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UNIVERSITY OF NORTHERN COLORADO

Greeley, Colorado

The Graduate School

DESIGN, DEVELOPMENT AND, PSYCHOMETRIC
ASSESSMENT OF AN INVENTORY
ON CONCEPTS PERTINENT TO
DEVELOPING PROFICIENCY
IN ORGANIC REACTION
MECHANISMS

A Dissertation Submitted in Partial Fulfillment
of the Requirements for the Degree of
Doctor of Philosophy

Sachin Nedungadi

College of Natural and Health Sciences
Department of Chemistry and Biochemistry
Chemical Education

May 2020

This Dissertation by: Sachin Nedungadi

Entitled: *Design, Development and, Psychometric Assessment of an Inventory on Concepts Pertinent to Developing Proficiency in Organic Reaction Mechanisms.*

has been approved as meeting the requirement for the Degree of Doctor of Philosophy in the College of Natural and Health Sciences in the Department of Chemistry and Biochemistry, Program of Chemical Education

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ABSTRACT

Nedungadi, Sachin. *Design, Development, and Psychometric Assessment of an Inventory on Concepts Pertinent to Developing Proficiency in Organic Reaction Mechanisms*. Published Doctor of Philosophy Dissertation, University of Northern Colorado, 2020.

This three-phase study was conducted to design, develop, and psychometrically analyze the Reaction Mechanisms Concept Proficiency Inventory (RMCPI). In the first phase, open-ended interviews were conducted with organic chemistry instructors ($N=11$) to obtain their opinion on concepts pertinent to developing proficiency in organic reaction mechanisms. The results yielded 11 pertinent concepts. Additionally, participants believed that organic reaction mechanisms are essential for mastering organic chemistry and students have difficulty with understanding the meaning and utility of the curved-arrows. The difficulties that students have with reaction mechanisms could be due to a lack of understanding of fundamental general chemistry and organic chemistry concepts.

The second phase of this study consisted of a national survey of organic chemistry instructors ($N=183$) to generalize the results obtained from the first phase. Organic chemistry instructors were asked to rate the importance of the concepts identified in phase 1. The results indicated a general consensus at the national level regarding these concepts and a list of 10 concepts was obtained. Additionally, there was a consensus at the national level regarding the importance of organic reaction mechanisms and the difficulties students face with this important area of organic chemistry education.

The third phase of this study consisted of the development of the inventory, test administration, and psychometric analysis. During the development of the inventory, open-ended questions under each of the pertinent concepts identified were administered to first-semester organic chemistry students ($N=138$) to obtain distractors from their alternate conceptions. Open-ended interviews were conducted with first-semester organic chemistry students ($N=22$) to obtain information on their thought process while answering the questions and identify additional alternate conceptions. These alternate conceptions were used as distractors for the two-tier items in the inventory. A pilot version, and a beta version of the inventory were administered to 109 and 359 first-semester organic chemistry students respectively. The 26-item alpha version of the RMCPI was administered to 753 first-semester organic chemistry students from 14 different universities across the U.S.A. At the item level, Classical Test Theory and Rasch analysis were used to assess item functioning. At the test level, face validity, content validity, and construct validity using Rasch analysis were utilized to establish the validity of the data obtained using the RMCPI. The reliability of the data obtained using the RMCPI was assessed by computing the Cronbach's alpha value, and the item and person separation reliability. The results indicate that the items on the alpha version of the RMCPI are functioning well and the instrument is measuring a unidimensional construct which suggests that the RMCPI could be used by organic chemistry instructors as an effective assessment tool to detect students' alternate conceptions on concepts pertinent to developing proficiency in organic reaction mechanisms. Additionally, the validity and reliability of the data meet the acceptable standards for a concept inventory.

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“No matter what we get out of this, I know we’ll never forget.”

- Blackmore, Gillan, Glover, Lord, and Paice

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CHAPTER I

INTRODUCTION

Introduction

Organic chemistry, has been found to be difficult and complex for undergraduate students (Grove, Cooper, & Cox, 2012). Students with a variety of majors including pre-health, and biology, are required to take at least one semester of organic chemistry (Seymour & Hewitt, 1997). Organic chemistry has even been described as a gatekeeper course for medical school (Baum & Axtell, 2005). Failure in organic chemistry usually means having to give up the dream of pursuing a career in a professional school.

One important topic in an organic chemistry course is the mechanisms of reactions. The use of curved-arrow notation in the electron-pushing formalism (EPF) to convey electron flow during mechanistic processes has had a great impact on the teaching and learning of organic chemistry (Grove, Cooper, & Rush, 2012). In this formalism, a single-headed or double-headed curved arrow is drawn with its tail at the electron source – usually a lone pair of electrons or a bond – to the electron sink – usually an electron-deficient atom (Bhattacharyya, 2014). An example of a mechanism showing the EPF is shown in Figure 1.1.

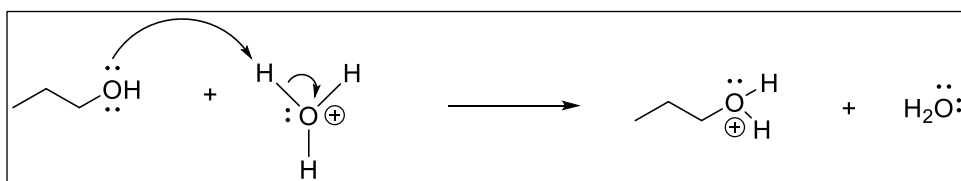


Figure 1.1. Mechanism showing the electron-pushing formalism (EPF).

This flow of electrons shows how bonds are broken and how bonds are formed in a reaction (Galloway, Stoyanovich, & Flynn, 2017). The ability to use this EPF is an extremely useful skill for organic chemists to possess (Bhattacharyya & Bodner, 2005). They use this as their primary tool to explain and/or predict reaction outcomes including the generation of side products, regioselectivity, and stereochemistry (Bhattacharyya, 2013). As such, electron-pushing is an efficient and effective mode of communication for expert organic chemists (Bhattacharyya, 2014).

The topic of organic reaction mechanisms is especially challenging for students in an organic chemistry course due to the abstract nature of the concept. There have been several studies done to show that undergraduate students and even graduate students encounter many difficulties when trying to use the EPF to propose reaction mechanisms which include a failure to understand the basic purpose of the EPF and how to effectively utilize it for problem-solving (Anderson & Bodner, 2008; Bhattacharyya & Bodner, 2005; Ferguson & Bodner, 2008; Grove, Cooper, & Rush, 2012; Kraft, Strickland, & Bhattacharyya, 2010). An understanding of such alternate conceptions that students develop with organic reaction mechanisms is important to assist students in overcoming difficulties with this important area in organic chemistry education.

Statement of Problem

The importance of reaction mechanisms in an organic chemistry class has been demonstrated (Duis, 2011). For students to gain a good understanding of organic chemistry, they have to be able to think mechanistically which involves visualizing how electrons flow during the making and breaking of bonds in chemical reactions. This thinking is very different from what undergraduate students have encountered in other

chemistry courses. Students often take two classes of general chemistry before they can enroll in an organic chemistry class. The general chemistry courses are much more algorithmic and when students come into an organic chemistry class, they struggle with the more conceptual way of thinking which is what is needed for a good understanding of reaction mechanisms (Cartrette & Mayo, 2011). Students also struggle with the abstract nature of chemistry. Students tend to give up and resort to rote memorization while studying organic reaction mechanisms (Bhattacharyya & Bodner, 2005). This affects their long-term understanding of the subject.

Qualitative studies have explored the difficulties students face with reaction mechanisms and how students approach mechanistic problems (Anderson & Bodner, 2008; Bhattacharyya & Bodner, 2005; Bhattacharyya, 2014; Ferguson & Bodner, 2008). There have also been some studies done on changing the organic chemistry curriculum to a more mechanistic based one as opposed to a functional group approach (Flynn & Ogilvie, 2015). While these qualitative studies are important to gain an understanding of how students view reaction mechanisms, no intervention tools have been developed to conduct a large-scale assessment of students' understanding of concepts that are pertinent to developing proficiency in organic reaction mechanisms.

This research project was conducted for two reasons: to gain a better understanding of students' alternate conceptions on topics pertinent to developing proficiency in organic reaction mechanisms and, thereby, help students overcome these alternate conceptions and better understand organic chemistry.

Research Questions

The research questions that guide this study are:

- Q1 What are the chemistry concepts perceived by experts to be pertinent to developing proficiency in organic reaction mechanisms?
- Q2 Is there a consensus at the national level regarding the concepts perceived to be pertinent to developing proficiency in organic reaction mechanisms?
- Q3 How can one appropriately assess organic chemistry students' conceptual understanding of the concepts perceived by the experts to be pertinent to developing proficiency in organic reaction mechanisms?

Theoretical Framework

Constructivism theorizes that meaning is constructed from prior knowledge by individuals rather than discovered (Crotty, 2015). As instructors, we should help students construct knowledge and meaning from their experiences thereby helping them overcome the difficulties they face. To do this we need to explore how students approach certain concepts and we need to understand how students develop alternate conceptions regarding certain concepts. This study will be covered by the broad framework of the constructivist theory.

Significance of the Study

The purpose of this study was to develop an assessment instrument in the form of an inventory on concepts that are perceived by experts to be pertinent to developing proficiency in organic reaction mechanisms. This inventory could serve as an intervention tool for organic chemistry instructors to assess their students' understanding of these pertinent concepts. Organic chemistry instructors could administer this inventory just prior to the point in the semester when students are first introduced to reaction mechanisms. By administering the concept inventory at this point in the semester, instructors will be informed about the concepts with which the students are having

difficulty and the alternate conceptions that they have developed before they get into the study of reaction mechanisms. Instructors can then decide if they need to review some of these concepts before introducing the topic of reaction mechanisms to their students. Instructors could also use this information to modify their syllabi for future classes and incorporate some of these concepts prior to teaching reaction mechanisms. Additionally, the inventory could help inform the general chemistry instructors on concepts further used in organic chemistry.

Description of the Organic Chemistry Course

Three different levels of organic chemistry courses are prevalent at various universities in the U.S.A. The general, organic and biochemistry (GOB) courses are usually taken by students looking to pursue a career in allied health. The survey of organic chemistry courses are single semester organic chemistry courses taken by students who are nutrition and dietetics majors. The sophomore-level organic chemistry courses are two-semester courses taken by students who are chemistry majors, other science majors, and students who are looking to pursue a pre-health career in professional schools like medical and dental schools. This inventory was designed to target students in the first semester of sophomore-level organic chemistry courses.

Limitations

The participants for the qualitative phase of this study were chosen only from universities within the state of Colorado and therefore the results from the qualitative phase may not be generalizable. This was overcome by conducting a national survey to increase generalizability. The quantitative phase of this study was limited by the validity and reliability of the instrument being tested.

Researcher's Personal Stance

As an organic chemistry student, I always found reaction mechanisms to be especially challenging. It was not until I was a graduate student and took advanced classes in organic reaction mechanisms and physical organic chemistry that I gained a wholesome understanding of reaction mechanisms. When I started teaching organic chemistry I found that my students had the same difficulties as I did when I was an undergraduate student. There was an added difficulty for them in that most of them were not chemistry majors and they were not going to go on to take advanced organic chemistry courses. With some students, their alternate conceptions were very clear and I could address them but with others, it was not always clear. As an organic chemistry instructor, my biggest struggle was how far back do I go with the review of concepts from previous courses? I did not know which general chemistry and introductory organic chemistry concepts I had to spend more time on before I could introduce reaction mechanisms. I also needed to use my time wisely during a busy semester. I always thought that some sort of a diagnostic tool would be helpful to quickly assess the concepts that needed to be strengthened.

The data for this project was collected from sophomore-level organic chemistry classes and being an instructor of organic chemistry myself, I collected data in some of my classes. As an instructor, I have always wanted to see my students succeed in classes and it gives me great joy to see students overcoming difficulties to understand complex concepts. While interviewing students I did not give them leading questions even if I could see that they were very close to the answer thereby eliminating any bias in their responses. The participants in this study were from diverse cultural backgrounds and

there was no bias shown towards people from a particular culture. I strived to conduct unbiased research.

