UNDERSTANDING STUDENT PROBLEM SOLVING IN ORGANIC CHEMISTRY

A Thesis in

Educational Psychology

by

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ABSTRACT

The purpose of this study is to better inform the Chemical Education community regarding the struggles that students face when problem solving in organic chemistry. Participants in an organic chemistry course at a large Mid-Eastern university were asked to think aloud while solving chemical resonance problems. Participants’ written work was scored to determine a high-performance grouping and a low-performance grouping, and think-aloud data (in video form) coded for content knowledge, problem solving strategies, and metacognitive regulation. Only one statistical association was found between performance grouping and the use of any of these codes related to content knowledge or problem solving. The scoring of each participant into their particular grouping was deemed to be with respect to an individual combination of the coded behaviors. These findings and additional observations of the researchers are discussed, and recommendations for instruction are made based on these findings.
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Chapter 1

INTRODUCTION

At the Spring 2016 American Chemical Society (ACS) meeting in San Diego, the symposium organizers highlighted a controversial session entitled “Is There a Crisis in Organic Chemistry Education?” Many of the publishers who presented at this session responded with a resounding “No.” How could we be experiencing a crisis when more resources than ever, including “a wealth of textbooks, electronic study guides, and databases with tens of thousands of questions,” are available to students (Chemical & Engineering News, 2016)? Educators in the audience disagreed with this perspective. They argued that organic chemistry has always been notoriously difficult, and that more students were coming into the classroom with less time to commit to learning than ever before. Given this argument, one educator, Jerome Haky, challenged publishers to move away from materials development to spend more time working with educational researchers to examine how their students learn and what strategies work best when teaching organic chemistry (Chemical & Engineering News, 2016).

To answer the question of what works requires an understanding of the struggles faced by organic chemistry students while learning and problem solving in this discipline. Currently, chemical education research primarily consists of materials development based on assumptions that we are making about why students are struggling. Despite the increasing availability of new materials, students still are not thriving in this discipline.

The purpose of the current study is to examine students’ problem solving in organic chemistry in order to identify the source of their struggles. College students enrolled in an organic chemistry course thought aloud while solving problems. These think-alouds, along with participants’ written work, were coded to reveal aspects of problem-solving that cause the
greatest difficulty. Although this coding began with no assumptions about these causes, our research is guided by an understanding of both the content-specific conceptual and procedural components of problem solving and the general problem solving skills that are necessary. Studying students’ actions as they go through this process will allow us to develop a better understanding of their learning and guide our future research, choice of materials, and teaching practices.

**Defining Problem Solving and Knowledge**

A student solving an organic chemistry problem has many opportunities to make mistakes in both their general problem solving approach and their understanding of the chemistry content, so instructors need to understand each of these factors and how they relate. First, we will define the problem-solving process, and second, we will define types of knowledge.

**Problem solving.** There are many ways in which problem solving has been described in the Educational Psychology literature, but for the purposes of this work, a simple description given by Litzinger, Van Meter, Wright, and Kulikowich (2006) will suffice. They describe the process as four sub-processes, including problem representation, goal setting and planning, plan execution, and solution evaluation. Because it is extremely difficult through observation to differentiate between problem representation and planning, we will be discussing these two processes together, bringing the total number of problem solving steps down to three. One thing to note is that although we are labelling these sub-processes as steps, they are likely to be recursive for a student rather than strictly sequential.

**Knowledge.** Within each problem-solving step, a student must be proficient with the types of knowledge required to complete it successfully. The framework that we will be using to describe the knowledge needed while problem solving includes four knowledge types and two
levels of knowledge quality (de Jong, 1996). The types of knowledge, each based upon the function they are fulfilling in the students’ problem solution, include situational knowledge, conceptual knowledge, procedural knowledge, and strategic knowledge. de Jong (1996) describes the two levels of knowledge quality described are “deep” and “surface” (p. 107). A student’s quality of knowledge is said to be deep if they have “…thoroughly processed, structured, and stored [it] in memory in a way that makes it useful for application and task performance” (de Jong, 1996, p. 107). Deep knowledge is closely tied to a students’ ability to think critically and make inferences. A surface-level quality of knowledge “…is stored in memory more or less as a copy of external information” (de Jong, 1996, p. 107) and is associated with memorization and a trial and error approach to solving problems. Ideally, we are interested in helping our students to develop a deep quality of knowledge that they can draw upon to think critically while solving organic chemistry problems.

**Problem Solving in the Context of Organic Chemistry**

Now that we have defined the structure of the process and types of knowledge that we are interested in, what does problem-solving ideally look like in the domain of organic chemistry? The topic of this study is chemical resonance, so we will be using a resonance problem taken from the study problem set as an example (Figure 1).

Figure 1. Sample problem from the Chemical Resonance Problem Set

For each benzene derivative, determine if the substituent is either electron donating or electron withdrawing using resonance as your justification.

(a) 

![Chemical structure](image)
Planning and problem representation. When attempting to solve a problem, the first step of the process, problem representation and planning, is thought to possibly be the most important (Litzinger et al., 2006). What is meant by problem representation and planning is taking the time to understand the problem’s structure and a probable solution path before beginning to solve it. Forming this initial representation can help the problem solver identify the underlying deep structure of the problem. Problem solvers who fail to execute this step, or do so only minimally, may fail to perceive this deep structure and consequently miss the problem features and principles that are critical for generating an effective solution (Hardiman, Dufresne, & Mestre, 1989). The reason that problem representation and planning are not separated for the purposes of this study is because of the difficulty in separating these constructs from the context of the organic chemistry content and the dynamic nature of the problem-solving process.

Going back to the example given in Figure 1 and de Jong’s (1996) types of knowledge, the representation of this problem would involve the use of situational knowledge, conceptual knowledge, and strategic knowledge. Situational knowledge refers to the knowledge required to accurately dissect the problem statement to identify relevant information. For this problem that information would be the terms “benzene derivative,” “electron donating,” “electron withdrawing,” and “using resonance as your justification.” Independently, the first three terms are types of conceptual knowledge, meaning that they are terms with an associated meaning that the student would need to know to understand the problem. By understanding these terms, the student would know that they need to bring in outside knowledge of the electronic properties of a benzene molecule, and that the problem is asking them whether the electrons belonging to the substituent group flow away from or towards the molecular ring.
A unique quality of organic chemistry content that needs to be discussed, is the coexistence of both text and molecular representations throughout the domain. Because of this coexistence, it is necessary for a student to use molecular representations in the same way that they might use the information given to them in the problem statement itself. To do this, they have to treat the individual atoms, pieces of a molecular structure, or the entire structure as conceptual knowledge. For this example, a student needs to be able to recognize the ring in the structure as being a representation of benzene, therefore connecting this image to what they know about the electronic properties of benzene, and they need to know that the presence of heteroatoms (nitrogen and oxygen, here) means the presence of unseen lone pairs. These lone pairs are shown in Figure 2 and are crucial to a student’s ability to plan and begin a solution approach.

Figure 2. Sample problem from the Chemical Resonance Problem Set with lone pairs assigned.

For each benzene derivative, determine if the substituent is either electron donating or electron withdrawing using resonance as your justification.

