deeper understanding of the ways problems are solved within and across domains. Identifying those behaviors which lead to problem solving success will directly address improved science instruction in the form of enhanced problem solving skills. While we recognize that the vehicle of this project is domain specific, we believe that our outcomes will add to the body of evidence which has sought to describe mechanisms of problem solving across the scientific spectrum.

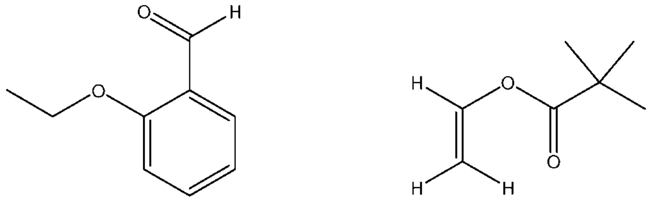
Methodology

The sample population for this study consisted of 13 Ph.D. students and two faculty from the organic chemistry division at a research oriented midwestern university who volunteered to participate in this study. Participants were recruited from organic chemistry research laboratories throughout the department. The interviewer approached 20 graduate students and four faculty; these numbers represented approximately one quarter of the total population of the organic chemistry division in terms of students and faculty at the time of data acquisition. Purposeful sampling (Patton, 2002) was used to ensure that the sample population reflected the demographics of the organic chemistry division in terms of both gender and ethnicity. Each participant took part in two semi-structured interviews. The first interview was a short, background-gathering session, which led to a description of each participant's prior and current training in chemistry. The first half of the interview focused on each participant's undergraduate training. Questions included the type of institution at which they studied, the extent and specialty of research participation, and the extent to which they had used spectroscopy in both classroom and laboratory settings. Participants were also asked to describe their first hands-on experience with various spectroscopic instruments, including their initial perceptions and confidence with the instrument. The second half of the interview focused on the participants' graduate training. Questions related to research projects, frequency of instrument usage, and year of graduate study were asked. The first interview was audiotaped so that the interviews could be transcribed.

For the second interview, the participants were asked to solve five spectroscopy problems while being audiotaped and videotaped. For each problem, the participants were given the IR and ^{1}H NMR spectra and the molecular formula of one of the compounds shown in Figure 1 and asked to deduce the molecular structure of the compound from these data. The problems were chosen to span a range of complexity, each with varying spectral characteristics. Given that content knowledge can be a confounding variable in problem solving interviews (Bowen & Bodner, 1991), the participants had access to the following supplementary materials for use at any time: a compass, a ruler, a calculator, and a textbook on spectroscopy. They were also told that they were free to ask the interviewer any questions of a factual or content nature.

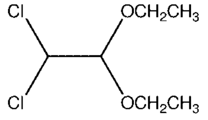
Problem 1: ethyl acetate

Problem 2: 3-pentanone



Problem 3: 2-ethoxybenzaldehyde

Problem 4: vinyl pyvalate



Problem 5: dichlorodiethoxyacetal

Figure 1. Molecular structures and names of the five compounds tested in the second interview.

The interviewer used standard think-aloud techniques (Ericsson & Simon, 1993; Pressley & Afflerbach, 1995). Participants experienced minimal interruptions from the interviewer, and were encouraged to talk about the processes of problem solving as they were involved in each task. While the think-aloud protocol is a particularly useful tool for gathering data ‘‘in the moment,’’ there are limitations to the technique. Participants often must become accustomed to the process of concurrently discussing thought processes while actually solving problems. Those unfamiliar with the task often require prompting from the interviewer. The main drawback associated with this method of data collection is the risk of incomplete reporting of steps in the problem solving process, which is automatic for many well-versed participants.

The second interviews were both audiotaped and videotaped. The videotapes were used to minimize confusion over ambiguous terms such as *this*, *that*, or *it* when the interviews were transcribed. The videotapes also provided a visual record of the order in which molecular fragments or structures were drawn. The worksheets upon which the participants solved the problems were kept as artifacts, as well. Together, the transcripts from the audiotape, the videotapes from the second interview, field notes kept by the researcher, and the participants’ worksheets comprised the data set analyzed.

After each interview, the audiotapes were transcribed. Transcripts from the problem solving interview were then reviewed while viewing the videotape of the interview. The researcher made notes that clarified any ambiguous referrals to the spectral data and recorded the order in which molecular fragments were drawn in the problem-solving process.

The completed transcripts were read and reviewed for common emergent themes. Analysis occurred under the phenomenographic framework (Marton, 1986, 1994), which allowed the researcher to focus on both the similarities and differences that exist among this set of problem solvers. As former practicing chemists, both authors had considerable experience with interpretation of infrared (IR) and proton nuclear magnetic resonance (^{1}H NMR) spectra. This experiential knowledge allowed the interviewer to act as an expert source for the participants, if they chose to ask questions about a given problem.

As a form of member checking (Lincoln & Guba, 1985), the interviewer randomly selected four of the participants with whom to have an informal follow-up conversation that addressed participants’ comments in the problem solving interviews. The interviewer shared with these four participants his interpretations of their work and asked if these interpretations were accurate. Each of the participants polled agreed with the interpretations of the researcher.