CHAPTER II

LITERATURE REVIEW

The literature reviewed in this chapter describes the work that has been reported on the utility of reaction mechanisms in an organic chemistry course and students' understanding of organic reaction mechanisms. It also describes statistical procedures performed on concept inventories developed in chemical education. The need for an intervention tool in the area of organic chemistry and its advantages are also discussed.

Background and History of Curved-Arrow Notation

A reaction mechanism is a set of sequential steps that depict the changes a reactant undergoes when it is converted to a product. The curved-arrow notation in organic chemistry is a symbolic representation of the movement of electrons during the process of bond-forming and bond-breaking which helps visualize the steps in a reaction mechanism. The study of reaction mechanisms is a major component of sophomore-level organic chemistry. Kermack and Robinson (1922) were the first to use the curved-arrow notation to show electron flow. From this point on the use of the curved-arrow notation in organic chemistry became widespread and it quickly gained an iconic status.

The curved-arrow notation became a useful tool for students studying organic chemistry to keep track of electron flow although earlier textbooks used it minimally and relied on descriptions to explain reaction mechanisms (Morrison & Boyd, 1966; Streitwieser & Heathcock, 1976). Over the years, textbooks included more information on the curved-arrow notation, and currently, the discussion of reaction mechanisms and

curved-arrow notation has become standard material in organic chemistry textbooks (Bruice, 2014; Loudon & Parise, 2016).

As the study of reaction mechanisms and the curved-arrow notation gained prominence, there were arguments made against the usefulness of the tool mainly in courses for non-chemistry majors (Laszlo, 2002). The author argued that students who do not intend to become chemists do not need to become proficient in such a specialized language to understand reactions since they may never utilize it in the future. Despite this, the study of reaction mechanisms is an integral part of undergraduate organic chemistry, and as long as students are in the course they need to learn to speak the language of organic chemistry to solve conceptual problems.

Different Approaches to Teaching Mechanisms

Due to the emphasis on reaction mechanisms in the study of organic chemistry and due to the difficulty of the content, different approaches to teaching mechanisms have been developed. It was proposed by Friesen (2008) and Ault (2010) that the best way to teach organic reaction mechanisms is to “say it the way it is.” Friesen (2008) states that the best approach to teaching reaction mechanisms is to consistently show students the most complete way of writing mechanisms so that they can appreciate the language of organic chemistry. In his study he discusses avoiding shortcut notations, fully balancing reaction equations and reaction mechanisms, writing clear structural representations that reveal key electrons and bonds, and distinguish between covalent and ionic bonds. Friesen believes that oversimplification of reaction mechanisms is harmful since it does not provide students with the complete picture.

Ault (2010) builds on this opinion, and he states that more than half of the steps in a mechanism involve a proton transfer so one must know the two rules of proton transfer namely proton transfers in aqueous acid and proton transfers in aqueous base. Ault uses the example of the acid-catalyzed hydrolysis of ethyl acetate, shown in Figure 2.1, where four out of the six steps in the mechanism involve a proton transfer step.

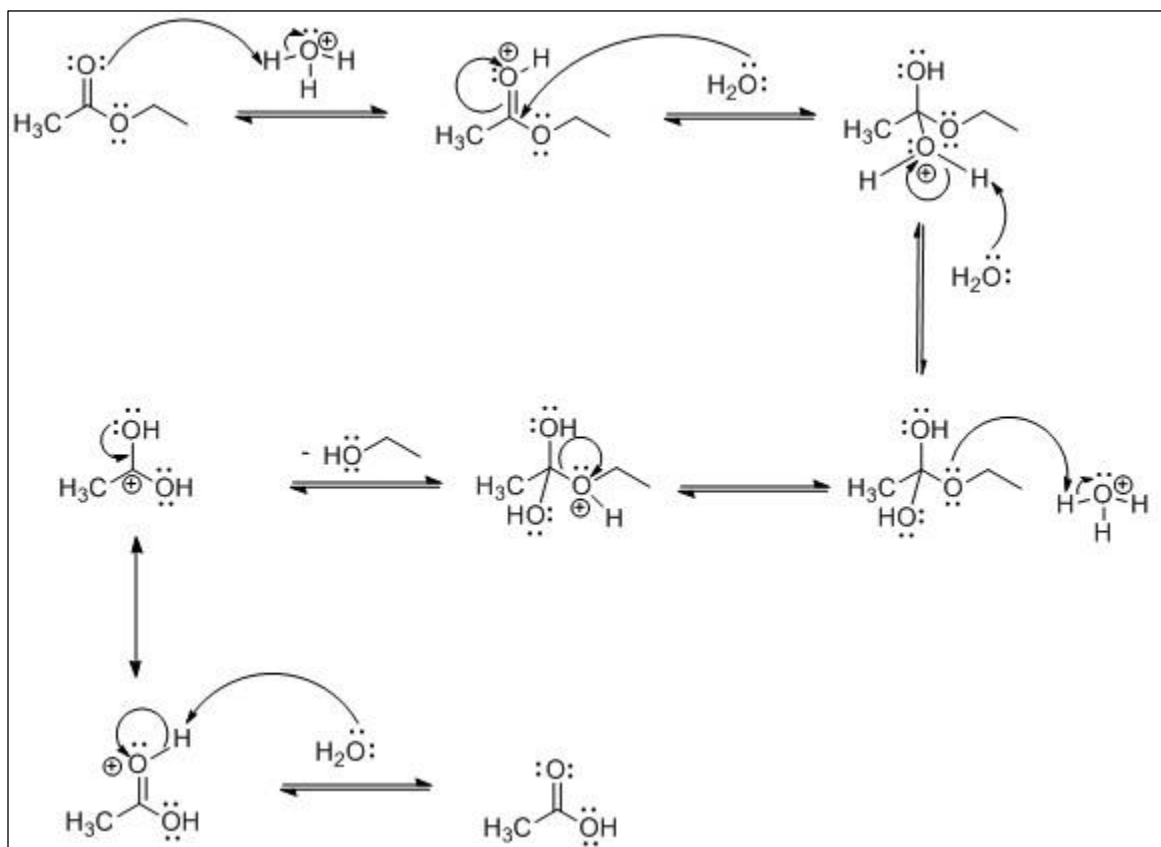


Figure 2.1. Reaction mechanism for acid-catalyzed hydrolysis of ethyl acetate.

Students must be introduced to the idea that reactions involve a set of equilibria and students need help visualizing these equilibria. Ault believes that students should first learn the proton transfer steps well before being introduced to the slower steps, but to do this instructors will have to use only hydronium ion and water as proton donors and only water and hydroxide ions as proton acceptors. This approach according to Ault is “saying it the way it is”.

There have been other studies (Penn & Al-Shammari, 2008; Straumanis & Ruder, 2009; Wentland, 1994) done on different approaches to teaching organic reaction mechanisms. The study done by Wentland (1994) reports five operations that help make the features of a reaction more clear. These are ionization, neutralization, 1,3-electron pair displacement, 1,3-electron pair abstraction and 1,5-electron pair displacement. Wentland suggests that these can be tied into the functional group based approach of teaching organic chemistry which most textbooks employ. Using these five approaches to describe reactions will help students see complex mechanisms as mere elaborations of simpler ones.

Straumanis and Ruder (2009) surveyed instructors and students to get their opinion on a novel method to depict electron flow called the bouncing curved-arrow technique as opposed to the traditional curved-arrow. In this depiction of electron flow, the arrows trace the movement of electrons and more explicitly show bond formation as opposed to the traditional curved-arrow. This type of depiction helps in understanding carbocation rearrangements and regiospecific reactions such as electrophilic additions to terminal alkenes. Electronic surveys were given to 261 second-quarter organic chemistry students to get information on which depiction of curved-arrows they preferred and 62.8% of students preferred the bouncing curved-arrow notation to the traditional notation showing that students understood reactions, especially regiospecific ones, better with this technique. Faculty (N=12) who used both methods of representation were also surveyed and they spoke highly about the effectiveness of the bouncing curved-arrow notation (Straumanis & Ruder, 2009).

The approaches described above are limited to single reaction types. A new approach of teaching mechanisms called the curved-arrow neglect method was put forth by Penn and Al-Shammari (2008). This method was suggested with the intent of using it as part of a computer-assisted instruction environment. In this method, students were given tasks of drawing intermediates and products for reactions without having to use the curved arrow as a method of keeping track of electrons. A comparison between a mechanism using curved-arrows and using the curved-arrow neglect method is shown in Figure 2.2.

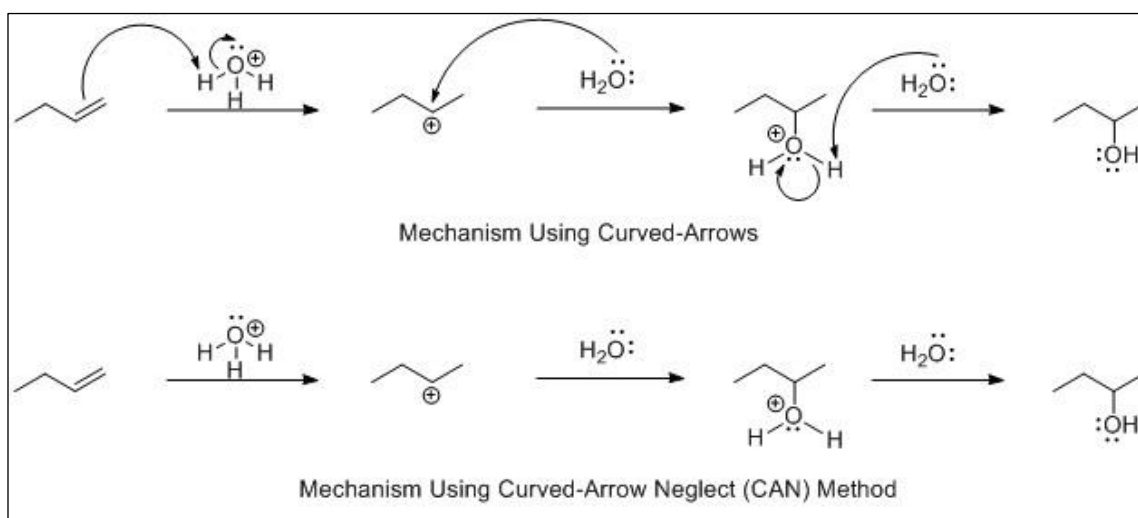


Figure 2.2. Mechanism for hydration of 1-butene using curved-arrows and the curved-arrow neglect method.

It was found that students who were given this type of instruction showed enhanced capabilities for drawing mechanisms even if they had to use curved-arrows to depict electron flow. This method of instruction can, therefore, be applied to a wide range of reaction types and will not be limited to only one reaction type.

The utilization of puzzles to assist in the learning of reaction mechanisms has been reported (Erdik, 2005; Starkey, Horowitz, & Schwartz, 2004). Erdik (2005) reported the use of building-block puzzles to get practice drawing reaction mechanisms. The

puzzles were designed using acetone as a ketone, and depicting the reaction of acetone-derived carbanions with electrophiles and the reaction of acetone itself with carbanions. These puzzles could be used as an in-class activity or homework for second-semester organic chemistry students. Starkey et al. (2004) reported the use of molecular modeling puzzles to help in the understanding of reaction mechanisms. In this study, students worked in groups to propose a suitable reaction mechanism, including intermediates and transition states, for the conversion of a reactant to a product. They then used molecular modeling software to make a model of their mechanism, optimize it and calculate the heats of formation. They were then asked to predict which product was kinetically and thermodynamically favorable, and they mapped an energy diagram. These projects gave students practice drawing mechanisms, and also identified gaps in their knowledge regarding reaction mechanisms. These studies put forth different methods to teach organic reaction mechanisms; however, understanding the importance that instructors and students place on organic reaction mechanisms would be beneficial.

The Utility of Organic Reaction Mechanisms

The use of the curved-arrow notation to describe mechanisms in organic chemistry is extremely important to the practicing organic chemist and is considered an integral part of organic chemistry education, which is one of the reasons educators are continuously trying to find novel methods of teaching this concept. The qualitative study done by Duis (2011) explored organic chemistry instructors' opinions on concepts that are important, core, or foundational in organic chemistry. The results indicated that 16 out of the 18 participants identified reaction mechanisms as a fundamental organic chemistry topic and 7 out of the 18 participants identified reaction mechanisms as an

organic chemistry topic that is important for later use. In addition to this, it was reported that 15 out of the 18 participants stated that reaction mechanisms is a difficult topic for organic chemistry students. The importance of reaction mechanisms is clear, but how do students benefit from their use?