(a) ![Chemical structure](attachment:image.png)

This approach is generated from the information gathered during the student’s representation of what the problem actually is and their knowledge of what strategy they should apply to begin their solution. The phrase “using resonance as your justification” would let the
student know that resonant electron movement should drive their solution, and the identification of the lone pairs on the molecule would be their starting point for this solution strategy.

**Plan execution and solution evaluation.** Once a plan has been determined and execution begins, solving a problem rarely proceeds in a linear fashion. Instead, the problem solver will ideally engage in plan execution and monitoring simultaneously as they work through the problem. Monitoring and evaluation represent two components of a recursive process known as metacognitive regulation of problem solving (Winne & Perry, 2000). Planning, as discussed previously, is the first step in this cycle. Monitoring, the second step, takes place when students check their progress while executing a solution. This occurs both when they stop to make sure they are proceeding correctly and when they stop because they detect a mistake or reach an impasse. Evaluation is the third and final step, and it is very similar to monitoring, but instead refers to the determination of whether or not a final problem solution is satisfactory or needs to be revised.

The difficulty that lies here is in whether or not students productively engage in this regulative process effectively as they are problem solving; do students stop to check their progress at all or even take notice when they have made a mistake? In theory, the closer students are to the level of an expert the more automatically they will engage in productive metacognitive regulation, as this process depends on students’ domain knowledge to both determine a mistake and correct it (Schraw, 2006).

Returning to our example, the next step students would take is beginning to execute the plan they formed after representing the problem. Plan execution will require students to use conceptual, procedural, and strategic knowledge. Conceptual knowledge comes into play in the interpretation of what static components of the molecular representations mean, as described in
the previous step. Procedural knowledge is the active combination of these conceptual pieces in a strategic way (de Jong, 1996). As the students continue their solution, they will need to use the identified lone pair electrons as a starting point and then add in electron movement arrows that will indicate what the next form of the molecule will look like. The way that an electron movement arrow is allowed to flow is an example of a constraining function of this representation (Ainsworth, 1999). In other words, the arrow is bound by chemical principles saying that it may only move electrons away from a more negative location towards a more positive location.

Once the next molecular representation has been determined by the students, they will need to use the process of monitoring to determine whether the actions taken have been correct, and if they determine that a mistake has been made, they will need to re-engage in problem representation to determine a new strategy if necessary, subsequently invoking their strategic knowledge once again. This type of knowledge also comes into play in determining the overall order in which solution steps should be taken (de Jong, 1996). The final step in this process is the evaluation of their solution. This is done for a resonance problem by assigning the formal charges of any heteroatoms in the molecule that resulted from electron movement in the previous step, combining the use of both conceptual and procedural knowledge (Figure 3). These three conceptual and, when combined, procedural components—lone pair electrons, electron flow arrows, and formal charges—are visual representations of the types of knowledge that we have discussed here, so in our experimental coding scheme we will be referring to the labelling of these components as content knowledge codes. This does not indicate that they represent all content knowledge in the domain of organic chemistry, but that they represent three fundamental and necessary components of this domain.
Other strategies of importance. From start to finish, ideal students solving a problem will go through the process by first planning their solution, monitoring their progress as they move forward, stopping to correct any errors or change their solution approach, and finally confirming that their final solution is accurate. However, engaging in this regulative process is not necessarily an easy or automatic behavior for students, and it has been shown that providing them with training in using this strategy is an effective way to improve their problem-solving performance (Bielaczyk, Pirolli, & Brown, 1995). The same study that demonstrated this finding also found that training students in another strategy, self-explanation, further increased their ability to solve problems using the deep structure of content with which we want our students to engage.

Self-explanation describes the use of the underlying principles of material to generate inferences while learning or solving problems (Chi, 1994). It is a learning strategy that has been found to increase students’ ability to learn in contexts where multiple representations are present (Berthold, Eysink, & Renkl, 2009) and has been found to be utilized heavily to increase the
understanding of students who are good problem solvers (Chi, Bassok, Lewis, Reimann, & Glasser, 1989). Self-explanation may be further broken down into two types that may be used effectively by learners: principle based and anticipatory (Renkl, 2002). Principal-based self-explanation refers to a student’s ability to explain an aspect of or allowable move within a problem using the deep structure of the domain. Anticipatory self-explanation is said to have occurred when a student uses the fundamental domain principles to predict events that will occur or actions that will need to be taken down the road in a problem solution.

While this strategy has frequently been described as an effective learning technique, the question has been asked, “Is self-explanation while solving problems helpful?” (Neuman & Schwarz, 1998). The answer to this question is yes, because the strategy performs the same cognitive function—filling in knowledge gaps through principle-based inference—whether the student is learning material or reasoning through a problem. In addition to the benefits of self-explanation mentioned thus far, it has also been shown to promote both near and far transfer of knowledge while problem-solving and an improved ability to perform the metacognitive self-regulation that has been discussed (Rittle-Johnson, 2006; Wong, Lawson, & Keeves, 2002; Crippen & Earl, 2007). One final behavior that has been noted by Chi (1989) while studying students’ self-explanation abilities is information seeking. She reported that more successful students, those who presented the highest number of self-explanations while problem-solving, also sought out additional information most frequently when they reached an impasse.

**Current Study**

As described, there are many potential sources for students’ difficulty solving problems in organic chemistry, making it difficult for us to determine which materials or teaching practices will be the most effective. To address this problem, the current study employed a think-aloud
protocol combined with observation of the participants’ problem solving behaviors using first-person perspective video data. Additionally, through scoring of the participants’ paper answers to the study problem set, both a high and low-performing participant group was determined.

The overarching research question guiding the analysis was, “Why do students struggle when problem solving in organic chemistry?” We hypothesized that there would be three possible ways in which this question could be further explored, which became three additional sub questions:

- Is there an association between performance grouping and content knowledge codes?
- Is there an association between performance grouping and participants’ application of problem solving codes?
- Are participants within each group using content knowledge codes and problem solving codes in similar ways to one another or different ways from one another?

Based on what is known about the problem-solving constructs described in our introduction, we expected to find an association between grouping and both content knowledge codes and application of problem solving processes. Additionally, we expected to observe themes in the way participants within each group approached solving these problems.
Chapter 2

METHODS

Participants

A total of 20 students from an Organic Chemistry I course at a large Mid-Atlantic research university participated in the experiment. Of these students, 12 provided sufficient data for analysis. Five students experienced technical malfunctions resulting in the loss of data, two students failed to provide adequate verbalization for analysis of the think-aloud portion of the experiment, and one student was considered to be an outlier for the experimental analysis due to lack of prior knowledge. Of the 12 participants included in study, 2 were in their third or fourth semester of college, 7 were in their fifth or sixth semester of college, and 3 were in their seventh or eighth semester of college. The reported majors of these students included Kinesiology, Pre-Medicine, Immunology and Infectious Disease, Biomedical Engineering, Biobehavioral Health, Chemical Engineering, and Biological Engineering. Five students identified as male, seven identified as female, and they had an average age of 19.7 years. Twenty-five percent of these students reported their ethnicity as Asian, and the remaining 75% reported their ethnicity as Caucasian.