Analysis of the data set included scoring the correctness of the answers put forth by the participants according to a rubric that included both technical and logic points that took into account the major points of interpreting the IR and ^{1}H NMR spectra, the correctness of molecular fragments deduced during the problem-solving process, the correctness of the connections made between these molecular fragments, and whether the correct structure was deduced. For each problem, six technical points were awarded for correct interpretation of spectral data and correct connections between molecular fragments, three technical points were awarded for correct interpretation of spectral data but incorrect connections between fragments, and zero points were awarded for an incorrect interpretation of spectral data. One logic point was awarded in each of the following categories, for a maximum of six logic points: unsaturation calculation, IR signal identification, multiplicity of signal in the ^{1}H NMR, chemical shift of signal in the ^{1}H NMR, integration of signal intensity in the ^{1}H NMR, and consideration of coupling constants in the ^{1}H NMR. A Pearson product moment correlation coefficient was calculated to determine if there was sufficient correlation between the two parts of the scoring rubric to warrant adding them to obtain a total score that could be used to judge success. Deduction of the correct molecular fragments was the dependent variable, while items such as ‘‘use of shift and splitting patterns’’ was the independent variable. The calculation gave an $r = 0.60$ at the 95% confidence level. Thus, while a given problem may have been answered incorrectly, it was still possible to amass points for it via the solution path. Scores calculated from the grading rubric were then normalized to a maximum of 100%. Normalization of overall score to 100% was necessary due to participants’ lack of use of certain information (to which points were assigned) during the problem solving tasks. For instance, if no participant indicated the use of unsaturation calculation when solving a specific problem, normalization prevented penalization of points for the entire population for that problem.

Once the scores for each participant were calculated, the participants were divided into two primary categories labeled ‘‘more successful’’ or ‘‘less successful.’’ Participants were placed in each category on the basis of their overall score. The "more successful" participants had an average score above 82%, while the "less successful" participants scored on average below 70%. These limits were the product of a natural break in the scores of the participant pool.

Two participants, however, obtained overall scores between 70% and 82%. These participants did not fit neatly into either category of success, which required the creation of a third category labeled "intermediate success." The two participants in this category demonstrated problem-solving behaviors that were not wholly consistent with either the "more successful" or "less successful" participants. Once classified, each participant was given a designator code consisting of a number and a letter in parentheses after their names. The number indicates the year of graduate study at the time of data acquisition—with the exception of faculty, for whom an "F" was used—while the letter indicates whether the participant was classified as "more successful" (S), "less successful" (U), or of intermediate success (I). The purpose of the designator code was to clarify any discussion of individual participants, rather than referring to tables or figures. Table 1 summarizes the grouping of the participants.

Once the participants were grouped into these categories, the transcripts were again reviewed to determine both similarities and differences in problem solving behaviors between the groups. Coding of these patterns was accomplished by an extensive reading and review of all transcripts over the course of several months, comparing subjects within and across groups on the same problem. Since five problems were given, five such iterations through the data set were required. Finally, each participant's performance was examined across all problems to provide a global description of how these types of problems are solved among this set of participants.

Results and Discussion

During the first interview, participants were asked to rate their confidence in solving combined spectroscopy problems on a scale of one to ten, where ten was very confident. This question was asked to gain an understanding of participants' views of their own problem solving ability. Interesting results were obtained when the participants' self-reports of confidence in their ability to solve spectra interpretation problems were compared with the participant's actual rate of success on these tasks. The average reported confidence across the 15 participants was 7.19 out of 10. The average of their actual performance was 7.59. Yet, examination of the same data by success group revealed that the "more successful" participants consistently underestimated their problem-solving skills, whereas the "less successful" individuals consistently overestimated their skills. On average, the "more successful" participants reported an average confidence level of 7.25 and achieved an average performance of 8.54. Their "less successful" counterparts reported an average confidence level of 7.2 and achieved an average performance of 6.0.

Table 1
Participants' year of study, overall score, and success rating

Name	Year of Study	Score[a] (%)	Rating
Roxanne	1	78	Intermediate
Albert	2	85	More successful
Mark	2	78	Intermediate
Matilda	2	35	Less successful
Nicole	3	70	Less successful
Tina	3	67	Less successful
Cathy	4	82	More successful
David	4	83	More successful
Daniel	5	87	More successful
Joseph	5	82	More successful
Monique	5	58	Less successful
Brad	6	70	Less successful
James	6	90	More successful
Pat	F	92	More successful
Robin	F	92	More successful

[a] Scores were calculated from grading rubric and normalized to 100%.

A list of the participants, their undergraduate and graduate research projects, and their relative success in solving the combined spectra problems in this study is given in Table 2. Among the eight participants who were more successful, six of them participated in undergraduate research projects which focused on synthesis, or building complex molecules from more simple starting materials. Seven of the eight more successful participants continued to study synthesis upon entering graduate school. This is important to note, because newly synthesized compounds must be fully characterized using spectroscopic methods, including IR and ^{1}H NMR spectroscopy. Synthetic chemists should, as a consequence of their work in the area, have more experience in interpreting spectral data. With greater experience, skills in spectral interpretation likely improve. Therefore, the amount of time spent interpreting spectra in a research setting was likely influential in placing these participants into the more successful category.