The benefits that students gain from using the curved-arrow notation were the aim of the study done by Grove, Cooper, and Cox (2012). In this study, second-semester organic chemistry students were asked to provide the mechanism for six organic reactions and to predict the product of the reactions. It was found that 51% of the students did not use mechanisms for the six tasks or they used it for only one of the six tasks. The success rates on the tasks were compared between mechanism users and non-mechanism users, and it was found that there was a significant difference only for two of the six tasks. These two tasks were more complex. The other four tasks were fairly straightforward and the cognitive demands associated with the curved-arrow notation might have prevented students from utilizing the curved-arrow notation. These results suggest that there is a need to better understand the barriers students face when trying to use mechanisms and the curved-arrow notation.

Grove, Cooper, and Rush (2012) examined how students' understanding of the curved-arrow notation, evolved with time. Students in a second-year two-semester organic chemistry course were followed for the duration of the academic year. Their use of mechanistic reasoning was studied by giving the students tasks at four different times during the course of the year, and these tasks were based on the material they were studying in the lecture. Students were asked to use a structure drawing software to predict the product of reactions and give a mechanism to show the formation of the products. The

results showed that there were a large number of students who just predicted the product without actually drawing the mechanism. Most of the others predicted the product first and then drew a mechanism in a so-called "decorating with arrows" technique. This indicates the need for more extensive training and instruction on the use of organic reaction mechanisms.

The importance of organic reaction mechanisms and the emphasis they have to be given in undergraduate chemistry education has been well established. What tasks can be performed using reaction mechanisms? Bodé and Flynn (2016) used grounded theory to examine the problem-solving strategies employed by second-semester organic chemistry students at a research-intensive university while solving organic synthesis problems. More than 700 responses to synthesis problems from final exams were analyzed using an open-coding method to yield six key strategies for successfully solving synthesis problems. One of the strategies identified was drawing reaction mechanisms while solving synthesis problems. Students who used this strategy together with other strategies such as mapping the atoms of the starting material on to the target or identifying newly formed bonds were found to have a higher rate of success when solving synthesis problems. The results indicated that mechanistic reasoning assists in solving synthetic problems in organic chemistry.

The utility of reaction mechanisms in solving advanced problems in organic chemistry is well established. Different methods of teaching reaction mechanisms have been explored. Given the importance of reaction mechanisms, the difficulties students face with reaction mechanisms have been a source of great interest in chemistry education.

Students' Difficulties with Reaction Mechanisms

One of the main concerns is that many students are unable to understand the importance of reaction mechanisms. Anderson and Bodner's (2008) work focuses on an organic chemistry student with the pseudonym Parker who was part of a qualitative study conducted on seven organic chemistry students enrolled in a two-semester course. The participants took part in two to four interviews during the two-semester course and their understanding of certain general chemistry concepts such as reaction rates, equilibrium and the process of dissolution, and fundamental organic chemistry topics were probed. Narrative analysis was conducted to identify areas where students struggle and reaction mechanisms seemed to be one common area. Parker did not have trouble with individual reaction mechanisms but he had trouble understanding the purpose of reaction mechanisms. He did not use mechanistic reasoning to answer questions. This shows that instructors need to first and foremost help students gain a deeper understanding as to why they are expected to learn reaction mechanisms.

Ferguson and Bodner (2008) reported a qualitative study done on sixteen second-year organic chemistry students to make sense of how they use the arrow-pushing formalism to represent reaction mechanisms. Data were collected using the think-aloud protocol and participants were asked to propose reaction mechanisms to seven questions when they were given the reactants and the products. The results showed that students lacked a fundamental understanding of chemical concepts and therefore approached the arrow-pushing formalism as a meaningless exercise. They resorted to drawing arrows to make the mechanism look real to hide their lack of understanding. These results indicate the need for instructors to focus more on the core concepts that run through organic

chemistry and to help students by giving more meaning to the symbols used when drawing reaction mechanisms.

Rushton, Hardy, Gwaltney, and Lewis (2008) utilized semi-structured, think-aloud interviews to interview 19 fourth-year chemistry students to examine the alternate conceptions they had developed in organic chemistry. The results indicated that even fourth-year students who are about to graduate with a chemistry degree possess a lot of confusion regarding models specific to organic chemistry and the discernment of appropriate reaction mechanisms.

Bhattacharyya and Harris (2018) studied the verbal descriptions of mechanism diagrams in seven pairs of second-semester organic chemistry students. The students were asked to describe and draw electron-pushing mechanisms for three problems. The results indicated that students have the most difficulty with describing the structural representations of the compounds involved in the reactions. The students seemed to be able to describe the movement of electrons during the mechanistic steps quite adequately. This indicates that students need help understanding how to draw Lewis structures which is a fundamental topic taught in general chemistry courses. These results are consistent with another qualitative study (Galloway et al., 2017) where 29 first-semester organic chemistry students were interviewed to analyze their verbal descriptions of reaction mechanisms and the meanings they give to the symbolism used. The results showed that students struggled the most with describing the structural representations, and different students used a different language to describe the same reactions which implies that again instructors have to give meaning to the symbols and establish a common language of descriptions from the beginning.

These studies indicate that students are not attributing any meaning to the curved-arrows when they are utilized to depict reaction mechanisms. The study done by Flynn and Featherstone (2017) explored students' answers to exam questions. Two types of questions were analyzed, one where the students had to give the arrow-pushing mechanism and the other where students had to predict the product. The results showed that students fared much better on the questions with arrows rather than the product questions with averages of 72% and 55%, respectively. On the arrows question, students were having difficulty mapping and expanding atoms and electrons. But most students were drawing arrows in the correct direction showing the movement of electrons. This suggests that students are attaching meaning to the arrows when drawing reaction mechanisms. Flynn and Ogilvie (2015) even reported the use of a mechanisms-first approach to teaching organic chemistry where students are introduced to the electron-pushing formalism even before they are taught reactions. This differs from the traditional functional group approach where the mechanisms of reactions are taught under each class of functional groups. This way they can use their mechanistic knowledge to learn new reactions and propose mechanisms for unknown reactions.

The difficulties students face with reaction mechanisms seem to stem from their lack of understanding of fundamental concepts as demonstrated by other studies (Anzovino & Bretz, 2016; Cruz-Ramírez De Arellano & Towns, 2014; Popova & Bretz, 2018). Anzovino and Bretz, (2016) studied students' ideas of electrophiles and nucleophiles which are key to understanding reaction mechanisms. Second-semester organic chemistry students were interviewed and asked to give examples of electrophiles and nucleophiles. Concept maps were generated and these were compared to concept

maps from experts. The results indicated that students have very fragmented ideas regarding electrophiles and nucleophiles. Popova and Bretz (2018) interviewed 36 second-semester organic chemistry students to see how they make connections between substitution and elimination reactions and their corresponding reaction coordinate diagrams. They found that one of the fundamental difficulties students have with reaction coordinate diagrams is that they do not have a firm understanding of the mechanism of these fundamental organic chemistry reactions. The students were either creating their own mechanisms or they were omitting crucial steps in the mechanism because they lacked the knowledge needed. A similar study (Cruz-Ramirez De Arrellano & Towns, 2014) used qualitative think-aloud interviews to study students' understanding of substitution and elimination reactions of alkyl halides. It was found that students possessed fundamental gaps in their knowledge such as classifying substances as nucleophiles and/or bases, assessing the basic or nucleophilic strength of species and accurately describing the steps that take place and the intermediates that are formed during the course of the reaction. These studies further demonstrate that students lack the fundamental skills needed to solve mechanistic questions.

The difficulties students face with organic reaction mechanisms are not limited to undergraduate students. Bhattacharyya and Bodner (2005) used the think-aloud protocol to study fourteen graduate students as they solved eight mechanism problems. These problems were based on simple variations of substitution reactions. The results indicate that the curved-arrows bore no physical meaning to the graduate students. They used it only because "it gets me to the product." Some students were able to propose the mechanism but they could not explain the steps which indicate that they just memorized

the steps. This study indicates that there is a big disconnect between the organic chemistry knowledge students possess and how they utilize it to solve problems.

Two studies (Kraft et al., 2010; Strickland, Kraft, & Bhattacharyya, 2010) examined the reasoning and representations used by graduate students when solving mechanistic problems. Results indicated that students exhibit representational incompetence when solving mechanistic problems (Kraft et al., 2010). The students have a very difficult time expressing their mental models of commonly used terms while describing reaction mechanisms like functional groups and electrophiles and nucleophiles (Strickland et al., 2010). These studies show that graduate students also struggle with the fundamental knowledge needed to solve mechanistic problems which suggests that the problem permeates to higher levels of education.

The trials and tribulations that students face with organic reaction mechanisms were the focus of Bhattacharyya's (2014) meta-analysis work. The study investigated articles published on students' difficulties with reaction mechanisms in top chemical education journals. The common theme found in most studies is that students' conceptions are consistent with a deterministic approach, and they have great difficulties with multi-variate thinking. The second part of the manuscript contained a tentative sketch for students' strategies for solving electron-pushing problems, and it demonstrated that students tend to approach these tasks algorithmically regardless of their conceptual understanding. This could be attributed more to metacognition, thus students should be given training in metacognition to improve multi-variate thinking.

As demonstrated here, the difficulties that students face with reaction mechanisms and their approaches to solving these problems have been the source of great interest in

chemical education research. What is the understanding of electron-pushing formalism among experts and how do they use it? Bhattacharyya (2013) reported a nationwide survey administered to organic chemistry instructors to get insight into their understanding of electron-pushing formalism, content knowledge, representational skills and important uses of this formalism. The results indicate that the focus should be on applied skills rather than theoretical ones. The emphasis was more on the understanding of electrophiles and nucleophiles than on acid-base chemistry. The primary use for this type of reasoning was more of an explanatory one. The results raise questions about the use of mechanistic reasoning and at what point during the course of an organic chemistry class should students develop mechanistic reasoning.

The studies presented indicate that considerable work has been done on the difficulties students face with organic reaction mechanisms. The results from these studies propose different approaches to use while teaching students reaction mechanisms. However, intervention tools for large scale assessment of students are lacking. A concept inventory on concepts pertinent to developing proficiency in reaction mechanisms would be one type of intervention tool that could be useful to instructors. The importance of reaction mechanisms in the study of organic chemistry and how instructors use it should be further explored.

Concept Inventories in Chemistry

Concept inventories have been utilized in chemical education research for over 30 years (Treagust, 1988). Concept inventories are usually multiple-choice assessments that use identified student alternative conceptions as distractors (Richardson, 2004). Research findings in science education take considerable time to be applied in the classroom, and

the development of tests that incorporate these research findings which can be readily used in the classroom will increase the rate of this application (Treagust, 1988). The alternative of interviewing students to identify alternate conceptions is time-consuming, but administering a pencil and paper multiple-choice test that identifies alternate conceptions in a limited time would be very useful (Treagust, 1988).

There have been several concept inventories developed in general chemistry as diagnostic tools to determine students' alternate conceptions. The Quantum Chemistry Concept Inventory (QCCI) (Dick-Perez, Luxford, Windus, & Holme, 2016) is a 14-item multiple-choice test developed to test physical chemistry students' alternate conceptions of quantum mechanics concepts. The QCCI was designed to be administered as a short duration test and the 12-item instrument was piloted on a small group of undergraduate students before the modified 14-item instrument was administered online to a larger number of students. The distractors for the items were devised from literature, and the results indicated that the researchers were capable of recognizing alternate conceptions. One of the most widely used concept inventories is the Chemistry Concepts Inventory (CCI) (Mulford & Robinson, 2002). A review of alternate conceptions present in the literature on general chemistry topics helped develop distractors for this 22-item concept inventory.