During analysis, these 12 participants were divided into two groups through the scoring of their written work from the experiment. Four participants scored into the high-performance group, five participants scored into the low-performance group, and two scored between these groupings and were removed from the data analysis to make sure that the two groups were removed from one another with regard to score. One other participant was removed from the analysis as an outlier because her performance was much lower than the other participants in the low-performance group, indicating insufficient knowledge of the topic to be useful for this
analysis. A more detailed description of the demographic characteristics of each participant within the high and low groups are given in Table 1 and Table 2. In addition to these descriptions, the high-performance group received an average final course grade of 95.7 (90.59 - 97.82) and the low-performance group received an average final course grade of 86.7 (83.42 - 90.71). It is important to note that the low-performance participants are not struggling significantly in their organic chemistry course, indicating that they do have a grasp of the content in general, but still have room for improvement in their understanding.

Table 1

<table>
<thead>
<tr>
<th>Participant</th>
<th>Gender</th>
<th>Ethnicity</th>
<th>Age</th>
<th>Semester Standing</th>
<th>Major</th>
<th>Cumulative GPA</th>
<th>Sciences Courses</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Male</td>
<td>Caucasian</td>
<td>20</td>
<td>5th-6th</td>
<td>N/A</td>
<td>3.54</td>
<td>9</td>
</tr>
<tr>
<td>9</td>
<td>Female</td>
<td>Caucasian</td>
<td>21</td>
<td>7th-8th</td>
<td>Biobehavioral Health</td>
<td>3.56</td>
<td>17</td>
</tr>
<tr>
<td>17</td>
<td>Male</td>
<td>Caucasian</td>
<td>20</td>
<td>5th-6th</td>
<td>Biological Engineering</td>
<td>3.75</td>
<td>N/A</td>
</tr>
<tr>
<td>18</td>
<td>Male</td>
<td>Caucasian</td>
<td>N/A</td>
<td>5th-6th</td>
<td>N/A</td>
<td>3.8</td>
<td>11</td>
</tr>
</tbody>
</table>
Significantly more females in this study scored into the low-performance group than the high-performance group. While there is no hypothesis provided as for why this might have occurred, it is important to mention that spatial ability plays a significant role when learning organic chemistry (Bodner & Domin, 2000). Although this is not something that is addressed in this study, others have found that women tend to possess lower rotational spatial ability than men (Dabbs, Chang, Strong, & Milun, 1998), which could in some cases be related to lower performance in an organic chemistry course.

### Materials

The experiment consisted of two parts for each participant: eye-tracking in Part I and problem-solving while thinking-aloud in Part II. The topic of the experiment, chemical resonance, had been taught in the course prior to the start of the data collection, and the students’ knowledge of resonance had recently been tested in class. This topic was chosen by the instructor, who we had asked to reflect upon areas of consistent difficulty for students in the

<table>
<thead>
<tr>
<th>Participant</th>
<th>Gender</th>
<th>Ethnicity</th>
<th>Age</th>
<th>Semester Standing</th>
<th>Major</th>
<th>Cumulative GPA</th>
<th>Sciences Courses</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Female</td>
<td>Caucasian</td>
<td>19</td>
<td>5th-6th</td>
<td>Immunology</td>
<td>3.3</td>
<td>13</td>
</tr>
<tr>
<td>10</td>
<td>Female</td>
<td>Asian</td>
<td>20</td>
<td>5th-6th</td>
<td>N/A</td>
<td>3.5</td>
<td>20</td>
</tr>
<tr>
<td>11</td>
<td>Female</td>
<td>Caucasian</td>
<td>20</td>
<td>7th-8th</td>
<td>N/A</td>
<td>3.46</td>
<td>13</td>
</tr>
<tr>
<td>16</td>
<td>Male</td>
<td>Caucasian</td>
<td>N/A</td>
<td>3rd-4th</td>
<td>Chemical Engineering</td>
<td>3.6</td>
<td>9</td>
</tr>
<tr>
<td>19</td>
<td>Female</td>
<td>Caucasian</td>
<td>19</td>
<td>5th-6th</td>
<td>Biomedical Engineering</td>
<td>3.55</td>
<td>14</td>
</tr>
</tbody>
</table>
years she had been teaching the course. As mentioned, this topic is unique in that students struggle to identify a definitive endpoint for resonance problems in the same way that they can for other Organic Chemistry problems.

**Demographic survey.** Before beginning the experiment, the participants were asked to provide written consent and complete a demographic survey (Appendix A). This survey included questions asking participants about their semester standing, gender, ethnic background, grade point average, major, Scholastic Aptitude Test (SAT) scores, and the number of science courses they had taken including any taken in high school. Many participants either were not certain of or did not provide their SAT scores, so these data were not used for this experiment.

**Experimental text.** The text used in the experiment contained a general description of chemical resonance and was taken from an Organic Chemistry textbook (Appendix B). This text was selected in consultation with the course instructor because it provided information beyond what had been taught in the course and was of the same comprehension level as the students’ other course materials. Originally, we had intended to use the study of this text to gain insight into participants’ learning processes. However, the students perceived the experimental text to be too similar to their course text, and did not engage with it meaningfully.

**Experimental problem set.** Participants also received a packet containing four open-ended problems, written by the instructor, pertaining to chemical resonance (three of which were broken into two parts, a and b). For the purpose of subsequent data analysis, there were seven problems total. The first two problems, taken from an optional homework set in the course, served as practice for thinking aloud. The remaining five problems presented to the participants were more applied than the problems they had previously encountered in class in that they asked...
them to use resonance in conjunction with other organic concepts. A sample problem from this set is given in Figure 1, and the full problem set is provided in Appendix C.

**Think-aloud recording device.** To record participants’ think-aloud data, a GoPro HERO4 was utilized. The participants were asked to wear this on their heads so that the lens was pointing down at their written work as they progressed. This provided the researchers with both audio data and a visual of the participants’ actions.

**Procedures**

Each experimental session was held individually in a university lab, and there were two parts per session: eye gaze tracking and think-aloud protocol while problem solving.

**Part I.** In Part I of the experiment, each participant was asked to read the text on the topic of chemical resonance while having their eye gaze pattern tracked using a Tobii Pro eye gaze instrument. Before beginning, they were instructed that they could take as much time as needed to complete the task and that they could move forward in the text but not back. They were also informed that they would be asked to complete a post-test after reading this information. The students spent approximately 5 minutes completing this portion of the experiment, ensuring that each participant had exposure to the experimental text. Participants did not use this text in the manner intended, and thus data associated with this portion of the experiment were not analyzed further.

**Part II.** After completing the reading, all participants were asked to place the GoPro camera on their heads so that the lens pointed down at the materials with which they would be working. They were then provided with the same text that they had just read in Part I and the resonance problem set. The text was provided so that the participants would be able to search for any relevant material while trying to complete the problem set, and they were instructed that they
could use this text as little or as much as they liked while they were working. Each participant was then asked to think aloud while working through these problems at their own pace, with the ability to go back to a problem or skip ahead at any point in time. The first two problems in the problem set (problems 1a and 1b) were provided as practice problems for the think-aloud procedure and were later determined to be useful for the experimental analysis after all of the participants had completed the experiment. The think-aloud sessions were conducted without interference by the researcher, other than prompting of the student to continue to think aloud as needed.