Four distinct patterns were observed in problem-solving behaviors that differentiate the ‘‘more successful’’ and ‘‘less successful’’ participants in this study. The ‘‘more successful’’ participants had a tendency to take a consistent approach to the problems; to use the available information effectively; to draw fragments of the structure deduced during intermediate stages in the problem-solving process; and to check their proposed structures against the spectroscopic data when they thought they had deduced the correct structure. Each of these patterns is discussed below in terms of comparisons of the observed behaviors of the ‘‘more successful’’ and ‘‘less successful’’ participants.

Consistency in Problem Solving

In general, the ‘‘more successful’’ participants attacked the problems methodically, following the same strategy no matter how simple or difficult they perceived the problem to be. They tended to start by calculating the unsaturation number from the molecular formula in order to determine the presence (or absence) of multiple bonds. They then looked for the presence or absence of absorptions in the IR spectrum that occur at characteristic frequencies, such as a C=O double bond (or carbonyl group) at roughly 1,700 cm^{-1}, which often led them to draw potential molecular fragments. They then picked out important aspects of the ^{1}H NMR spectrum, such as the number of signals, the splitting of peaks, the integration of the signals, and the chemical shift of a particular set of peaks.

Occasionally, the order in which these tasks were carried out varied, depending on several factors. For example, Daniel (5S) followed his strategy for solving problems consistently except for 3-pentanone, which has ^{1}H NMR characteristics that reflect the symmetric nature of this compound. For this problem, Daniel calculated the unsaturation number, followed by correctly deducing the presence of a carbonyl group from the IR spectrum. His usual strategy from this point was to assess the peaks in the NMR, but from looking at the spectrum he correctly assumed a symmetric ketone:

Table 2
Participants' undergraduate (UR) and graduate research (GR) projects as a function of success grouping

Participant	UR	GR	Grouping
Albert	Organometallic synthesis	Carbohydrate synthesis	More successful
Brad	Organic synthesis	Protein conformations	Less successful
Cathy	Organic synthesis	Organic synthesis	More successful
David	Organic synthesis	Organic synthesis	More successful
Daniel	Biochemistry	NMR of unique materials	More successful
James	Organic synthesis	Organic synthesis	More successful
Joseph	Biochemistry	Bioorganic synthesis	More successful
Monique	Biochemistry	Organic synthesis	Less successful
Mark	Host/guest chem.	Bioorganic synthesis	Intermediate
Matilda	Photochemistry	Carbohydrate synthesis	Less successful
Nicole	Host/guest chem.	Organic synthesis	Less successful
Pat	Biochemistry	Organic synthesis	More successful
Robin	Biochemistry	Bioorganic synthesis	More successful
Roxanne	Host/guest chem.	Gas phase reactions	Intermediate
Tina	Inorganic chemistry	Organic synthesis	Less successful

> Uh, the symmetry is really what helps you out in this one. I mean, because each side is the same when you look at this, you say you have ten hydrogens, and you only have two peaks, that means, that's a clue right away that you have symmetry. It's a very symmetric molecule. So you just start building from that.

Robin (FS), Pat (FS), Albert (2S), Cathy (4S), Joseph (5S), and James (6S) also recognized the symmetric nature of this compound almost immediately. This reduced the need to examine other pieces of information available because deducing the structure of half of the molecule automatically gave the participant the other half. This problem exemplifies the need to normalize the scores to 100%. Recognition of the symmetry element obviates the need for an analysis of coupling constants. For this problem, no participant mentioned coupling constants during the problem solving process, so they were rated equally for it by normalizing the scores.

David (4S) gave correct structures for three of the five problems. His approach first involved taking the relevant peaks from the IR spectrum, including the fingerprint region. This behavior is of note because the fingerprint region is not relied upon as heavily for spectral interpretation by practicing organic chemists as it was before the advent of techniques, such as NMR, that convey structural information in a more explicit fashion. After considering the IR, David (4S) calculated the unsaturation number and moved on to the NMR spectrum, where he relied mostly on splitting and integration. In each problem, David was able to deduce the correct molecular fragments from the spectra, but pieced them together incorrectly and only sometimes arrived at the accepted structure. While he did not answer each question correctly, his consistent approach allowed him to isolate fragments of the molecule about which he was confident.

The "less successful" participants displayed problem-solving strategies that varied greatly from problem to problem. Monique (5U), for example, varied her approach with nearly every problem. While interpreting the spectra for 3-pentanone, she first identified the carbonyl stretch at 1,750 cm^{-1}, and used it as her starting point to deducing a structure. After looking at the NMR, she too recognized the symmetry element:

> Well, yeah. The triplet/quartet, um, first of all that those are the only signals there, so that means that this molecule is probably symmetrical. It's reading the same thing. All the protons are in the same environment one way or the other. Um, and this molecule (her proposed structure) is in fact symmetrical.

However, her strategy changed when the problems became more difficult. She began her attack by examining the NMR spectrum of vinyl pivalate:

> I: What is your immediate reaction?
>
> Monique: (laughs) Um, that this (referring to signal at a chemical shift of 4.8 ppm) is not a quartet but a doublet of doublets. So that means that I have protons that partially overlap in signal.