The 19-item Flame Test Concept Inventory (FTCI) (Bretz & Murata Mayo, 2018) was developed to test students' understanding of atomic emission. Students (N=52) enrolled in secondary and postsecondary chemistry courses were interviewed about atomic emission and they were specifically asked to explain flame test demonstrations and energy level diagrams. The analysis of students' explanations yielded alternate

conceptions which were developed into distractors for the concept inventory. A similar methodology of interviewing students to obtain alternate conceptions was employed to develop the Redox Concept Inventory (ROXCI) (Brandriet & Bretz, 2014). The inventory was administered to first- and second-semester general chemistry students and the results identified several alternate conceptions that students developed concerning oxidation numbers, electron transfer, and bonding.

The alternate conceptions that students possess regarding particulate nature of matter and understanding of chemical bonding together with answers to open-ended questions were used to generate distractors to create a two-tier inventory to test these concepts (Othman, Treagust, & Chandrasegaran, 2008). The first tier required a content response and the second tier required a reason for that response (Treagust, 1988). The inventory was administered to 260 grade 9 and 10 students and the results showed that the instrument was functioning well to give insight into students' alternate conceptions on this content area. The instrument was administered to college students in a first-semester general chemistry class as part of another study (Heredia, Xu, & Lewis, 2012). The students were divided into three groups. One group with preparatory chemistry, one group who were repeating the course without preparatory chemistry, and a third who were taking it for the first time without preparatory chemistry. ANCOVA analysis showed that preparatory chemistry had a statistically significant but small effect on students' scores. All three groups yielded similar alternate conceptions as those that were seen in the original study (Othman et al., 2008).

The Bonding Representations Inventory (BRI) is a 23-item inventory which was developed to test the alternate conceptions students developed about covalent and ionic

bonding representations (Luxford & Bretz, 2014). Interviews were conducted with 28 high school physical science, high school chemistry, and general chemistry students to identify common alternate conceptions held regarding concepts of bonding. Four general themes in alternate conceptions were identified and these were periodic trends, electrostatic interactions, the octet rule, and surface features. Analysis of the themes from the interviews led to the creation of the items on the BRI and it was administered to 1072 high school chemistry students and general chemistry students across the U.S.A. The descriptive statistics and psychometrics suggest that the items on the BRI were generating valid and reliable data regarding the alternate conceptions that students develop in the area of chemical bonding.

In the area of thermochemistry and thermodynamics several concept inventories have been developed namely the Thermal Concepts in Everyday Contexts (TCE) (Chu, Treagust, Yeo, & Zadnik, 2012), Thermodynamics Diagnostic Instrument (THEDI) (Sreenivasulu & Subramaniam, 2013), and Heat and Energy Concepts Inventory (HECI) (Prince, Vigeant, & Nottis, 2012). The TCE is mainly targeted at secondary school students, the HECI is targeted at engineering students, and the THEDI is mainly focused on concepts in thermodynamics and not thermochemistry. A Thermochemistry Concept Inventory (TCI) (Wren & Barbera, 2013) was developed to assess alternate conceptions in thermochemistry. An online survey was administered to experts in the field to identify important thermochemistry concepts. Open-ended questions were designed based on these concepts and students were interviewed to obtain their alternate conceptions which were used to develop multiple-choice items for the inventory. The Thermodynamic Diagnostic Test (TDT) was developed to assess students' understanding of thermal

physics (Kamcharean & Wattanakasiwich, 2016). The 15 items were converted into a multiple-choice format using qualitative and quantitative approaches where students were interviewed to obtain their alternate conceptions for use as distractors.

In addition to general chemistry and physical chemistry, concept inventories have also been developed in the area of biochemistry. Bretz and Linenberger (2012) reported the development of a 15-item Enzyme-Substrate Interactions Concept Inventory (ESICI) that measures student understanding of enzyme-substrate interactions. Alternate conceptions of student understanding were derived from interviews with undergraduate and graduate biochemistry students (N=25). Analysis of the interviews revealed five categories of alternate conceptions including enzyme and substrate characteristics, the role of shape and charge in selectivity, how the enzyme interacts with the substrate, competitive vs. non-competitive inhibition, and conformational change. These categories were used to develop the items for the ESICI which was then administered to 707 undergraduate biochemistry students. The analysis of the items suggested that the ESICI was functioning appropriately to determine students' alternate conceptions in enzyme-substrate interactions.

An instrument to assess student understanding of foundational concepts before biochemistry coursework has been reported (Villafañe, Bailey, Loertscher, Minderhout & Lewis, 2011). The instrument was developed through an iterative process employing content validity. A list of concepts from chemistry and general biology were generated and a set of incorrect ideas that are commonly developed were listed. These incorrect ideas were reviewed by 20 biochemistry instructors and they narrowed it down to five chemistry topics and three biology topics. The chemistry topics were bond energy, free

energy, London dispersion forces, pH/pK_a, and hydrogen bonding. The biology topics were alpha helix, amino acids, and protein function. Based on these topics 24 multiple-choice questions were developed and administered to 166 undergraduate biochemistry students. Descriptive statistics, confirmatory factor analysis, and reliability results indicate that the items had excellent fit and they were functioning well to identify difficulties students face with these general chemistry and biology topics.

Brown, Hyslop, and Barbera (2015) reported the development of an instrument that was designed to assess students' understanding of chemistry topics important to the clinical nursing practice. The General, Organic, and Biological Chemistry Knowledge Assessment (GOB-CKA) is a 45-item multiple-choice instrument where the items were built on essential topics which were identified from interviews with experts in the field of nursing. These essential topics were confirmed through a national survey. The individual items were tested through qualitative studies with students from the target population. The psychometric analysis performed on this instrument reported the validity and the reliability of the data collected with the instrument in assessing nursing students' understanding of essential chemistry topics.

These inventories have been extensively developed for general chemistry, physical chemistry, biochemistry, and general, organic, and biological chemistry. However, except for a diagnostic tool developed to measure organic chemistry students' alternate conceptions of acid strength (McClary & Bretz, 2012) and a tool to assess organic chemistry students' knowledge of stereochemical concepts (Leontyev, 2015), there are no concept inventories developed in the area of organic chemistry. The diagnostic tool developed by McClary and Bretz (2012) is a nine-item, multiple-tier,

multiple-choice test where the distractors were derived from deep structure prediction tasks and student interviews. When administered, this ACID I inventory identified two alternate conceptions that students possess with regards to acidity. One is that functional groups determine acid strength, and the other is that stability determined acid strength. There is a need for more such diagnostic tools in organic chemistry. The diagnostic tool developed by Leontyev (2015) is a 20-item Stereochemistry Concept Inventory (SCI) where the items were developed based on important stereochemistry concepts that were identified from two national surveys. Several pilot tests were conducted and the psychometric quality of the items was assessed before revisions were made to problematic items. The final version of the SCI proved to be a useful tool in providing information about the abundance of different incorrect ideas that students had developed regarding stereochemistry.

In these studies, the distractors for the inventory items were either derived from students' alternate conceptions present in literature, qualitative interviews to discern students' alternate conceptions, answers to open-ended questions, or a combination of these approaches to develop items for the concept inventory. Most of these inventories are two-tier based on Treagust's (1988) design where the questions are in linked pairs with an answer tier followed by a response tier. According to Treagust (1988), the items in two-tier instruments help understand the mental models students create even more than think-aloud interviews do.

In addition to strengthening concept inventories by designing them with two-tiers, it is important to develop items that involve three-dimensional thinking. Lavery et al. (2016) reported the development of the Three-Dimensional Learning Assessment

Protocol (3D-LAP) which uses the National Research Council's (NRC) report "A Framework for K-12 Science Education: Practices, Crosscutting Concepts, and Core Ideas" (2012), referred to as the Framework, to redesign science curricula, instruction and the way student learning is assessed in higher education. The Framework outlines three dimensions namely scientific and engineering practices, crosscutting concepts, and disciplinary core ideas which should be incorporated in all aspects of learning. A development team consisting of educators in biology, chemistry, and physics worked to develop the protocol to test assessments as exhibiting three-dimensional learning and they established the validity of the protocol by testing exams in the three disciplines to see how many items exhibited three-dimensional learning. This three-dimensional learning focuses not only on what students should know but how they know it and how they use this knowledge. The 3D-LAP could be used by educators to design items but a more practical application would be to assess existing items and modify them for them to exhibit three-dimensional learning (Underwood, Posey, Herrington, Carmel, & Cooper, 2018). The design of such items exhibiting three-dimensional learning could prove very valuable while developing concept inventories and could strengthen these assessments.

Psychometric Analysis of Concept Inventories

A crucial component of developing instruments is establishing psychometric properties that provide robust information about the instrument and its functionality (Barbera, 2013). Establishing the validity and reliability of instruments like concept inventories gives valuable information to the users regarding the quality of the items which is useful when using these instruments as diagnostic tools (Barbera, 2013). Instruments developed in chemical education utilize Classical Test Theory (CTT) to

establish validity and reliability of concept inventories (Brandriet & Bretz, 2014; Bretz & Murata Mayo, 2018; Chu et al., 2012; Dick-Perez et al., 2016; Kamcharean & Wattanakasiwich, 2016; McClary & Bretz, 2012; Othman et al., 2008; Prince et al., 2012; Sreenivasulu & Subramaniam, 2013)

CTT is utilized routinely by researchers as the first step in establishing validity and reliability because it is based on relatively weak assumptions that are easily met by test data, simple mathematical techniques are used, and moderate sample sizes are needed (Hambleton & Jones, 1993). The major drawback is that item and person parameters are sample dependent. Item Response Theory (IRT) on the other hand is based on strong assumptions that are not easily met by the data, but if the model fits the data then item and person parameters are sample independent (Hambleton & Jones, 1993). IRT models like the Rasch model, generally require larger sample sizes, and this tends to be a drawback for researchers (Hambleton & Jones, 1993).

Boone and Scantlebury (2006), used a science achievement test to describe the strengths of using the Rasch model as a psychometric tool and analysis technique. They state that Rasch techniques help researchers improve the quality of quantitative measurements by assisting them in monitoring scales and improving scales over time. This is especially useful for norm-referenced tests that are used in various areas of science. Boone, Townsend, and Staver (2011) reported the strengths of using Rasch analysis to develop higher-quality science education instruments that help science educators increase the rigor of attitudinal instrument development and analysis.

In chemical education research, most of the instruments developed are relatively new (Arjoon, Xu, & Lewis, 2013). Therefore reporting the validity and reliability of the

data collected with these instruments is of great importance. Arjoon and co-workers (2013) investigated the psychometric evidence reported in articles regarding concept inventories published in the *Journal of Chemical Education* between 2002 and 2011. It was found that researchers favor reporting test-retest reliability, internal consistency, and internal structure over response process validity. Thus there is a need for a detailed report of the quality of assessment tools that would assist future researchers.

The Rasch model has been utilized sparingly while designing concept inventories. Rasch analysis was used on a thermochemistry concept inventory (TCI) (Wren & Barbera, 2014). It was reported that all the items showed good functioning. The TCI was well targeted to the ability of students and the TCI was a measure of overall student ability providing evidence of concurrent validity. Rasch analysis was also used for investigating instrument functioning, item difficulty and person ability which helped validate an ordered multiple-choice test for assessing students' understanding of matter (Hadenfeldt, Bernholt, Liu, Neumann, & Parchmann, 2013). A similar study (Wei, Liu, Wang, & Wang, 2012) used a partial-credit Rasch model to determine the validity and reliability of a computer-modeling based instrument to assess students' understanding of matter. These studies demonstrate that the Rasch model has been used sparingly in chemical education research.

The Rasch model, however, has been used to add to psychometric data on existing concept inventories. The Chemical Concepts Inventory (CCI) (Mulford & Robinson, 2002) has been the source of further investigations. A method based on Rasch modeling to measure learning gains in chemistry was introduced (Pentecost & Barbera, 2013). Learning gain analysis was compared using normalized learning gain calculations and

Rasch modeling on data using the CCI, and it was found that Rasch modeling gave information on students' learning of specific content by comparing item difficulty and student ability on the same scale. Additions were made to the existing psychometric data on the CCI by conducting CTT and Rasch analysis (Barbera, 2013). The unidimensionality, item fit, and reliability were reported using Rasch analysis.