**Coding and Scoring**

Both the written work and video data collected for each participant were analyzed independently. The following schemes describe the way in which this was done.

**Problem solving scores.** To determine performance groups, the participants’ written work was scored using a key provided by the instructor of the course (Appendix D) and a rubric developed by the researchers (Table 3).

<table>
<thead>
<tr>
<th>Problem</th>
<th>Score of 0</th>
<th>Score of 1</th>
<th>Score of 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Incorrect or incomplete answer provided.</td>
<td>Correct answer is provided, but the participant either continued to provide incorrect resonance structures beyond the final answer set or failed to label the correct formal charges on their final answer.</td>
<td>Correct answer is provided and labelled with the correct formal charges.</td>
</tr>
<tr>
<td>1b</td>
<td>Incorrect or incomplete answer provided.</td>
<td>Correct answer is provided, but the participant either continued to provide incorrect resonance structures beyond the answer or failed to label the correct charges on their final answer.</td>
<td>Correct answer is provided and labelled with the correct formal charges.</td>
</tr>
</tbody>
</table>
In the process of scoring the paper data, two of the questions (problems 3a and 3b) were removed from the analysis, and thus are not included in the rubric given above. These questions were not consistently responded to by the participants on paper, with several participants responding verbally, because there was no required molecular structure to be drawn in the solution. Because the written responses were scored separately from the video data, the responses to these questions were not considered to be reliable by the researchers. A maximum total score of 10 points was possible for the entire problem set.

**Problem solving codes.** Two categories of codes were used in the analysis of the video data: content knowledge codes and problem solving codes. The codes describing participants’ use of content knowledge represented the three concepts described previously: lone pairs, electron flow arrows, and formal charges. Each participant could receive 1 point per problem for the correct use of each concept. This resulted in a maximum score of 21 points per participant for the entire problem set (3 points per question).
The problem-solving codes included both codes representing strategies and codes representing metacognitive actions. The problem-solving strategies included procedural organization of content knowledge, information seeking, self-explanation, and planning/problem representation. These codes were not all assigned in the same way. One point was assigned for the use of procedural organization and information seeking per problem, resulting in a maximum score of 7 for each independent strategy (maximum score of 14 per participant combined). Self-explanation and planning/problem representation were scored differently. There was no limit for how many times these events could be recorded, so scores had the potential to range from zero to infinity for each participant.

Finally, metacognitive events, which were represented by a singular monitoring and evaluation code, were coded for each participant. Similar to self-explanation and planning/problem representation events, there was no limit on the number of codes assigned for metacognitive events. These codes were developed through the consultation of two raters, both of whom possessed a background in chemistry; furthermore, a summary of the codes, their counts, and examples from the video data are given in Table 4.

Table 4

*Codes describing participant behaviors*

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
<th>Counts</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Content Knowledge</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Lone Pairs</em></td>
<td>Participant correctly assigns lone pair electrons on nitrogen and oxygen atoms in each molecule.</td>
<td>0 – 21</td>
<td>• The participant is observed assigning the lone pair electrons and may or may not describe what they are doing.</td>
</tr>
<tr>
<td>Electron Flow Arrows</td>
<td>Participant correctly draws in arrows indicating electron movement.</td>
<td>0 – 21</td>
<td></td>
</tr>
<tr>
<td>----------------------</td>
<td>---------------------------------------------------------------------</td>
<td>--------</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• The participant is observed assigning all electron flow arrows and may or may not describe what they are doing.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Formal Charges</th>
<th>Participant correctly assigns formal charges present in each molecule.</th>
<th>0 - 21</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• The participant is observed assigning all formal charges and may or may not describe what they are doing.</td>
<td></td>
</tr>
</tbody>
</table>

**Problem Solving**

**Strategies**

<table>
<thead>
<tr>
<th>Procedural Organization</th>
<th>Participant assigns all three content knowledge codes (Lone Pairs, Electron Flow Arrows, and Formal Charges) in an organized and meaningful way.</th>
<th>0 - 7</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• The participant is observed assigning the lone pairs, electron flow arrows, and formal charges methodically for the entire problem. They may or may not describe what they are doing.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Information Seeking</th>
<th>Participant seeks additional information to assist them in solving the problem.</th>
<th>0 - 7</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• The participant is observed either looking through the text that was provided or looking back at their previous work to help them solve a new problem.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Self-Explanation</th>
<th>Participant explains an aspect of the problem or their solution process using content knowledge principles. All observed instances of self-explanation</th>
<th>0 - Unlimited</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• The participant describes why something would or would not be allowed using the ideas of formal charge, octet,</td>
<td></td>
</tr>
</tbody>
</table>
were principle-based, rather than anticipatory.

**Planning/Problem Representation**

Participant uses either general knowledge about the type of problem or content specific knowledge to plan how they will generate a solution or begin the problem. As described in the introduction, problem representation is not separated from this code, because of the difficulty in separating these two constructs.

### Metacognition

**Monitoring/Evaluation**

Participant checks their progress as they move through a problem. This includes instances in which no error is detected through the process and instances in which an error is detected. Evaluation, or checking that a final answer to a problem was satisfactory, is included in this code.

**Detected Error:**

- The participant stops and says “…wait.” (Indicating that something is wrong.)
- The participant verbally indicates that their current step or final solution is wrong in some way.

**Did not Detect Error**

- The participant says, “Yeah,” after checking their works then moves on.
- The participant is observed moving their pen to silently check over the structure they have
The participant mumbles while moving their pen to count bonds or electrons. (They did this while making solution progress, not as a reaction to making a mistake.)

The coding of these data was performed in three cycles to provide an increasingly comprehensive picture of the participants. In the first cycle, all of the codes provided in Table 4 were assigned for each participant to determine any statistical differences in the performance of each group. During the second cycle, the monitoring and evaluation codes were separated into instances in which a participant detected an error and instances in which they detected no error after monitoring or evaluation (also described in Table 4). Once this separation was completed, the researchers recorded the participants’ responses to each instance of error detection to determine any differences in response between groups. Finally, in the third phase of coding, the researchers recorded a comprehensive picture of each participant to understand how each of the individual components that were measured up to this point were working together.
Chapter 3

RESULTS

Before beginning the analysis, performance scores were derived from the rubric described in Table 3, and the participants were mapped onto a distribution (Figure 4). This distribution was then used to determine performance groupings for subsequent analyses.

Participants scoring a 3 or 4 were considered to be the low-performance group, and participants scoring a 6 or 7 were considered to be the high-performance group. The participant who scored a 1 was considered to be an outlier on the basis of her performance characteristics in comparison to the other participants in the low-performance group. The middle group of participants with a score of 5 (3 participants) were excluded from further analysis on the basis that their inclusion had the potential to confound any true differences between the groups.

Once groups had been determined, the analysis proceeded in three cycles that were parallel to the coding cycles described in the methods section. The first cycle examined
statistical differences between the participant groups, the second examined the participants’ responses to errors in their solutions and looked for differences in responses between the groups, and the third cycle examined the participants holistically to determine any differences by group.