Initially, Monique focused on the pattern of the splitting of signals in the NMR. When that approach did not lead her to the solution, she moved back to an examination of the IR, from which she deduced a carbonyl, but with trepidation:

> Monique: That's really close to 18 (referring to stretch at 1767 cm^{-1}).
>
> I: What are you thinking it could be?
>
> Monique: Um, we're only working with carbons, hydrogens, and oxygens. Um, its awfully close to 18 and usually I'm used to seeing carbonyl stretches at least 17 wavenumbers, 16 or 17, I'm just hesitant to call this a carbonyl. It may be, but I'm not convinced because it is registering so high.

After these initial steps, Monique moved back and forth between the two spectra. At points along her solution pathway she drew possible structures, amending them as necessary when she thought she had another piece of information deduced from the spectra. Well into her solution of vinyl pivalate, she was still not convinced of the presence of a carbonyl: "…and I haven't even started adding my carbonyl group yet, if in fact it is a carbonyl group at all."

Monique's lack of a consistent solving strategy hindered her ability to recognize a slightly shifted carbonyl stretch in Problem 4, which one would expect when the molecule is an ester. Whereas she deduced the correct answer for ethyl acetate and 3-pentanone, Monique did not determine correct structures for the remainder of the problems. Clearly, one of the obstacles that Monique faced was a distrust of her instincts, as evidenced by the above quotations, in spite of the fact that she was a fifth-year graduate student.

Effective Use of Embedded Information

Coupling constants obtained from an NMR spectrum provide skilled spectroscopists with detailed information about the arrangement of neighboring hydrogen atoms in the molecular structure of a compound. This information therefore plays an invaluable role in interpreting ^{1}H NMR spectra of molecules encountered in the real world of the practicing organic chemist. Such real world molecules are usually significantly more complex than the five problems on which this study was based. Many participants did not use coupling constant information in their solution strategies when other information led them to a viable answer. The "more successful" problem solvers, however, resorted to analysis of coupling constant information in their solution pathways for vinyl pivalate and dichloroacetaldehyde diethyl acetal, the two most difficult problems in the study.

Pat (F) and Daniel (5S) made coupling constant measurements to help them make the correct connections between the molecular fragments they had deduced from other spectral information. After measuring the coupling constants for the signals with chemical shifts at 4.6 and 4.9 ppm in the NMR spectrum of vinyl pivalate, for example, Pat reached the correct answer after having been tempted to choose another structure from prior information:

> So, if I have t-butyl acrylate … one question is: Do the coupling constants here (δ4.6) match with the coupling constants there (δ4.9)? So what we would have, we would have a very small geminal coupling of these two (δ4.6 and δ4.9), and then these two would be coupled to this (δ7.2). And assuming they're all done on the same scale, we should be able to answer that question rather quickly. So it's about, yeah, it's about 20 mm that separates these two peaks. Do I see a 20 Hz coupling here (δ7.2)? And the answer is yes, going from peak to … so yes, this proton is coupled to each of these two by vicinal coupling. These two are coupled to each other by geminal coupling. Instead of t-butyl acrylate, we would have a vinyl ester of pivalic acid.

A similar phenomenon occurred when Pat worked on the dichloroacetaldehyde diethyl acetal problem. In the absence of an analysis of the coupling constant information, Pat would have likely ended up with the wrong structure; the path Pat was following would have led toward an incorrect solution until the coupling constants were properly measured.

Daniel experienced much the same situation in the dichloroacetaldehyde diethyl acetal problem. Without calculating coupling constants, he would have ended up choosing a structure which matched most of the spectral data, but not the coupling constants. After measuring the coupling constants and deciding on a structure, he rethought his conclusion:

> You know what? It's not right… In this coupling, there is, I've been saying all along that these couplings (δ4.6 and δ5.7) match each other Anyway, they're not even close to these (the multiplet), you know. None of them. They're all so small. And so, these are just coupled to themselves and nothing else, so they're off in happy go lucky land, by themselves. From this (δ4.6 and δ5.7), there are two protons coupled with a coupling constant of 5 Hz, and they are coupled to nothing else. So if I did it that way, it would mean that it would have to be something like that. But that's the only way I can fit them in.

Albert (2S) was able to recite from memory the coupling constants for ortho-, meta-, para-protons on a monosubstituted benzene ring when considering how to answer the 2-ethoxybenzaldehyde problem. He measured the coupling constants as best as he could, considering the poor resolution of the NMR spectrum, and compared them to those he recited from memory. He then discussed how he chose the best structure from three possible choices:

> Assuming that it's not para, because that is almost nothing, the coupling constant, this one could be ortho and this one meta. These two could be ortho, and here I would say that roughly the same case is here. So these two are ortho, and this one meta. Triplet, triplet, doublet, I think that structure is the one that makes the most sense from what I see here.

Four different kinds of information can be mined from an NMR spectrum. The chemical shift (e.g., $\delta4.6$ or $\delta5.7$) can provide insight into the presence of electron-withdrawing substituents attached to the atom whose signal is being examined. The intensity of a peak or multiplet of peaks is directly proportional to the number of spectroscopically equivalent atoms that give rise to the signal. The splitting pattern—whether a doublet, triplet, quartet, doublet of doublets, etc.—reflects the number of spectroscopically active nuclei on atoms that are directly bound to the atom whose signal is being examined. (As a rule, the number of lines into which a ^{1}H NMR signal is split is equal to $n + 1$, where n is the number of equivalent hydrogen atoms and a neighboring carbon atom.) The magnitude of the coupling constant (J_{HH})—the separation between the lines in a splitting pattern—can provide information about the exact stereochemical relationship between the positions of atoms that give rise to a splitting pattern. The chemical shift data, integration and splitting patterns are all surface-level information that are readily apparent from the spectrum. Determining coupling constants, however, requires an element of data-mining, in this case, measuring the distance between peaks in the NMR spectrum with the ruler that was available for participants to use during the problem-solving process.