In addition to Barbera's (2013) work, utilizing CTT and Rasch analysis to validate a concept inventory, these two models have been used together in chemical education research. CTT and Rasch analysis were employed to study the impact of the flipped classroom on students' performance and retention rate where ACS general chemistry exam scores were used from pretest and posttest data, and the items on the exam were validated using CTT and Rasch analysis (Ryan & Reid, 2016). CTT and Rasch analysis was also used to test the validity of the Chemical Representations Inventory (CRI) when administered to students and instructors, and it was reported that the test functioned reasonably well for the intended purpose (Taskin, Bernholt, & Parchmann, 2015).

The presence of published concept inventories in organic chemistry is lacking except for ACID I (McClary & Bretz, 2012), which was used to test organic chemistry students' alternate conceptions of acids and bases, and it was validated using only CTT. The SCI (Leontyev, 2015) was validated using CTT, and Rasch analysis was used to provide additional information regarding item functioning. An exploratory study during the development of the inventory on concepts pertinent for developing proficiency in organic reaction mechanisms used Rasch analysis to establish the psychometric properties of the instrument, and it was found that useful information regarding item fit,

construct validity, and reliability was obtained (Nedungadi, Paek, & Brown, 2019). These studies demonstrate the utility of Rasch techniques but it is sparingly used in organic chemistry education. Rasch analysis was used to explore the relationship between person ability and item difficulty on a questionnaire studying teaching assistants' pedagogical content knowledge in ^1H NMR spectroscopy (Connor & Shultz, 2018). Rasch techniques were used to validate an instrument developed to measure graduate students' pedagogical content knowledge of thin layer chromatography (Hale, Lutter, & Shultz, 2016). These studies demonstrate that there are examples of Rasch analysis being utilized in organic chemistry education, but none have utilized Rasch analysis to validate concept inventories.

These studies support the importance of using Rasch analysis techniques to determine the quality of assessment tools in chemical education. Rasch analysis will help establish the quality of the RMCPI instrument when administered to students from different universities and give psychometric data on an assessment tool in the field of organic chemistry which lacks such diagnostic tools.

Summary

In this chapter, a review of relevant literature regarding the history of the curved-arrow notation, the different approaches to teaching reaction mechanisms, and the difficulties students face with reaction mechanisms were presented. Additionally, relevant literature regarding concept inventories in chemical education and methods to establish psychometric properties of these inventories were discussed. This study aims to fill the gap in the literature by designing and validating a diagnostic tool for large-scale assessment of students' alternate conceptions of concepts pertinent to developing

proficiency in organic reaction mechanisms. The next chapter outlines the methods which were employed in this study.

CHAPTER III

METHODOLOGY

The methodology utilized to answer the research questions that guided this study are discussed in this chapter. The purpose of this study was to develop a two-tier concept inventory on concepts that are pertinent to developing proficiency in organic reaction mechanisms. The participants, data collection, and data analysis for each of the three phases are discussed in this chapter along with the validity and reliability of the study.

The methodology employed was mixed methods, which was conducted in three main phases. Phase 1 was a qualitative study in which semi-structured, in-depth interviews with organic chemistry instructors were conducted to identify concepts that are pertinent to developing proficiency in organic reaction mechanisms. Phase 2 was a quantitative study where a national survey was administered to organic chemistry instructors across the U.S.A. to determine what the national consensus was regarding these concepts identified by experts in phase 1 as pertinent to developing proficiency in organic reaction mechanisms. Phase 3 consisted of three sub-phases. In the exploratory phase, questions were written representing each of the concepts identified from phase 2, and they were administered in an open-ended format to organic chemistry students to evaluate students' understanding of these concepts. Semi-structured interviews were also conducted with students to explore their thought process while answering the questions. Incorrect answers revealed alternate conceptions and were used as distractors for multiple-choice questions which constituted a two-tier concept inventory. This concept

inventory was administered to first-semester organic chemistry students one month into the semester as part of the pilot study. A full study was conducted on a larger sample as part of an iterative process after the items on the inventory were modified to create the final version of the concept inventory.

Protection of Human Subjects

Before data collection, Institutional Review Board approval was obtained for each phase of the project (see Appendix A).

For phase 1 all participants were given a code to maintain their anonymity, and all participants were given two consent forms (see Appendix A), one to be signed and returned and the other to be kept for their records. All interviews were digitally recorded and saved on a password-protected device. Backups of these interviews were saved on password-protected devices.

For phase 2 all participants were asked to give their consent before responding to the national survey (see Appendix A). The consent form was included as part of the survey; if participants chose not to give their consent, they were directed to the end of the survey and were not allowed to submit their responses. Although Qualtrics records the email addresses, the location, and the IP addresses of the participants, this information was deleted immediately after data collection was stopped to preserve the anonymity of the participants.

For student interviews and data collection in phase 3, all participants were given a code to maintain their anonymity and two consent forms (see Appendix A), one to be signed and returned and the other to be kept for their records.

Phase 1: Semi-Structured, In-Depth Interviews

In-Depth Interviews

“The qualitative research interview seeks to describe the meanings of central themes in the life world of the subjects. The main task in interviewing is to understand the meaning of what the interviewees say” (Kvale, 1996). The in-depth interview is a technique designed to elicit a vivid picture of the participant’s perspective and experience on the research topic. In this first phase of the study, in-depth interviews were conducted with organic chemistry instructors to obtain their opinions on organic reaction mechanisms and the concepts involved in the process.

Participants

Interviews were conducted with a purposeful sample (Creswell, 2013) of organic chemistry instructors. The main criterion for participation was that the instructors must have either been teaching organic chemistry at the time of the interview or must have taught organic chemistry at some point. An invitation was sent via email to instructors at universities in the Rocky Mountain region of the U.S.A.

Data Collection

The data were collected using semi-structured, in-depth interviews (Creswell, 2013). The interviews with instructors lasted approximately 30 minutes. The participants were asked to give their opinions on the importance of organic reaction mechanisms, the concepts that are pertinent to developing proficiency in organic reaction mechanisms, and the difficulties students face with organic reaction mechanisms. Additionally, they were asked about their approach to teaching organic reaction mechanisms and problems that can be solved in organic chemistry with the electron-pushing formalism. All participants

were asked to provide demographic information before the interview was conducted. The full interview protocol is shown in Appendix B.

Data Analysis

The interviews were transcribed verbatim except for stammering phrases such as ‘uh’ and ‘um’ which were removed for clarity. The data were analyzed using thematic analysis which is a process by which the researcher analyzes “what” is spoken or written during data collection (Riessman, 2008). An inductive approach to analysis was used where codes and themes were created from the data. The validity and reliability of the data obtained were established by member check and inter-rater reliability (Creswell, 2013). The transcripts were sent back to the participants as a form of member-check for them to make sure the information was accurate. They were also asked to add details if they felt that it would help clarify their ideas. The transcripts were sent to other researchers with experience in chemical education as a form of inter-rater reliability to check the reliability of the identified themes.

Phase 2: National Survey

Participants

A national survey was administered to organic chemistry instructors across the U.S.A. An email list of organic chemistry instructors at different universities across the U.S.A. was compiled using the research group indices database from the organic chemistry division of the American Chemical Society (ACS) (Organic Synthetic Faculty, 2020; OrganiclinksPUI, 2018). The sample consisted of those who were willing and able to take part in the survey.

Survey Instrument

The survey was designed on Qualtrics and consisted of five sections including the consent form, a screening question, questions on concepts, questions on the participants' opinions regarding reaction mechanisms, and demographic questions (see Appendix C). The participants were asked to give their consent on the first page of the survey and if they have taught or were currently teaching an undergraduate organic chemistry course. If they failed to give their consent or answered no to the question of teaching an undergraduate organic chemistry course, they were directed to the end of the survey. The concepts identified by experts from phase 1 were included in the national survey. Participants were asked to classify the concepts in terms of their pertinence to developing proficiency in organic reaction mechanisms using a scale of important (critical for proficiency in organic reaction mechanisms), foundational (moderately critical for proficiency in organic reaction mechanisms) and not important (not critical for proficiency in organic reaction mechanisms). The participants were asked for their opinions regarding the importance of organic reaction mechanisms, their approach to teaching organic reaction mechanisms, and the barriers that students face when learning reaction mechanisms. Finally, the participants were asked demographic questions regarding the highest chemistry degree they had earned, their area of specialization in organic chemistry, their teaching experience in organic chemistry, the type of university where they were employed, whether the organic chemistry course they were teaching was one semester or two semesters, whether they used the ACS standardized test for their organic chemistry course, and their gender.

Data Collection

The participants were asked to complete the survey online. An initial email with a link to the survey was sent to all organic chemistry instructors from the compiled list of organic chemistry instructors across the U.S.A. The link to the survey was kept open for one month and a reminder email was sent two weeks after the initial email to those who had not completed the survey.

Data Analysis

The percentage of responses for each concept was analyzed. Concepts that were identified as important were retained and concepts that were identified as foundational were further analyzed by considering the additional comments made by the participants.

Phase 3: Development of the Concept Inventory

Exploratory Study

Participants. Approximately three questions representing each concept identified by participants from the national survey were developed (see Appendix D) and administered in an open-ended format to first-semester organic chemistry students at a mid-sized university in the Rocky Mountain region of the U.S.A. Open-ended interviews were conducted with first-semester organic chemistry students at the same mid-sized university in the Rocky Mountain region of the U.S.A. to obtain information on their thought processes while answering the questions.

Data collection. Each question asked for an answer and an explanation. The explanation constituted the second tier of the concept inventory. The questions were administered to the participants one month into the semester immediately prior to the study of organic reaction mechanisms. The participants were provided with a periodic

table and were not allowed to use any other instructional materials while answering the questions. The participants were given approximately 30 minutes to complete the questions during their regular class period. The participants also answered demographic questions.

The open-ended interviews with students lasted approximately 45 minutes. Participants were presented with the questions on the inventory in an open-ended format first and then the multiple-choice format. Participants were asked to answer the questions and explain their thought process. All interviews were digitally recorded and saved on a password-protected device. All written answers to questions were recorded using a digital pen and paper (Livescribe, 2016). Backups of these interviews were saved on password-protected devices.

Data analysis. The responses to the questions were analyzed for common alternate conceptions. Some of the most commonly occurring alternate conceptions were used as distractors for the multiple-choice format of the questions which constituted the two-tier concept inventory.

The interviews with participants were transcribed verbatim except for stammering phrases such as 'uh' and 'um'. These were removed for clarity. The data were analyzed using thematic analysis (Riessman, 2008). The thought processes that students use for answering the questions were analyzed to further understand students' alternate conceptions and if new potential distractors emerged from their alternate conceptions.

Pilot Study

Participants. The pilot version of the two-tier concept inventory was administered to first-semester organic chemistry students at a mid-sized university in the

Rocky Mountain region of the U.S.A. The beta version of the inventory was administered to first-semester organic chemistry students at three different universities in the Rocky Mountain region of the U.S.A.

Data collection. The questions were administered to the participants one month into the semester immediately prior to the study of organic reaction mechanisms. The participants were provided with a periodic table and were not allowed to use any other instructional materials while answering the questions. The participants were given approximately 45 minutes for the pilot version and approximately 20 minutes for the beta version to complete the questions during their regular class period on a bubble sheet which was scanned by the researcher at the university. The participants also answered demographic questions.

Data analysis. The responses to the multiple-choice questions were scored as correct or incorrect and were aggregated to yield the total score. Classical Test Theory (CTT) was used to analyze item difficulty (P) and item discrimination (D). The distractors were also analyzed to gain insight into which distractors functioned well and which ones were under-utilized.

Item difficulty (P) represents the proportion of those responding correctly (Doran, 1980). It is given by the formula shown in equation 1.

$$P = \frac{\text{Number of correct responses}}{\text{Total number of responses}} \quad (1)$$

Items that are said to be of appropriate difficulty level will have item difficulty values between 0.3 and 0.8 for a criterion-referenced test with very easy items being above 0.8 and very difficult items being below 0.3 (Kaplan & Saccuzzo, 1997).