**Cycle I**

Cycle I corresponded with two research questions: “Is there an association between performance grouping and content knowledge,” and “Is there an association between performance grouping and problem solving ability.” This cycle specifically looked for any statistical differences between the content knowledge and problem solving codes of the two performance groups.

**Grouping associations with content knowledge.** The first research question, “Is there an association between performance grouping and content knowledge,” was answered by performing Chi Square independent samples testing, because of the non-continuous nature of the data. These tests examined the frequency of the high and low groups’ accurate use of each of the content knowledge codes; three separate tests were performed. A perfect score for a participant for one of these categories (meaning that they used a single concept correctly for each problem) is a frequency of 7, so the maximum frequency for each code for the low-performance group as a whole is 35 and the maximum frequency for the high-performance group is 28. As described in the introduction and methods, consistent use of these concepts is a positive behavior, so a higher score is desirable. Table 5 contains the data used to perform this testing. Uncorrected Chi Square values were used, and each of the expected cell values was proportionally corrected for the difference in high-performance and low-performance group sizes.
Table 5.

**Counts of high- and low-performance participants’ use of content knowledge codes.**

<table>
<thead>
<tr>
<th></th>
<th>High N=4</th>
<th>Low N=5</th>
<th>Combined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lone Pairs</td>
<td>21</td>
<td>27</td>
<td>48</td>
</tr>
<tr>
<td>Electron Pushing Arrows</td>
<td>23</td>
<td>28</td>
<td>51</td>
</tr>
<tr>
<td>Formal Charges</td>
<td>22</td>
<td>26</td>
<td>48</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>66</strong></td>
<td><strong>81</strong></td>
<td><strong>147</strong></td>
</tr>
</tbody>
</table>

The calculated Chi Square values for lone pairs (0.01, \( p = 1.00 \)), electron pushing arrows (0.01, \( p = 1.00 \)), and formal charges (0.04, \( p = 1.00 \)) did not reach significance, indicating that there was no association between performance grouping and the use of any of these concepts. This and the high usage of each concept by both groups was surprising because there is an implicit assumption amongst instructors in this discipline that students struggle to identify, label, and use these molecular characteristics. The current data shows that this is not the case.

**Grouping association with problem solving ability.** The second research question, “Is there an association between performance grouping and problem solving ability,” was answered by two separate analyses. First, Chi Square independent samples testing was used to examine associations between performance grouping and use of each problem-solving code (four separate tests, each corrected for the uneven ratio between groups). Tables 6 and 7 contain the raw cell values used to perform the Chi Square tests. Uncorrected Chi Square values were used with the exception of the Planning code, and each of the expected cell values was proportionally corrected for the difference in high-performance and low-performance group sizes. Because there was a count of 4 in the cell representing the Planning events coded for the high-performance group, the corrected Chi Square value was used.
Table 6.

**Counts of high- and low-performance participants’ use of problem solving codes.**

<table>
<thead>
<tr>
<th></th>
<th>High N = 4</th>
<th>Low N = 5</th>
<th>Combined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Procedural Organization</td>
<td>16</td>
<td>26</td>
<td>42</td>
</tr>
<tr>
<td>Information Seeking</td>
<td>4</td>
<td>10</td>
<td>14</td>
</tr>
<tr>
<td>Self-Explanation</td>
<td>27</td>
<td>47</td>
<td>74</td>
</tr>
<tr>
<td>Planning/Problem Rep.</td>
<td>4</td>
<td>17</td>
<td>21</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>51</strong></td>
<td><strong>100</strong></td>
<td><strong>151</strong></td>
</tr>
</tbody>
</table>

The Chi Square values calculated for organization (.69, \( p = .502 \)), information seeking (1.43, \( p = .354 \)), and self-explanation (1.9, \( p = .207 \)) did not reach significance. The Chi Square value calculated for planning/problem representation (5.49, \( p = .034 \)) was found to be statistically significant, indicating more frequent performance of this behavior by the low-performance participants. Previous research indicates that, typically, higher performance is associated with a greater degree of information seeking, self-explanation, and planning/problem representation behaviors (Chi, Feltovich, & Glaser, 1981; Chi, Bassok, Lewis, Reimann, & Glaser, 1989). In this case, however, the trends observed were opposite to that expectation despite not reaching significance, particularly with regard to information seeking. This theme will be discussed in greater detail when describing participants’ behaviors upon encountering an error.

Table 7.

**Counts of high- and low-performance participants’ use of metacognitive codes.**

<table>
<thead>
<tr>
<th></th>
<th>High N = 4</th>
<th>Low N = 5</th>
<th>Combined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monitoring/Evaluation (No Error)</td>
<td>49</td>
<td>58</td>
<td>107</td>
</tr>
<tr>
<td>Monitoring/Evaluation (Error)</td>
<td>22</td>
<td>26</td>
<td>48</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>75</strong></td>
<td><strong>101</strong></td>
<td><strong>176</strong></td>
</tr>
</tbody>
</table>
The Chi Square values calculated for monitoring and evaluating when an error was not detected (.08, \( p = .863 \)) and monitoring and evaluating when an error was detected (.04, \( p = 1.00 \)) did not reach significance. By definition, the low-performance group made a greater number of mistakes than the high-performers and thus should have had more opportunities to detect error, which makes a lack of difference in the two groups’ metacognitive codes interesting.

**Phase II**

Phase II consisted of the second analysis used to answer the research question: “Is there an association between performance grouping and problem solving ability.” The purpose of this phase was to determine if there was a difference in the response of participants within each group to the detection of an error in their problem solutions.

**Responses to error.** The second analysis examining the participants’ problem solving ability was a content analysis of their actions following an error. After a participant was observed detecting an error while monitoring or evaluating, their response was recorded by the researchers. Those responses were then coded for general themes to further explore the groups’ problem solving abilities. These themes are organized in Table 8, along with the number of instances each response was recorded per group (total number of times as opposed to number of individuals who performed the behavior).
Table 8.

*Participant responses to error detection, and the number of times the response was recorded per group.*

<table>
<thead>
<tr>
<th>Response</th>
<th>High N = 4</th>
<th>Low N = 5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>22 Total Responses</td>
<td>26 Total Responses</td>
</tr>
<tr>
<td>The participant asks the researcher a clarifying question about the problem.</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>The participant moves on without further progress towards a solution.</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>The participant moves on from the problem and later returns to solve it.</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>The participant thinks silently before moving forward with a problem solution.</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>The participant seeks information in the text or previous solutions to help solve the problem.</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>The participant verbally talks through their current problem scenario.</td>
<td>0</td>
<td>6</td>
</tr>
<tr>
<td>The participant returns to a previous solution attempt that they had discarded or decides their current solution is not incorrect.</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>The participant responds to error detection with trial and error.</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>

Within the high-performance group, 22 total responses and 5 of the major themes were observed. From these observations, the high-performance participants appeared more likely to
either move on entirely or jump straight into trying another solution route than the low-performance participants. This suggests that they may be more confident in the boundaries of their content knowledge. Additionally, many of the students in this group paused for long periods of silence, which may have been indicative of periods of internal self-explanation that we were not able to code.