While the ‘‘more successful’’ solvers depended on coupling information to overcome barriers toward the solution of the more difficult problems, the ‘‘less successful’’ solvers either did not use coupling constants at all, or only cursorily mentioned them. Brad (6U) exhibited the latter behavior in the following extract from the dichloroacetaldehyde diethyl acetal problem.

> The J couplings are usually, you can calculate the coupling or J values. They're sort of a guide, but I never paid that much attention to it. But in this case, they ($\delta4.6$ and $\delta5.7$) are split by each other, and they have exactly the same J values so its one peak, split by all kinds of long range couplings.

Despite his inability to use coupling constants to help him, Brad reached the correct structure anyway. Monique (5U), however, did not obtain the correct answer while working on the vinyl pivalate problem.

> Um, that this is not a quartet but a doublet of doublets, separated by the same J value. So that means I have protons that partially overlap in signal. And, uh, perhaps it's what the J values are supposed to tell me, cis or trans.

This is the only instance where Monique discussed coupling, and here she did not measure the coupling constants; she estimated their magnitude. As coupling constants are usually very small, a slight over- or under-estimation could result in a skewed interpretation, resulting in choosing one erroneous structure over the correct one. In this instance, Monique did not arrive at the correct structure. The other ‘‘less successful’’ problem solvers made no mention of coupling constants at all.

Fragments Versus Whole Molecules

One of the most interesting differences between the ‘‘more successful’’ and ‘‘less successful’’ problem solvers' behaviors was the way they started the process of proposing structural solutions. The ‘‘more successful’’ participants generally deduced fragments of the molecular structure from one aspect of the spectral data, wrote them down, and repeated the process in the same manner until all the information was written on article. It was at this point that they started thinking about possible connections between the fragments. Their ‘‘less successful’’ counterparts tried to start by drawing possible molecules in their entirety.

This can be seen by comparing answers to 2-ethoxybenzaldehyde given by Robin (FS) and Matilda (2U), shown in Figures 2 and 3 respectively.

The tendency for the "more successful" participants to draw pieces of molecules rather than entire molecules may have been responsible for at least part of their success. As they examined the spectra, certain aspects of one of the spectra provided clues about the functional groups or molecular fragments that could be present in the structure of the molecule. By writing this information down, working memory space was freed to search for hints about the next piece of the molecular structure. Maintaining an inventory of possible fragments also helps the individual solving the problem to focus on the most likely functional groups. For example, if no –OH group stretching appears in the 3,200–3,500 cm^{-1} range of the IR spectrum, one can automatically eliminate alcohols and carboxylic acids from the possible solutions to the problem. In effect, this process of elimination allows the solver to focus his/her efforts on deducing how the pieces are put together, rather than a more random guessing approach.

Final Checks Performed

Without exception, every participant in the "more successful" category made certain that their chosen structures would match the actual spectral data, as a means of checking their work. Three methods of checking answers were observed among the "more successful" participants: drawing hypothetical NMR spectra to match their proposed structure; counting atoms in the structure and comparing the result to the molecular formula; and providing a verbal explanation of spectral characteristics in terms of their proposed structure. Cathy (4S) used all three checking mechanisms upon completion of each problem. For instance, when explaining her answer to the 3-pentanone problem, she added the atoms in the structure to determine if they matched the molecular formula. She also devised and discussed the theoretical splitting patterns she would expect from her chosen answer, pointing out each piece of evidence in the spectral information:

> I would say I have my carbonyl here, and since this is a quartet, it must be near the CH_3 group. This would be a triplet, a triplet near a CH_2. This atom has to be closest to the carbonyl. And this one is going to be like a quartet. Add it all to the carbonyl, and it's symmetric. I have expended all of my atoms, and I think that's it.

As a consequence of testing the goodness of the final answer, each of the "more successful" participants was better able to explain their answers verbally than were their "less successful" counterparts.

The "less successful" participants rarely checked their final answers. When pressed to explain their final answers in terms of the spectral data, most experienced difficulty in their reasoning. Brad (6U) provided the following answer when asked to review his proposed structures for vinyl pivalate:

> Brad: I think I'm going to go with one of these. I can't explain everything in it, but I sort of answered some of the observations, I suppose.
>
> I: Why don't you explain that structure and its spectrum, I mean as much as you can.
>
> Brad: In my structure they're equivalent, but there's quite a bit of difference in chemical splitting which I cannot explain. This hydrogen, being next to two carbonyl groups, is shifted down to $\delta 7.2$. But, uh, again the splitting patterns I can't explain.