Item discrimination indices (D) are measures of the degree to which an item distinguishes between the high performers and low performers, and values above 0.3 are said to be acceptable (Doran, 1980). Item discrimination is calculated using the formula shown in equation 2 where D_i is the discrimination index for item i , P_u is the proportion of those in the upper group who respond to the item correctly and P_l is the proportion of those in the lower group who respond to the item correctly.

$$D_i = P_u - P_l \quad (2)$$

For larger samples ($N > 200$), the upper and lower groups are created from the top and bottom 27% of respondents, but for smaller samples, they are created from the top and bottom 50% of respondents (Kelley, 1939).

Based on the item difficulty, item discrimination, and distractor analysis, the items were analyzed and either modified or omitted to create the alpha version of the concept inventory which was administered to a larger sample.

Full Study

Participants. The alpha version of the Reaction Mechanisms Concept Proficiency Inventory (RMCPI) was administered to first-semester organic chemistry students at universities in the Rocky Mountain region and universities in other regions of the U.S.A.

Data collection. The instrument was administered to the participants one month into the semester immediately prior to the study of organic reaction mechanisms. The participants were provided with a periodic table and were not allowed to use any other instructional materials while answering the questions. The participants were given approximately 25 minutes to complete the test. The participants answered the questions during their regular class period on a bubble sheet which was then mailed back to the

researcher by the instructor at the university where the data were collected. The participants also answered demographic questions on their gender, major, year of study, high school graduation year, and whether they were taking the organic chemistry course for the first time or retaking it.

Data analysis. The responses to the questions were scored as correct or incorrect. CTT was used to conduct item difficulty, item discrimination, and distractor analysis on the items. Additionally, the validity and reliability of the concept inventory were established using Rasch analysis which gave additional psychometric information.

The Rasch model is a probabilistic model; the principle is that a person with a greater ability than another person should have a greater probability of correctly answering any item. Also, if one item is more difficult than another, the probability of correctly answering the easier item is higher (Bond & Fox, 2015). The general equation for the dichotomous Rasch model is given in equation 3 where item difficulty is denoted by δ_i and person ability is denoted by β_n .

$$P_{ni}(x = 1) = \frac{\exp(\beta_n - \delta_i)}{1 + \exp(\beta_n - \delta_i)} \quad (3)$$

Equation 3 shows that the probability of correctly answering an item $P_{ni}(x = 1)$, where n is person number and i is item number, is equal to the function of the difference between a person's ability (β_n) and the difficulty of the item (δ_i) (Rasch, 1980).

The principal component analysis (PCA) was used to conclude if the data are unidimensional and fit well to the Rasch model. Wright maps were used to assess item difficulty in relation to person ability. Wright maps place item difficulty and person ability on the same log-odds scale. Fit statistics were used to analyze the item fit to the Rasch model. This estimation begins with calculating the response residual for each

person n and each item i . This is calculated as the difference between the actual response and the Rasch model expectation. These residuals are summarized in a fit statistic either as a mean square fit statistic (MNSQ) or a standardized fit statistic (Z-STD). These fit statistics are characterized as outfit and infit statistics. The outfit statistic is an average of the standardized residual variance across both persons and items and emphasizes unexpected responses far from a person's or item's measure (Wright & Masters, 1982). The infit statistic is one where the residuals are weighted by their individual variance to emphasize unexpected responses close to a person's or item's measure. Both types of fit statistics have an expected value of 1, but infit statistics are used more routinely because they are weighted and hence not sensitive to outlying scores. For a criterion-referenced test, the critical values for mean square fit statistics should be in the range of 0.70 – 1.30 (Bond & Fox, 2015). These fit statistics indicate whether the data accurately fit the dichotomous Rasch model.

Assessment of Validity

The validity of the data obtained using the RMCPI focused on construct validity which employs subjective measures such as face validity, and content validity. The face validity was established with the input of both chemistry graduate students, and undergraduate students who took part in the open-ended interviews in phase 3 of the study. The chemistry graduate students and the undergraduate students were asked to review the clarity of the questions on the instrument. The content validity refers to the coverage of a certain content domain presented in the blueprint of the instrument and the questions, and this was established by sending the instrument to organic chemistry

faculty and having them review and revise if necessary the content for clarity, correctness, and relevance.

Additionally, the RMCPI items were compared to similar items on the American Chemical Society (ACS) Organic Chemistry Exam (Form 2014, Form 2016) and General Chemistry Exam (Form 2015, Form 2017). The performance of students on these similar items on the ACS exam was compared to their performance on those RMCPI items in order to evaluate the degree to which two or more measures that theoretically should be related to each other are observed to be related to each other (Kaplan & Saccuzzo, 1997). The RMCPI items were also compared to the ACS Exams Institute anchoring concepts content map for undergraduate organic chemistry (Raker, Holme & Murphy, 2013) to explore the content coverage and notice similarities in content areas.

The construct validity was further established using the PCA of residuals to test the unidimensionality of the instrument. The unidimensionality of the RMCPI helps determine if the instrument is actually measuring the intended construct.

Assessment of Reliability

The reliability of the RMCPI was analyzed in terms of internal consistency which is represented through a Cronbach's alpha value. This type of reliability is concerned with the consistency of the data produced by an instrument, and it requires only a one-time administration of the instrument (Trochim & Donnelly, 2007). A high alpha value indicates a high correlation among items measuring the same construct. An acceptable Cronbach's alpha value is 0.70-1.00 (Nunnally & Bernstein, 1994).

Person separation reliability, which is an estimate of how well one can differentiate persons on the measured variable (Wright & Masters, 1982), was used to

establish the reliability of the items on the concept inventory. This estimate is based on the same concept as Cronbach's alpha, and it gives information regarding the reliability of the instrument. The reliability estimate for persons ranges from 0 to 1 (Wright & Masters, 1982).

Summary

In this chapter, the methods that were utilized to answer the research questions were discussed. A qualitative design was used to answer the first research question, a quantitative design was used to answer the second research question, and a mixed-methods design was used to answer the third research question. The assessment of the validity and reliability of the data collected using the instrument were also discussed in this chapter.

CHAPTER IV
THINKING LIKE AN ELECTRON: CONCEPTS
PERTINENT TO DEVELOPING
PROFICIENCY IN ORGANIC
REACTION MECHANISMS

Contribution of Authors and Co-Authors

Manuscript in Chapter IV

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Contributions: Helped conceive the study design. Provided feedback on data and early drafts of the manuscript.

Abstract

The difficulties students face with organic reaction mechanisms has been the subject of much research in chemical education however, no concept inventory has been reported in this area. The development of a concept inventory would be useful for the large-scale assessment of students' understanding of concepts pertinent to developing proficiency in reaction mechanisms. The first step in the design of such an inventory is identifying the pertinent concepts. In phase 1 of this study, open-ended interviews were carried out with organic chemistry instructors ($N=11$) in order to ascertain their opinions on concepts pertinent to developing proficiency in reaction mechanisms. Phase 2 of the study consisted of a national survey of organic chemistry instructors ($N=183$) to explore the general consensus regarding the concepts identified in phase 1. The results yielded 10 concepts identified by experts to be pertinent. The general consensus among organic chemistry instructors is that the topic of reaction mechanisms is important to the study of organic chemistry, but students have difficulty understanding the meaning of the curved-arrow notation. Future work will include the design and development of a concept inventory based on these identified concepts.

Introduction

Organic chemistry is a required course not just for chemistry majors but also for various other majors (Seymour & Hewitt, 1997). Pre-health students are required to take organic chemistry for medical and dental schools; however organic chemistry is usually perceived as a gatekeeper class that separates the students not qualified for medical school (Baum & Axtell, 2005). Among the organic chemistry students, the course has a reputation of being difficult, complex, and with some material that students may perceive as being irrelevant (Grove, Cooper, & Cox, 2012).

An important topic in undergraduate organic chemistry is reaction mechanisms. The use of the curved-arrow notation or the electron-pushing formalism to convey electron flow during bond breaking and bond making is of great importance in the teaching and learning of organic chemistry (Grove, Cooper, & Cox, 2012).

The importance of reaction mechanisms in an organic chemistry class was emphasized in the qualitative study by Duis (2011). In her study, organic chemistry instructors' opinions on concepts that are important, core, or foundational in organic chemistry were explored and the results indicated that 16 of the 18 participants identified reaction mechanisms as an important organic chemistry topic. It was further reported that 15 of the 18 participants stated that the topic of reaction mechanisms is difficult for organic chemistry students.

Bhattacharyya and Bodner (2005) have argued that the ability to use the curved-arrow notation in reaction mechanisms is a vital skill for organic chemists to possess.

Bhattacharyya (2013) has reported that students use this curved-arrow notation as their

primary tool to explain and/or predict reaction outcomes including the generation of side products, regioselectivity, and stereochemistry.

There are several qualitative studies showing that undergraduate students and even graduate students encounter difficulties when using the curved-arrow notation to propose reaction mechanisms; these difficulties include a failure to understand the basic purpose of the notation and how to utilize it effectively for problem-solving (Anderson & Bodner, 2008; Bhattacharyya & Bodner, 2005; Bhattacharyya, 2014; Ferguson & Bodner, 2008; Grove, Cooper, & Rush, 2012; Kraft et al., 2010). Flynn and Ogilvie (2015) reported a “mechanisms-first” approach to teaching organic chemistry rather than the traditional functional-group approach. The existing organic chemistry curriculum was modified to introduce reaction mechanisms before students learned a single organic reaction. This curricular change aims to ensure that students learn to interpret reactions based on patterns of reactivity which would assist them when they are faced with new reactions.

Studies have also shown that students are unable to attribute any meaning to the curved-arrows when utilized to depict reaction mechanisms (Bhattacharyya & Harris, 2018; Galloway et al., 2017). The results indicated that students struggled the most with describing the structural representations, and different students used a different language to describe the same reactions.

A recent study (Bodé, Deng, & Flynn, 2019) explored the causal mechanistic explanations that organic chemistry students provide when comparing two proposed reaction mechanisms. The results indicated that the majority of the students understood the need for providing causal arguments to support their claims but they did so

irrespective of whether the claims were correct or incorrect. Therefore the conclusion that can be drawn is that students tend to struggle with using mechanistic thinking to make claims and explain them.

The difficulties that students face with reaction mechanisms seem to stem from a lack of understanding of fundamental concepts. Studies exploring student understanding of fundamental organic chemistry topics (Anzovino & Bretz, 2016; Cruz-Ramirez De Arrellano & Towns 2014), indicate that students lack the understanding necessary for classifying substances as nucleophiles and/or bases and accurately describing the steps that take place during the course of the reaction. These studies demonstrate that students lack the fundamental skills needed to solve mechanistic questions.

While these qualitative studies are important to gain an understanding of how students view reaction mechanisms and the difficulties they face, no concept inventories with the exception of ACID I (McClary & Bretz, 2012) designed to test organic chemistry students' alternate conceptions of acids and bases, have been developed to conduct a large-scale assessment of students' understanding of concepts that are pertinent to developing proficiency in organic reaction mechanisms. The development of such an inventory would help organic chemistry instructors gain insight into their students' understanding of pertinent concepts before they start the study of reaction mechanisms. Instructors can then decide if they need to review some of these concepts before teaching reaction mechanisms or modify their course content to incorporate some of these concepts. Additionally, the inventory may inform the general chemistry instructors on concepts taught in general chemistry that are further used in organic chemistry. To

develop such an inventory, it is necessary to obtain information on the concepts that are pertinent to developing proficiency in organic reaction mechanisms.

The present study was divided into two phases. The first phase consisted of open-ended interviews with organic chemistry instructors to get their opinion on concepts that they consider pertinent to developing proficiency in organic reaction mechanisms. The second phase consisted of a national survey to generalize the results obtained from the first phase. With this aim in mind the research questions that govern this study are:

- Q1 What are the chemistry concepts perceived by experts to be pertinent to developing proficiency in organic reaction mechanisms?
- Q2 Is there a consensus at the national level regarding the concepts perceived to be pertinent to developing proficiency in organic reaction mechanisms?