Within the low-performance group, 26 total responses and 6 of the major themes were observed. Several points were interesting about the low-performance groupings responses to error detection. First, they sought out further information when needed, which was not observed at all in the high-performance group when they reached an impasse. However, when they did so, they were observed scanning only molecular structures in the text or previous problems for surface similarities. Second, this group talked throughout their responses, which in some cases coincided with a self-explanation code, which was not observed in response to error detection by the high-performers (although they may have been doing this silently). Third, this group exhibited more uncertainty in their content knowledge by moving backwards towards previous solutions when they detected an error in their current solution.

Phase III

Phase III consists of the third research question: “Are students within each group using content knowledge and problem solving skills in similar ways to one another or different ways from one another?” This question examines each participant as a whole to understand the way in which all of the factors looked at thus far worked together for each individual. It additionally looks at whether the participants in a group used all of these factors similarly to one another, and if so, how this compared between groups.
Similarity of participants within groupings. The third question was answered by looking at a holistic picture of each participant and how they used all of the factors measured thus far together (raw data for all participants given in Appendix E). Additionally, any interesting characteristics or reasonable inferences that might be made by the researchers were noted. We were primarily interested in noting whether or not the participants within each group were similar to one another holistically, and if so, whether there was a fundamental difference between groups. Holistic descriptions of two participants from each group are given.

High-performance group. Participants 9 and 17 will be described within the high-performance group

Participant 9. Participant 9 was a Caucasian, 21-year-old female who was a Biobehavioral Health major entering into her fourth year of college. Her cumulative GPA was a 3.56, and she reported having taken 17 science courses including those she took in high school. While completing the problem set, she used the content knowledge concepts coded in 20 out of 21 total instances, used these concepts procedurally for all 7 problems, did not seek outside information, and performed self-explanation 8 times. She performed metacognitive planning once, monitoring and evaluation 15 times with no error detection, and monitoring and evaluation with the detection of an error 4 times. When she did detect errors, she used trial and error to find a solution twice and decided to move on without attempting to find a solution at all twice.

Overall, this participant was very meticulous in labelling every important molecular characteristic as she went along, and this, in addition to the speed at which she moved, made her appear to be very procedurally practiced with these types of problems. Throughout the experiment, she gave the impression of low confidence in her own abilities by using phrases like, “I’m terrible at resonance so…,” and saying, “I suppose,” and, “I think,” very frequently. One
possible reason for this may be the difficulty of determining an endpoint for each problem at a novice level of knowledge. The only points at which she used inference and self-explanation were in the final two problems of the experiment, which were the most different from the work that the participants had encountered in class.

To the researchers, it appeared as though this participant scored into the high-performance group because of her diligence in studying these types of problems. She was very adept at the procedural steps required for each solution, but she did not frequently draw upon the chemical concepts underlying these procedures until the end of the problem set.

**Participant 17.** Participant 17 was a 20-year-old, Caucasian, male who was majoring in Biological Engineering and was entering into his third year of college with a 3.75 GPA. He did not report the number of science courses he has taken. As he completed the problem set, he assigned important molecular characteristics in 10 out of 21 total instances and did this in a procedural way for 4 out of the 7 problems. He sought information from the information packet or problem set 3 times, and he performed self-explanation 4 times. Additionally, he performed metacognitive planning once, monitoring and evaluation without error detection 4 times, and monitoring and evaluation with error detection 11 times. After error detection, he asked a clarifying question about the problem twice, took a trial and error approach towards solving the problem 4 times, silently considered his work for an extended period 4 times, and moved on to return to the problem later once.

This participant was not meticulous and procedurally competent in the same way as Participant 9. However, he very frequently caught himself when he made mistakes and was very comfortable using appropriate chemical language, which may indicate a greater conceptual understanding than Participant 9 possessed. He did not think-aloud comfortably, which seemed
to affect the number of codes that were present in his final data set. For example, he spent extended periods of time thinking silently before the start of every problem and every time he made a mistake, which may have been coded as self-explanation or metacognitive events if he had shared these thoughts. Overall, his placement into the high group appears to be less likely to do with practice with the surface features and procedural aspects of this material, and more likely to do with an understanding of the deep structure of the knowledge.

**Low-performance group.** Participants 10 and 16 will be described within the low-performance grouping.

**Participant 10.** Participant 10 was an Asian, 20-year-old female in her third year of college. She had a cumulative GPA of 3.5 and reported having taken 20 science courses, including those she took in high school. She assigned fundamental chemical concepts in 6 out of 21 instances and did this in a procedural way for 2 out of 7 total questions. She sought information 4 times and performed self-explanation once. She also used metacognitive planning twice, monitoring and evaluation 8 times without the detection of an error, and monitoring and evaluation with the detection of an error 5 times. Upon detection of an error she sought information three times and moved on without further attempts twice.

Participant 10 was very clearly uncomfortable with this topic. She made statements that indicated this several times and skipped over the two practices problems which were the most similar to the course content that had been covered recently. She also used phrases such as, “I think,” “I’m just gonna go with,” and “I’m guessing,” very frequently. When she assigned molecular characteristics, she did so in an uncertain way, and she used molecular terminology incorrectly towards the end of the problem set. Out of all of the participants studied, she spent the most time searching the text provided for surface similarities between the molecules provided
in the text and the problem solution she was generating. Her lack of strong content knowledge was most likely why she scored into the low-performance group.

Participant 16. Participant 16 was a Caucasian male who was in his second year of college as a Chemical Engineer. He had a cumulative GPA of 3.6 and reported having taken 9 science courses including those he had taken in high school. He assigned important molecular characteristics 18 out of 21 times and did so procedurally for 4 out of the 7 problems. He also used metacognitive monitoring 4 times, monitoring and evaluation without error detection 12 times, and monitoring and evaluation with the detection of an error 7 times. Upon detection of an error, he corrected his mistake using self-explanation 3 times, returned to an incorrect previous solution twice, and arrived at the correct answer after silent reevaluation of his solution twice.

This participant behaved very differently from Participant 10. He was very good at verbalizing his explanations using correct chemical principles, but he often focused his attention on isolated parts of molecules rather than a more global representation of the problem. This not only led him to the wrong answer for a few of the problem sections, but it also assisted him in cases where focusing on just the reactive site appropriately reduced his cognitive load. His low frequency of labelling important molecular characteristics appeared to contribute to his struggle in identifying the most important attributes of some of the molecules.

Summary. By examining two very different participants in both the high-performance group and the low-performance group, it becomes clear that there is no one factor separating the performance of these students. Instead, each student scored into their respective group through an individual combination of successful or unsuccessful behaviors.
Chapter 4

DISCUSSION

Summary of Findings

This experiment examined the content knowledge and problem-solving characteristics of students in organic chemistry, with the intent of clarifying which teaching practices might be the most effective for instructors to employ. Video data were collected in which a group of high-performing and low-performing participants thought aloud while solving organic chemistry problems, and through the use of both statistical and qualitative analyses, the problem-solving characteristics of these groups were examined. Chi square tests determined that there were no significant associations between grouping and number of observed content knowledge (lone pair electrons, electron pushing arrows, and formal charges), problem solving (procedural organization, information seeking, self-explanation, and planning/problem representation), and metacognitive (monitoring and evaluation) codes. However, qualitative analysis of all of these codes combined revealed that each participant within the high- and low-performance groupings exhibited a very unique combination of behaviors leading to their group placement.