Matilda (2U) explained her answer to the vinyl pivalate problem as follows:

> Matilda: Um, I mean I think if I knew how to read these things (NMR) a little better it would be pretty clear, because it's a really nice spectrum. I mean, you've got this, this doublet here. I forget, what is it called when you've got, because this is a doublet with two peaks, but what does it mean when they're paired like that?
>
> I: That's a doublet of doublets.
>
> Matilda: Of course it is. Hmm... well, I'm sure that means something. So they're probably in pretty similar environments, I'm guessing, especially since they're close to each other like that on the spectrum.

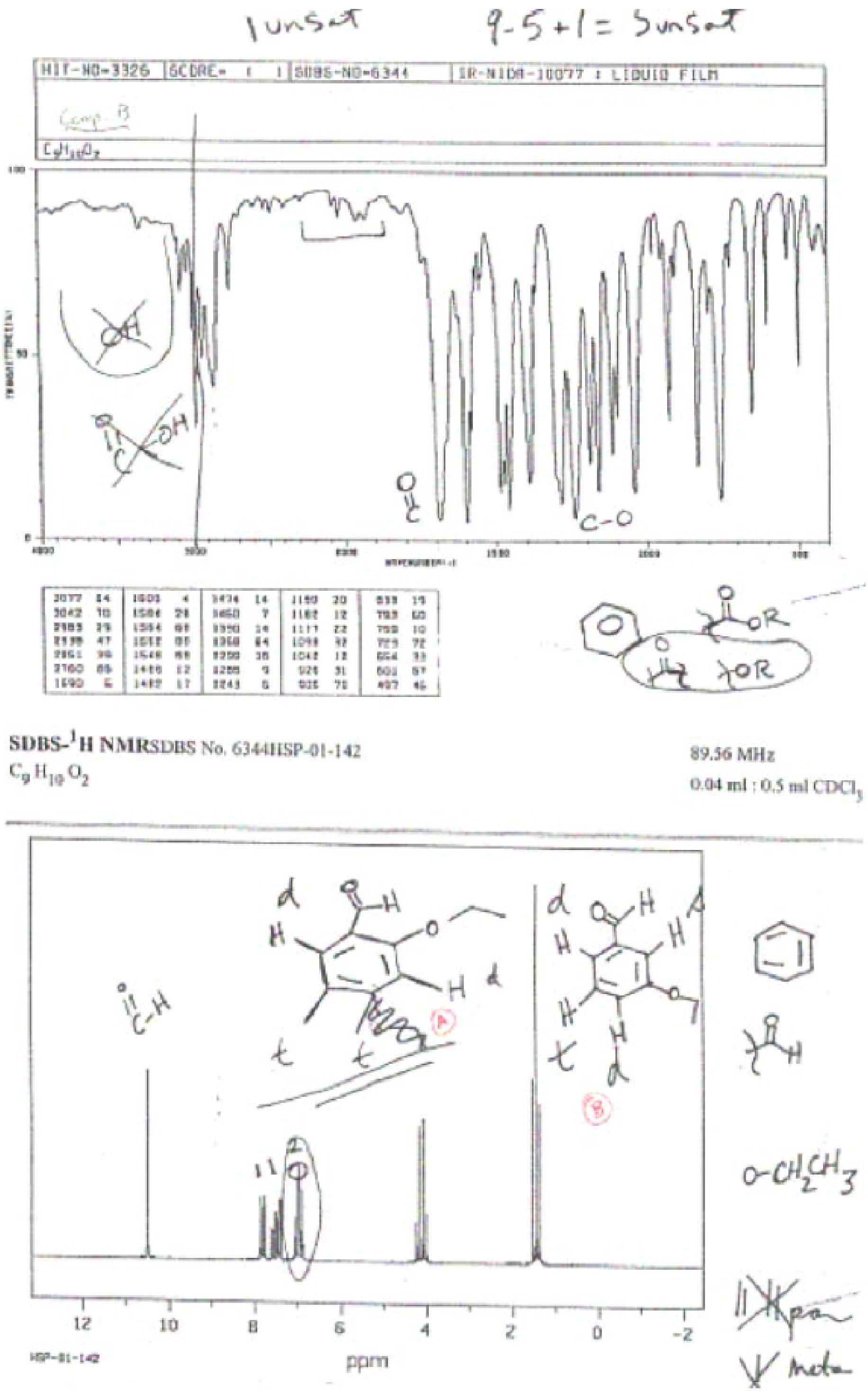


Figure 2. Robin's (FS) fragment drawings in solving 2-ethoxybenzaldehyde.