Methodology

Phase 1: Semi-Structured, Open-Ended Interviews

Participants. Interviews were conducted with a purposeful sample (Creswell, 2013) of organic chemistry instructors. The main criterion for participation was that the instructors had to have had experience with teaching the organic chemistry course. An invitation was sent via email to instructors at universities in the Rocky Mountain region of the U.S.A. The sample consisted of 11 organic chemistry instructors (five females and six males). Among the participants, 10 had doctorate degrees and one had a masters degree as their highest earned degrees in chemistry. Based on the Carnegie classification of universities, three participants were from an M1 university (masters colleges and universities – larger programs), six participants were from a D/PU university (doctoral/professional universities), and two participants were from an R1 university (doctoral universities – very high research activity). Among the 11 participants, eight

participants had over 10 years of teaching experience with the minimum being two years teaching experience and nine participants mentioned the use of the ACS standardized exams in their classes. Prior to data collection, Institutional Review Board approval was obtained through the University of Northern Colorado (see Appendix A).

Data collection. The data were collected using semi-structured, open-ended interviews (Creswell, 2013) with organic chemistry instructors to gain their opinions on organic reaction mechanisms and the concepts involved in the process (see Appendix B). All participants were asked to provide demographic information before the interview was conducted (see Appendix B). All participants were assigned a code (OI# for organic chemistry instructor followed by a number) to maintain their anonymity. The interviews lasted approximately 30-45 minutes. The participants were asked to provide their opinions on the importance of organic reaction mechanisms, the concepts that are pertinent to developing proficiency in organic reaction mechanisms, and the difficulties students face with organic reaction mechanisms. Additionally, they were asked about their approach to teaching organic reaction mechanisms and problems that can be solved in organic chemistry with the electron-pushing formalism.

Data analysis. The interviews were transcribed verbatim except for stammering phrases such as 'uh' and 'um' which were removed for clarity. An inductive approach to thematic analysis was used where codes and themes were created from the data (Riessman, 2008). The validity and reliability of the data obtained were established by member check and inter-rater reliability (Creswell, 2013). The transcripts were sent back to the participants as a form of member-check for them to make sure the information was accurate. They were also asked to add details to help clarify their ideas. The transcripts

were evaluated by four other researchers with experience in chemical education as a form of inter-rater reliability to check the reliability of the identified themes giving a percentage agreement of 95%.

Phase 2: National Survey

Participants. A national survey was administered to organic chemistry instructors across the U.S.A. An email list of organic chemistry instructors at different universities across the U.S.A. was compiled using the research group indices database from the organic chemistry division of the American Chemical Society (ACS) (Organic Synthetic Faculty, 2020; OrganiclinksPUI, 2018). A total of 1500 organic chemistry instructors were invited to participate and 183 completed the survey for a response rate of 12.2%. Of the participants who completed the survey, 127 were male, 181 had earned doctorate degrees in chemistry, 158 had over five years of organic chemistry teaching experience, 111 were from primarily undergraduate institutions (PUI), and 91 used the ACS standardized exams in their class. Prior to data collection, Institutional Review Board approval was obtained through the University of Northern Colorado (1245324-1).

Survey instrument. The survey was created on Qualtrics and consisted of five sections including a consent form, a screening question, questions on concepts, questions on the participants' opinions regarding reaction mechanisms, and demographic questions (see Appendix C). The participants were asked to give their consent on the first page of the survey and if they have taught or are currently teaching an undergraduate organic chemistry course. If they failed to give their consent or answered "no" to the question of teaching an undergraduate organic chemistry course, they were directed to the end of the survey. The concepts identified by experts from Phase 1 were included in the national

survey, and additionally, space was provided for comments or the addition of new concepts. Participants were asked to classify the concepts in terms of their relevance to developing proficiency in organic reaction mechanisms using a scale of important (critical for proficiency in organic reaction mechanisms), foundational (moderately critical for proficiency in organic reaction mechanisms) and not important (not critical for proficiency in organic reaction mechanisms). The participants were asked for their opinions regarding the importance of organic reaction mechanisms, their approach to teaching organic reaction mechanisms, and the barriers that students face when learning reaction mechanisms. Demographic information was also collected from the participants.

Data collection. An initial email with a link to the Qualtrics survey was sent to the participants. The survey was open for one month with a reminder email being sent two weeks after the initial email was sent. All participants were given a code (NS# for national survey followed by a number) to maintain their anonymity.

Data analysis. The data were analyzed in Qualtrics. The percentage of responses for each concept was analyzed. The concepts that were identified as important were retained. The concepts that were identified as foundational were further analyzed by examining the comments of the participants regarding the concepts.

Results and Discussion

Phase 1: Semi-Structured, Open-Ended Interviews

Importance of reaction mechanisms. Ten (91%) participants indicated that organic reaction mechanisms are important to the success of students in their organic chemistry courses. One of the organic chemistry instructors (OI 003) mentioned that organic reaction mechanisms are important only at the beginning of the course, and

students tend to use it as a tool for predicting the product of reactions only initially but they still require an understanding of reaction mechanisms:

What I find frequently is that once the students can understand the process of the movement of electrons they are more easily able to say okay this is very repetitive across different reaction styles. That's when they can rely less on completing a mechanism to predict the product of a reaction. OI 003

Nine (82%) participants said that understanding intermediates in reactions, reaction rates, and acid-base chemistry are the types of problems one can solve using the arrow-pushing formalism. Five (46%) participants mentioned that every problem in organic chemistry can be solved using the arrow-pushing formalism. These results confirmed and emphasized the importance of organic reaction mechanisms in the study of organic chemistry.

Approach to teaching the course. When asked whether they used the functional group approach or mechanisms based approach when teaching their course, two (18%) of the participants stated they use a mechanistic approach, five (46%) of the participants indicated they use a combination of both, and four (36%) of the participants mentioned teaching by using the functional group approach because traditionally in textbooks the organization of the chapters is based on functional groups. These four participants stated that ideally they would like to use more of a mechanistic approach to teaching their classes which further reiterates the importance of mechanisms in organic chemistry.

When asked how they introduce the topic of reaction mechanisms to their students, four (36%) of the participants stated using alkene reactions, and seven (64%) of the participants indicated using acid-base chemistry. These seven participants indicated

that their students are exposed to the arrow-pushing formalism when they are introduced to acid-base chemistry but the first time they see a complete mechanism is when they cover electrophilic addition reactions of alkenes or substitution reactions of alkyl halides. This suggests that a fundamental understanding of the arrow-pushing formalism is important for understanding other topics covered in the organic chemistry course.

Concepts pertinent to developing proficiency in reaction mechanisms. Of the total participants, seven (64%) mentioned that resonance and inductive effects are pertinent while six (54%) of the participants stated that electron density and polarity, acids and bases, and electrophiles and nucleophiles are pertinent for developing proficiency in reaction mechanisms. The full list of concepts identified, the number of participants who identified these concepts and the ranking based on percentage agreement are shown in Table 4.1.

Atomic structure, electronic configuration, Lewis structures, molecular geometry, and bonding are concepts covered in general chemistry and typically reviewed at the beginning of a first-semester organic chemistry course. Acids and bases, electron density and polarity, and hybridization are also covered in general chemistry but they are typically reviewed in detail in the first-semester organic chemistry class and their applicability to organic chemistry is introduced. Resonance and inductive effects, electrophiles and nucleophiles, and stability of intermediates are covered usually within the first month of a first-semester organic chemistry course.

Table 4.1.

Concepts Identified in Phase 1 as Pertinent to Developing Proficiency in Organic Reaction Mechanisms

Concepts Identified	Number of Participants (N=11)	Percentage Agreement (%)
Resonance & inductive effects	7	64
Acids & bases	6	54
Electrophiles & nucleophiles	6	54
Electron density & polarity	6	54
Atomic structure	5	46
Electronic configuration	5	46
Lewis structures	5	46
Hybridization	5	46
Molecular geometry	5	46
Stability of intermediates	4	36
Bonding	2	18

Difficulties students face. Of the participants, six (54%) mentioned that one of the main barriers to understanding reaction mechanisms that students face is the difficulty in understanding how the tool works and what the arrows represent. One of the participants (OI 011) explained how students in general are unable to give proper meaning to the curved-arrows:

I guess to some extent just arrow pushing backwards. A lot of the time people don't quite understand that arrows are electrons only, nothing else ever. And so you see arrows coming off of plus charges drifting around the molecule and arrows backwards for a step that would otherwise be valid. OI 011

Lack of understanding of fundamental general chemistry principles like Lewis structures and acid-base chemistry was identified as another reason why students struggle with reaction mechanisms by five (46%) of the faculty interviewed. This is one of the participant's (OI 004) opinion:

One big issue that people have is they don't actually pay attention to how many lone pairs are on heteroatoms. They don't think about the lone pairs unless they are really explicit and so that's one issue. Another issue is they don't actually understand really where the electrons are located. So they will kind of draw random arrows and you need to have the arrow pointing exactly who you are going to bond up to and they tend to be vague and sloppy on that. And that indicates to me that they don't really understand where the electrons are really located and that whole idea of breaking bonds and forming bonds it's not inculcated in their brain. They are just trying to memorize mechanisms as just like little lines on a little drawing type of thing you know. OI 004

This participant talked about students resorting to rote memorization of reaction mechanisms. Five other participants also mentioned that students seem to struggle with understanding reaction types such as nucleophilic substitution and electrophilic addition thereby resorting to rote memorization.

Phase 2: National Survey

The results from Phase 1 were limited to the 11 participants from universities in the Rocky Mountain region of the U.S.A. To generalize the results and gather information on what the consensus is at the national level regarding the concepts perceived to be pertinent to developing proficiency in reaction mechanisms, a national survey was conducted. The 183 participants in this phase of the study were asked the same questions as those used in Phase 1 of the study.

Importance of reaction mechanisms. Of the participants, 87% stated that reaction mechanisms are important for their students' success. One participant's (NS 047)

comment suggests that students could move forward with a limited familiarity of reaction mechanisms but it could affect their long-term understanding:

Students can be moderately successful in organic chemistry 1 but they will struggle in organic chemistry 2 without a good understanding of mechanisms.

NS 047

These results are consistent with the results from Phase 1 of the study where 91% of the participants indicated that reaction mechanisms are important for their students' success in organic chemistry.

Approach to teaching the course. As was the case in Phase 1 of the study, the participants were divided on their opinion of a functional group based approach versus a mechanisms based approach to teaching organic chemistry. Among the participants, 51% mentioned that they use a combination of both, 33% indicated they use a mechanisms based approach, and 16% stated they use a functional group approach. The instructors prefer to use a combination of both methods as suggested by one participant's (NS 127) comment:

Try to relate to mechanisms even when using a functional group approach.

Functional group approach helps later in synthesis problems. NS 127

When the participants were asked how they introduce the topic of mechanisms, 74% indicated using acid-base chemistry which is comparable to 64% of participants in Phase 1 who provided the same answer. These results indicate that most organic chemistry instructors use acid-base chemistry as the foundation for building an understanding of reaction mechanisms.

Concepts pertinent to developing proficiency in reaction mechanisms. Of the 11 concepts identified in Phase 1 of the study, nine were identified as important for developing proficiency in organic reaction mechanisms by more than 60% of the national survey participants. A larger percentage of participants stated that these concepts were important (critical) rather than foundational (moderately critical). For the concept of atomic structure, only 24% of the participants mentioned that it is important, 66% stated that it is foundational, and 10% stated that it is not important. Similarly, for the concept of electronic configuration 34% of the participants indicated that it is important, 58% stated that it is foundational, and 9% stated that it is not important. Since the number of participants identifying that the two concepts were not important was 10% or less, and since we defined foundational as moderately critical, the comments made by the participants who determined these two concepts to be foundational were further analyzed. It was found that 81% of these participants considered the concept of valence electrons to be more important to reaction mechanisms than the broad concepts of atomic structure and electronic configuration. The concept of valence electrons is related to both atomic structure and electronic configuration. Due to these results, the two concepts of atomic structure and electronic configuration were combined under the concept of valence electrons instead. A complete list of concepts and participants' opinions are presented in Table 4.2.

Table 4.2.

List of Concepts and Participants' Percentage Agreement on Each Concept from the National Survey

Concepts	Important	Foundational	Not Important
Resonance & inductive effects	86%	14%	<1%
Acids & bases	79%	21%	<1%
Electrophiles & nucleophiles	92%	8%	<1%
Electron density & polarity	81%	18%	<1%
Atomic structure	24%	66%	10%
Electronic configuration	34%	58%	9%
Lewis structures	87%	13%	<1%
Hybridization	68%	31%	1%
Molecular geometry	64%	35%	1%
Stability of intermediates	84%	16%	<1%
Bonding	82%	17%	1%

Note:

Important was defined as critical for developing proficiency in reaction mechanisms.