Implications

Findings. At the beginning this study, we had several expectations of what we would find, but were surprised that none of these hypotheses held. We expected the weaker participants to struggle to accurately and consistently engage with the procedural concepts of labelling lone pairs, electron pushing arrows, and formal charges, but instead found that these concepts were correctly used by both strong and weak problem-solvers. We also expected to find that the stronger problem-solvers were more frequently using problem solving strategies and metacognitive regulation. No significant differences were found between the groups with regard
to these aspects, which included procedural organization of their problem solutions, information seeking, self-explanation, and monitoring and evaluation of their work. Statistical significance was found when examining differences in the groups’ use of planning/problem representation, with low-performance students performing more instances of this behavior. Despite the lack of statistical significance in the differences between groups with regard to the use of problem solving strategies, such as procedural organization, information seeking, self-explanation and planning, the use of these behaviors was in fact more frequently observed in the weaker problem-solvers. The placement of participants into the low-performing and high-performing problem-solving groups ultimately appeared to be individual for each participant, with each participant possessing their own strengths and weaknesses, leading to their final scores.

Observations made by the researchers outside of the specific coding scheme used were also interesting. It was observed in several cases that the participants were not confident in their ability regardless of the ultimate group into which they ended up scoring. This was indicated by the use of phrases such as, “I can’t…this is like my hardest…” and “I’m terrible at resonance.” A similar finding was a lack of confidence in their final solutions. We noted in our introduction that resonance is a unique topic in organic chemistry, because a final solution state is not obvious to novice problem-solvers. This was most likely the cause of the uncertainty observed in participants when evaluating their solutions, including the solutions they provided to the first two problems in the set, which were taken from homework questions they had previously had access to in the course.

Other observations included frequent scanning of the surface features of molecular structures to generate solutions, both in the text provided and between problems in the set, a lack of problem representation in both groups, and a nearly equivalent occurrence of error detection
in both groups. We would have expected to see more error detection in the low-performing group because, by definition, they had a higher number of errors present in their work.

**Application to instruction.** The most important implication for instructors to take away from this work is that there appears to be no proverbial “magic bullet” for teaching organic chemistry. Furthermore, although it is frequently pre-supposed that very strongly emphasizing procedures will lead to the greatest success, this alone is not enough. These data show that students are very individual in their needs and abilities, and that they must be instructed in how to understand organic chemistry content, problem solving, and ways that they can strategically connect these pieces.

Teaching students a learning strategy, such as self-explanation, is a great way to promote the use of the deep structure of course content (Chi, De Leeuw, Chiu, & LaVancher, 1994). As previously mentioned, this learning strategy has been found to typically be used most frequently by strong learners and problem-solvers (Chi, Bassok, Lewis, & Reimman, 1989). Additionally, it has been found to promote better learning in scenarios where the integration of multiple representations is required (Berthold, Eysink, & Renkl, 2009), which is the case in an organic chemistry classroom.

Instructors can use two methods to teach students how to use this strategy. The simplest of these is to model their own thought processes while demonstrating a problem solution for students. By saying, “I’m moving the electrons from here to there because…,” the instructor is telling the students both that they procedurally move electrons and that they do it in a certain way that obeys fundamental organic principles. A way to get students to practice doing this on their own is to incorporate semi-structured leading questions into students’ homework or to give them a list of fundamental principles in addition to a problem set that they must use to explain
their actions as they generate a solution (Berthold, Eysink, & Renkl, 2009; Fiorella & Mayer, 2012). However, care is needed when wording these questions to make sure that they are not too open for student interpretation, as this has been found to be less effective than a more structured question that draws upon their knowledge of fundamental principles (Berthold, Eysink, & Renkl, 2009).

One additional finding important for instructors to be aware of is that the participants in this experiment were frequently unconfident that they had reached the final solution for each problem. Most interestingly, this was true for problems 1a and 1b in the experiment, which were taken directly from an optional homework set provided to the students online by their course instructor. As mentioned, chemical resonance is a topic that does not possess a clearly defined endpoint, and it will be necessarily to teach students how to determine when they have reached their final endpoint and then have them practice generating solutions with appropriate feedback until they begin to feel comfortable (Schunk, 1990).

Limitations. The small sample size of the groups included in this study limited our ability to determine statistical significance but allowed us the opportunity to engage deeply with each participant video. Additionally, no measure of spatial ability was obtained prior to data collection, which would have been interesting to compare between groups. Other limitations include the inability of the researchers to clearly separate problem representation from metacognitive planning and any error associated with each particular students’ level of comfort with thinking aloud (Fonteyn, Kuipers, & Grobe, 1993).

Conclusions

In conclusion, instructing organic chemistry students is no simple endeavor and will require that instructors teach content and problem-solving skills. Fortunately, work has been
done demonstrating strategies, such a self-explanation, that can assist students in bringing these pieces together and help them to learn to use the deep structure of their course material. In the future, this work could be further built upon by examining additional factors, such as spatial ability, or through the study of specific materials teaching students how to learn using all of the factors explored here.
References


Semester standing at Penn State:
- 1st – 2nd semester
- 3rd -4th semester
- 5th – 6th semester
- 7th – 8th semester
- 9th – higher semester

Major:

Ethnicity:
- Caucasian
- African-American
- Asian
- Hispanic
- Other

Gender:
- Male
- Female

Age:

Your current GPA:

**Your Verbal SAT score:

**Your Mathematics SAT score:

Including any courses that you completed in high school, please write the total number of courses you have completed in each area below:
- Biology
- Physics
- Chemistry
- Geology
- Other Science

**Student response rate to these questions was low, so they were not used by the researchers
Appendix B: Chemical Resonance Text

7.4 Drawing Resonance Contributors

We have seen that an organic compound with delocalized electrons is generally represented as a structure with localized electrons, so that we will know how many \( \pi \) electrons are present in the molecule. For example, nitroethane is represented as having a nitrogen-oxygen double bond and a nitrogen-oxygen single bond.

\[
\text{CH}_2\text{CH}_2\overset{\text{N}}{\text{O}}\overset{\text{O}}{\text{O}}
\]

However, the two nitrogen-oxygen bonds in nitroethane are identical; they each have the same bond length. A more accurate description of the molecule's structure is obtained by drawing the two resonance contributors. Both resonance contributors show the compound with a nitrogen-oxygen double bond and a nitrogen-oxygen single bond, but to show that the electrons are delocalized, the double bond in one contributor is the single bond in the other.

The resonance hybrid shows that the \( p \) orbital of nitrogen overlaps the \( p \) orbital of each oxygen. In other words, the two electrons are shared by three atoms. The resonance hybrid also shows that the two nitrogen-oxygen bonds are identical and that the negative charge is shared by both oxygen atoms. Although the resonance contributors tell us where the formal charges reside in a molecule and give us the approximate bond orders, we need to visualize and mentally average both resonance contributors to appreciate what the actual molecule—the resonance hybrid—looks like.