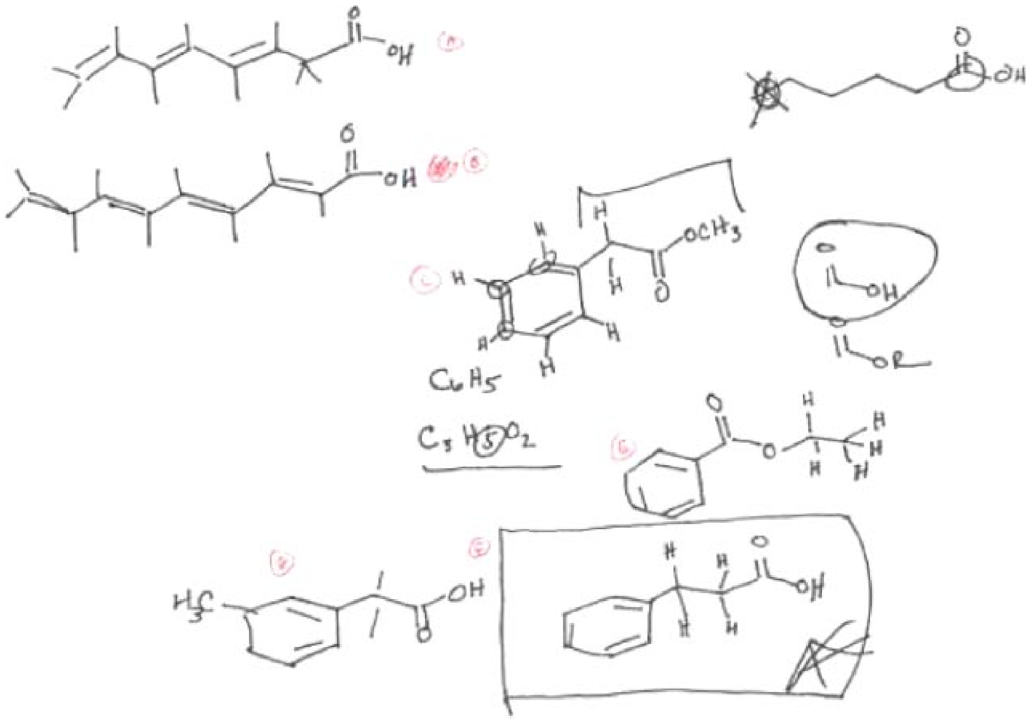


Figure 3. Matilda's (2U) attempts at solving 2-ethoxybenzaldehyde.

While most practicing chemists make use of the ''$n+1$ rule''—a rule that predicts the multiplicity of a signal based on the number of neighboring hydrogen atoms—when solving problems of this nature, this rule is not an infallible predictor of the splitting pattern in complex NMR spectra. The ''less successful'' solvers relied on the ''$n+1$ rule'' heavily, and could not explain which factors to consider in compensating for it. On the other hand, the ''more successful'' solvers could rationalize such adjustments of the ''$n+1$ rule.'' As noted above, some even drew out hypothetical ^{1}H NMR spectra based on their proposed structures, and compared these to the actual given spectra as a means of checking their answers.

Conclusions and Implications

One outcome of this study is a descriptive set of behaviors that help us differentiate between ''more successful'' and ''less successful'' problem solvers within the domain of organic spectral interpretation. The ''more successful'' individuals tended to:

- Take consistent, appropriate approaches to solving problems of this type.
- Make use of more given information, including coupling constants that must be deduced from analysis of the spectrum.
- Draw out fragments of molecules as they are deduced.
- Check their solutions against the spectral data.

The ''less successful'' individuals tended to exhibit the opposite behaviors.

The data obtained in this study also provided information about the factors that were likely to make an individual ''more successful'' or ''less successful.'' As might be expected, the main factor that appears to affect success is experience. Data from the first interview indicated three categories of experience: classroom, teaching, and research-related experience.

The results of this project also support those drawn from similar studies in other domains. For instance, the ‘‘more successful’’ participants tended to keep an accurate, detailed account of each molecular fragment as it was deduced from the spectra given. This behavior demonstrated that the original problem was broken into parts, or subproblems, the answers to which, when taken together, give the correct solution to the overall problem (Smith & Good, 1984). The ‘‘less successful’’ participants did not appear to be as diligent in keeping track of molecular fragments. These participants seemed to invest significantly less time and effort into restructuring the problem, to break it into subproblems.

Another reason which may account for the ‘‘less successful’’ participants not restructuring the problem is related to the declarative nature of their knowledge base. In the case of Matilda (2U), while she is able to deduce a splitting pattern in ^{1}H NMR via the ‘‘$n+1$ rule’’, she is unable to use the information to lead her further down the solution pathway:

> I’m really concerned about the NMR shifts and splits over here, but I can’t verify these two different types of protons using the NMR. But, just playing the numbers, I can’t think of any other structure.

The ‘‘more successful’’ participants, in contrast, exhibit a more sophisticated understanding of the guiding principles of spectroscopy. Consider Robin’s (FS) comment referring to the relationship between coupling constants and structural characteristics:

> That number is too big, so they are not in communication. It is in communication, though, with that. It is probably really two, there are probably really two ethyls. I mean, now the problem of where the attachments are is solved.

When narrowing down possible structures, Robin not only correctly recalled coupling constant facts correctly, it was also put to use correctly which led Robin to reach the structural solution to the problem. Matilda, on the other hand, factually indicated the splitting patterns found in the ^{1}H NMR spectrum, but could not apply this information in such a way which would advance her toward a solution. Matilda’s factual understanding and the procedural implications of it were not strong enough to allow her to reach a viable solution. Thus, Robin’s knowledge of coupling constants is richer and factually correct, and it is procedurally useful as well. Overall, the differences in declarative/procedural knowledge between the ‘‘more successful’’ and ‘‘less successful’’ participants were obvious, corroborating the conclusions of Camacho and Good (1989).

The observation that the ‘‘less successful’’ participants’ knowledge is more declarative may account for their tendency to focus on only one or two pieces of data (Smith & Good, 1984), as opposed to conducting something akin to a meta-analysis. Both Pat (FS) and James (6S) were observed to flip between the two spectra that were given in the problem statement, confirming features found in one with features in the other. In effect, they were analyzing the spectra simultaneously, devising a picture of what the overall molecule must look like to produce the spectra before them. None of the ‘‘less successful’’ participants were observed to behave this way. Instead, the ‘‘less successful’’ participants tended to focus on one or two characteristics in the data, and to devise a solution based on those pieces of information.

We also observed, particularly with Matilda, a reliance on the ‘‘$n+1$ rule’’ when such reliance would not prove fruitful to reaching an answer to the problem. The NMR spectrum of vinyl pivalate contains information that requires analysis beyond the ‘‘$n+1$ rule’’ to reach the correct structure. Matilda’s exclusive use of the ‘‘$n+1$ rule’’ indicated that for her, this rule is a weak heuristic. As a heuristic, it may be used with success on some occasions, but not all. Matilda was unable to recognize this nuance of interpreting NMR spectra, and did not reach a correct answer.

One conclusion that is unique to this study is the consistency of approach for the ‘‘more successful’’ participants. Each of the ‘‘more successful’’ participants attacked each problem following the same steps in roughly the same order: calculation of degree of unsaturation from the molecular formula, determination of functional group characteristics from IR, determination of molecular connectivity based on ^{1}H NMR, and checking their solutions against the given spectra. It would seem that the ‘‘more successful’’ participants had used prior experience with analysis of molecular structure via IR and NMR spectroscopy to develop an approach that might be viewed as almost algorithmic.

The results of this study also show that a continuum of problem solving ability exists, even among this set of similar participants. All participants were doctoral students or faculty in organic chemistry. All else being equal, these persons can and should be considered knowledgeable in the field. Yet, there were demonstrable differences in how they solved combined spectroscopy problems, leading ultimately to various levels of success in performance. This differential ability in solving problems has established a continuum of ability.

Further, the participants were shown to lie at various points along this continuum. As might be expected, more advanced graduate students exhibited problem solving behaviors and characteristics that were similar to those demonstrated by the faculty participants. The less successful participants, on the other hand, did not solve the problems like the faculty members did. This observation leads to the conclusion that experience with the type of problem being solved directly influences a problem solver's position along the continuum. While the results of this study offer an adequate beginning description of the problem solving continuum, further studies in the area are necessary to fully describe it.

While our conclusions reinforce those of other researchers, we believe our findings expand the understanding of problem solving in novel directions. This works adds to the body of research findings which suggest that problem solving, irrespective of domain, is governed by overriding principles. With this project we have begun to probe the continuum of problem solving abilities, including the characteristics of the continuum, where participants are situated on it, and the factors which affect movement along it. The problem solving behaviors of the participants also indicate that the continuum can be subdivided; our participants can be considered well-versed in organic chemistry, but even so we still see differential abilities in problem solving.

The outcomes of this study provide insight into problem solving within the domain of organic chemistry that might lead to changes in the way organic chemistry is taught that might help students become more like the practicing chemists who dominated the "more successful" category in this study. First, and perhaps foremost, we should consider teaching problem-solving techniques and strategies that are modeled after those of the "most successful" participants in studies of this nature. Robin, one of the faculty members who participated in this study, teaches organic spectroscopy. In observing Robin's approach to teaching combined spectral problems, we noted that she emphasized a consistent, methodical approach to these problems. It is interesting to note that, when faced with such a problem, Robin proceeded in the same consistent way. This strategy might prove more difficult for instructors for whom the knowledge they use in teaching is tacit and so well understood that subtle nuances may be overlooked in the classroom. Robin, however, teaches students to take a consistent approach and follow step-by-step the recommended solution pathway. Her students seem to enjoy the spectroscopy portion of the class, and perform well on the examination covering spectroscopy.

When teaching spectroscopy, Robin instructed students to follow certain steps in a certain order: determine unsaturation; pick salient peaks from IR spectrum to narrow possible functional groups, and draw those functional groups out; mine the ^{1}H NMR spectrum for the number of signals, the splitting of those signals, chemical shift, and integration of signals, and draw out possible connections; placing all draw fragments together to form a structure; and verifying the validity of the final structure against the spectra themselves. Every example Robin taught follows this sequence identically. Robin's participation in this project demonstrated that her expertise in the area of spectroscopy problem solving can (and in this case does) transfer directly into the classroom. Robin's approach to solving such problems mirrors all of the characteristics of the more successful participants in this study, and teaching which is based on these characteristics will promote greater problem solving ability among those just beginning to solve similar problems.

Despite this, sometimes in the classroom it is beneficial to allow students to initially reach conclusions that are incorrect, to illustrate the process which led them there. This teaching approach demonstrates that faulty problem solving strategies often lead to incorrect answers. When presented in the context of the conclusions of this project, such teaching methods will inform students of the most common errors associated with solving combined spectral analysis problems. Therefore, avoiding the problem solving behaviors demonstrated by the unsuccessful participants in this study will allow sophomore students to move toward the successful end of the problem solving continuum.

It would also be useful to consider shifting the focus of problem solving from solution generation to understanding of the process by which problem solving occurs. By thinking about the steps that one takes in solving a problem, the typical pitfalls that a student might face can be emphasized and sidestepped, which can help students avoid common mistakes that interfere with successful performance on the tasks they face in our courses.

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