Rules for Drawing Resonance Contributors

In drawing resonance contributors, the electrons in one resonance contributor are moved to generate the next resonance contributor. As you draw resonance contributors, keep in mind the following constraints:

1. Only electrons move. The nuclei of the atoms never move.
2. The only electrons that can move are \( \pi \) electrons (electrons in \( \pi \) bonds) and lone-pair electrons.
3. The total number of electrons in the molecule does not change, and neither do the numbers of paired and unpaired electrons.
The electrons can be moved in one of the following ways:

1. Move π electrons toward a positive charge or toward a π bond (Figures 7.2 and 7.3).
2. Move lone-pair electrons toward a π bond (Figure 7.4).
3. Move a single nonbonding electron toward a π bond (Figure 7.5).

**Figure 7.2**
Resonance contributors are obtained by moving π electrons toward a positive charge.

**Figure 7.3**
Resonance contributors are obtained by moving π electrons toward a π bond. (In the second example, the red arrows lead to the resonance contributor on the right, and the blue arrows lead to the resonance contributor on the left.)
Notice that in all cases, the electrons are moved toward an \( sp^2 \) hybridized atom. Remember that an \( sp^2 \) hybridized carbon is either a double-bonded carbon (it can accommodate the new electrons by breaking a \( \pi \) bond) or a carbon that has a positive charge or an unpaired electron (Sections 1.8 and 1.10). Electrons cannot be moved toward an \( sp^3 \) hybridized carbon because it cannot accommodate any more electrons.

Because electrons are neither added to nor removed from the molecule when resonance contributors are drawn, each of the resonance contributors for a particular compound must have the same net charge. If one resonance structure has a net charge of \(-1\), all the others must also have net charges of \(-1\); if one has a net charge of 0, all the others must also have net charges of 0. (A net charge of 0 does not necessarily mean that there is no charge on any of the atoms: A molecule with a positive charge on one atom and a negative charge on another atom has a net charge of 0.)

Radicals can also have delocalized electrons if the unpaired electron is on a carbon that is adjacent to an \( sp^2 \) hybridized atom. The arrows in Figure 7.5 are single barbed because they denote the movement of only one electron (Section 3.6).

One way to recognize compounds with delocalized electrons is to compare them with similar compounds in which all the electrons are localized. In the following example, the compound on the left has delocalized electrons because the lone-pair

\[ \text{Figure 7.4} \]
Resonance contributors are obtained by moving a lone pair toward a \( \pi \) bond.
Figure 7.5
Resonance structures for an allylic radical and for the benzyl radical.

Electrons on nitrogen can be shared with the adjacent \(sp^2\) carbon (since the carbon–carbon \(\pi\) bond can be broken):

\[
\text{CH}_3\text{CH=CH}^+\text{NHCH}_3 \leftrightarrow \text{CH}_3\text{CH=CH}^+\text{NHCH}_3^-
\]

delocalized electrons

\[
\text{CH}_3\text{CH=CH}^+\text{NHCH}_3 \rightarrow \text{CH}_3\text{CH=CH}^+\text{NHCH}_3^-
\]

localized electrons

In contrast, all the electrons in the compound on the right are localized. The lone-pair electrons on nitrogen cannot be shared with the adjacent \(sp^2\) carbon because carbon cannot form five bonds. The octet rule requires that second-row elements be surrounded by no more than eight electrons, so \(sp^2\) hybridized carbons cannot accept electrons. Because an \(sp^2\) hybridized carbon has a \(\pi\) bond that can break, has a positive charge, or has an unpaired electron, it can accept electrons without violating the octet rule.

The carbocation shown on the left in the next example has delocalized electrons because the \(\pi\) electrons can move into the empty \(p\) orbital of the adjacent \(sp^2\) carbon (Section 1.10). We know that this carbon has an empty \(p\) orbital since it has a positive charge.

\[
\text{CH}_2=\text{CH}^+\text{CHCH}_3 \leftrightarrow \text{CH}_2=\text{CH}^+\text{CHCH}_3^-
\]

delocalized electrons

\[
\text{CH}_2=\text{CH}^+\text{CHCH}_3 \rightarrow \text{CH}_2=\text{CH}^+\text{CHCH}_3^-
\]

localized electrons

The electrons in the carbocation on the right are localized because the \(\pi\) electrons cannot move. The carbon they would move to is \(sp^3\) hybridized, and \(sp^3\) hybridized carbons cannot accept electrons.

The next example shows a ketone with delocalized electrons (left) and a ketone with only localized electrons (right):

\[
\text{CH}_3\text{C}^+\text{CH=CHCH}_3 \leftrightarrow \text{CH}_3\text{C}^+\text{CH=CHCH}_3^-
\]

delocalized electrons

\[
\text{CH}_3\text{C}^+\text{CH=CHCH}_3 \rightarrow \text{CH}_3\text{C}^+\text{CH=CHCH}_3^-
\]

localized electrons
Appendix C: Chemical Resonance Problem Set

This problem is from a recent homework assignment in class. Practice thinking aloud while solving this problem.

1. Draw as many resonance structures as you can for the following organic molecules.

(a) ![Resonance structure for (a)]

(b) ![Resonance structure for (b)]

End of practice problem.

1. For each benzene derivative, determine if the substituent is either electron donating or electron withdrawing using resonance as your justification.

(a) ![Resonance structure for (a)]
2. For each compound below, there is an incorrect resonance form given. Explain why the resonance form is incorrect.

(a) ![Resonance forms for compound (a)]

(b) ![Resonance forms for compound (b)]
3. Consider the following reaction.

The reactant conjugated ketone has two electrophilic sites. The nucleophile can attack either electrophilic carbon resulting in two possible products. Using resonance drawings for the reactant structure, show how the carbons in the reactant can serve as electrophiles.
Appendix D: Chemical Resonance Problem Set Key

This problem is from a recent homework assignment in class. Practice thinking aloud while solving this problem.

1. Draw as many resonance structures as you can for the following organic molecules.

(a) \[
\begin{align*}
\text{N} & \quad \text{O} \\
& \quad \text{O}
\end{align*}
\]

(b) \[
\begin{align*}
\text{O} & \quad \text{C} \\
\text{C} & \quad \text{C}
\end{align*}
\]

End of practice problem.
1. For each benzene derivative, determine if the substituent is either electron donating or electron withdrawing using resonance as your justification.

(a) 

(b)
2. For each compound below, there is an incorrect resonance form given. Explain why the resonance form is incorrect.

(a) ![Diagram of benzaldehyde and its incorrect resonance form]

(b) ![Diagram of aniline and its incorrect resonance form]

- Charges are incorrect, which reveals that the electron push was incorrectly done.
- E should move towards oxygen more effectively.
- Again, charges are incorrect with nitrogen lone pair reacting into the alkene system.
3. Consider the following reaction.

The reactant conjugated ketone has two electrophilic sites. The nucleophile can attack either electrophilic carbon resulting in two possible products.

Using resonance drawings for the reactant structure, show how the carbons in the reactant can serve as electrophiles.
Appendix E: Raw Participant Data

Participants’ individual content knowledge counts.

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