Foundational was defined as moderately critical for developing proficiency in reaction mechanisms.

Not important was defined as not critical for developing proficiency in reaction mechanisms.

These results indicate that there is a general consensus at the national level regarding the concepts that are pertinent to developing proficiency in organic reaction mechanisms. A comparison between the results obtained from Phase 1 and Phase 2 of this study is shown in Table 4.3.

Table 4.3.

Comparison of Results from Phase 1 and Phase 2

Concepts Identified	Percentage Agreement (%)		
	Phase 1	Phase 2	
		Important	Foundational
Resonance & inductive effects	64	86	14
Acids & bases	54	79	21
Electrophiles & nucleophiles	54	92	8
Electron density & polarity	54	81	18
Atomic structure	46	24	66
Electronic configuration	46	34	58
Lewis structures	46	87	13
Hybridization	46	68	31
Molecular geometry	46	64	35
Stability of intermediates	36	84	16
Bonding	18	82	17

A comparison of the results from both phases of the study indicates that there is consistency among the opinions of experts on most of the concepts. There is a discrepancy in opinion regarding the concepts of stability of intermediates, bonding, and electrophiles and nucleophiles between participants in phase 1 and phase 2. A large percentage of participants in phase 2 indicated that these concepts are important whereas participants in phase 1 did not identify these concepts as pertinent. Participants in Phase 2 stated that stability of intermediates is helpful for predicting reaction outcomes as well as explaining mechanisms, bonding is important since an understanding of sigma and pi bonds is crucial to reaction mechanisms, and electrophiles and nucleophiles is what organic chemistry is all about. These three concepts were retained since a large percentage of participants in Phase 2 identified them as important.

Participants in Phase 2 were asked to provide other concepts they considered important for developing proficiency in reaction mechanisms. The topics that were provided are ones that are usually covered under the major concepts identified such as

understanding pK_a which is related to acid-base chemistry and formal charge, electron dot diagrams, and octet rule which are all related to Lewis structures. This information is useful while developing questions for the concept inventory since specific areas of each concept can be addressed.

Difficulties students face. Participants in Phase 2 of the study were asked to give their opinion on the difficulties students face with understanding reaction mechanisms. The most common difficulties stated were the lack of understanding of electron flow, failure in understanding the basics of bonding and valency, remembering fundamentals from general chemistry, and identifying electrophiles and nucleophiles. A consequence of these difficulties is that students resort to rote memorization. These results are consistent with those obtained in Phase 1.

Limitations

In Phase 2 of the study, 61% of the participants were from a primarily undergraduate institution (PUI) with only 18% from an R1 school and even less from other institution types; this was dictated by the number of participants who chose to complete the online survey. The final list of concepts represents the opinion of 183 participants out of 1500 that were invited to take part in the national survey giving a response rate of 12.2%. Although this response rate might seem low, it is comparable to the response rates reported for national surveys conducted in other studies (Bhattacharyya, 2013; Emenike, Schroeder, Murphy, & Holme, 2013).

Conclusions and Future Work

The purpose of this multi-step study was to gather the opinions of organic chemistry instructors regarding concepts that are considered pertinent to developing

proficiency in organic reaction mechanisms. The results from Phase 1 of this study identified 11 concepts perceived by experts to be pertinent to developing proficiency in reaction mechanisms. Among the 11 concepts identified in this phase five concepts, (electronic configuration, Lewis structures, polarity, acid-base chemistry, and electrophiles and nucleophiles), were found to be similar to those previously reported (Bhattacharyya, 2013). In addition to these concepts, six new concepts were identified in this study; these include resonance and inductive effects, atomic structure, hybridization, molecular geometry, stability of intermediates, and bonding. The results of phase 1 were compared to the results obtained at the national level (phase 2), and it was found that the general consensus is very similar. The concepts of atomic structure and electronic configuration were combined under the concept of valence electrons based on the comments of the participants in the national survey to yield a final list of 10 concepts that were retained. The concepts that are considered pertinent to developing proficiency in organic reaction mechanisms obtained from phase 2 of this study in decreasing order of importance are electrophiles and nucleophiles, Lewis structures, resonance and inductive effects, stability of intermediates, bonding, acids and bases, hybridization, molecular geometry, electron density and polarity, and valence electrons.

The results generated from this study indicate a general consensus among organic chemistry instructors regarding the importance of reaction mechanisms for gaining a comprehensive understanding of organic chemistry. From the instructors' perspective, students seem to have the greatest difficulty with understanding what the arrows in the curved-arrow notation mean, and consequently the students resort to rote memorization. A conclusion that can be drawn from these results is that the struggle with reaction

mechanisms can be attributed to a lack of understanding of fundamental general chemistry and organic chemistry concepts which is consistent with the literature (Anzovino & Bretz, 2016; Bhattacharyya & Bodner, 2005; Bhattacharyya, 2013). Additionally, these results indicate that before we can explore student thinking and thought processes that lead to this difficulty with reaction mechanisms, it is important to make sure we are providing them with the necessary tools needed to develop mechanistic thinking. It may be difficult for students to use mechanistic thinking to solve higher-order problems if they are struggling with fundamental chemistry concepts.

The development of a concept inventory for the large-scale assessment of students' understanding of these pertinent concepts would be useful for organic chemistry instructors to assess their students and address these alternate conceptions before introducing reaction mechanisms. The next phase of this research will be the design, development, and psychometric analysis of the inventory based on our findings and reported literature.

CHAPTER V

DEVELOPMENT AND PSYCHOMETRIC ANALYSIS OF AN INVENTORY ON CONCEPTS PERTINENT TO DEVELOPING PROFICIENCY IN ORGANIC REACTION MECHANISMS

Contributions of Authors and Co-Authors

Manuscript in Chapter V

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Contributions: Developed and implemented the study design. Collected and analyzed data in all phases of the study. Wrote the first draft of the manuscript.

Co-Author: Dr. Michael D. Mosher

Contributions: Assisted in designing and modifying the items for the inventory. Contributed manuscript revisions.

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Contributions: Assisted in modifying items for the inventory. Contributed manuscript revisions.

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Contributions: Directed the project, assisted in designing items, and assisted in analysis of data. Contributed manuscript revisions.

Abstract

The Reaction Mechanisms Concept Proficiency Inventory (RMCPI) is a multiple-choice instrument designed to assess students' understanding of concepts that are pertinent to developing proficiency in organic reaction mechanisms. This manuscript describes the development of the inventory items and the psychometric analysis of the instrument. In the development stage, open-ended questions were administered to first-semester organic chemistry students ($N=138$), and open-ended interviews were conducted with students ($N=22$) to gain insight into their thought process. The answers revealed alternate conceptions which were used to formulate distractors for the inventory. A pilot version and a beta version of the inventory were administered to 105 and 359 first-semester organic chemistry students, respectively. From these administrations the 26-item alpha version of the RMCPI was developed and administered to first-semester undergraduate organic chemistry students ($N=753$) from 14 different universities throughout the U.S.A. Psychometrics at the item level were conducted using item analysis in Classical Test Theory and Rasch analysis. Psychometrics at the test level were conducted by assessing the validity and reliability of the data obtained using the RMCPI. The results indicate that the items on the RMCPI function well to reveal students' alternate conceptions regarding concepts pertinent to developing proficiency in organic reaction mechanisms. The instrument meets the acceptable standards of validity and reliability for concept inventories.

Introduction

The difficulties students face with understanding organic reaction mechanisms have been a source of interest in chemical education research. Studies have focused on understanding how students use their organic chemistry knowledge to solve mechanistic problems (Anderson & Bodner, 2008; Bhattacharyya & Bodner, 2005; Bhattacharyya, 2013; Bhattacharyya, 2014; Ferguson & Bodner, 2008; Grove, Cooper, & Cox 2012; Grove, Cooper, & Rush, 2012; Kraft et al., 2010). However, no work has been reported on the development of a diagnostic tool in the form of a concept inventory for the large-scale assessment of students' understanding of concepts pertinent to developing proficiency in reaction mechanisms. Such a tool could assist instructors in identifying alternate conceptions that students have developed. The purpose of this study is the development and psychometric analysis of the Reaction Mechanisms Concept Proficiency Inventory (RMCPI) to assess students' understanding of concepts pertinent to developing proficiency in organic reaction mechanisms.

Concept inventories are usually multiple-choice assessments that use identified student alternate conceptions as distractors (Richardson, 2004). There have been several concept inventories developed in chemistry as diagnostic tools to determine students' alternate conceptions, and multiple methodologies have been utilized for developing suitable distractors (Brandriet & Bretz, 2014; Bretz & Linenberger, 2012; Bretz & Murata Mayo, 2018; Brown et al., 2015; Chu et al., 2012; Dick-Perez et al., 2016; Luxford & Bretz, 2014; McClary & Bretz; Mulford & Robinson, 2002; Othman et al., 2008; Villafañe et al., 2011; Wren & Barbera, 2013). Many of these inventories are two-tier based on Treagust's (1988) design where the questions are in linked pairs with an

answer tier followed by a response tier. These inventories have been extensively developed in different areas of chemistry; however, with the exception of the inventory developed by McClary and Bretz (2012) to assess organic chemistry students' understanding of acids and bases, there are no concept inventories developed and reported in the literature to assess students' understanding of other concepts pertinent to developing proficiency in organic reaction mechanisms.

An important step in the development of concept inventories is establishing the validity and reliability of the instrument (Bandalos, 2018). Classical Test Theory (CTT) is routinely used as the first step in exploring item functioning because it involves simple mathematical techniques, and it requires moderate sample sizes (Hambleton & Jones, 1993). The majority of the concept inventories developed in chemical education utilize CTT to establish validity and reliability (Brandriet & Bretz, 2014; Bretz & Linenberger, 2012; Bretz & Murata Mayo, 2018; Brown et al., 2015; Chu et al., 2012; Dick-Perez et al., 2016; Luxford & Bretz, 2014). The development of a concept inventory is an iterative process and CTT provides a quick method to check the functioning of items on a smaller sample which helps justify the modification or elimination of items during the developmental phases.

In CTT, item and person parameters are sample dependent; however, in Item Response Theory (IRT) if the model fits the data then item and person parameters are sample independent (Hambleton & Jones, 1993). IRT models, such as the Rasch model, generally require larger sample sizes. Rasch analysis helps researchers determine the probability of an examinee answering an item which gives details about item quality and person ability beyond just the test scores (Hambleton & Jones, 1993).

The utility of Rasch analysis for psychometric assessment and as an analysis technique in science education has been reported (Boone & Scantlebury, 2006; Boone et al., 2011). Other than a few exceptions (Hadenfeldt et al., 2013; Nedungadi et al., 2019; Wei et al., 2012; Wren & Barbera, 2014), Rasch analysis has not been used frequently when designing concept inventories in chemical education. However, it has been used to add to psychometric data on established concept inventories (Barbera, 2013; Pentecost & Barbera, 2013; Taskin et al., 2015). In chemical education, researchers tend to favor reporting particular types of evidence such as test-retest reliability and internal consistency over response process validity while developing concept inventories (Arjoon et al., 2013). There is a need for users of these instruments to have a more detailed report on the quality of the assessment tool to use the instrument effectively.

When developing concept inventories it is important to establish proper functioning of the instrument by conducting a rigorous psychometric analysis of the instrument. Rasch analysis together with CTT can provide adequate psychometric data thereby establishing the robustness of the RMCPI as an assessment instrument.

The present study was aimed at the design and development of the RMCPI, and psychometric assessment using CTT and Rasch analysis. The reliability and validity of the data obtained using the RMCPI were also established. The research question that governed this study was:

- Q3 How can one appropriately assess organic chemistry students' conceptual understanding of the concepts perceived by the experts to be pertinent to developing proficiency in organic reaction mechanisms?

Methodology

Protection of Human Subjects

Institutional Review Board approval was obtained before data collection for all phases of the study (see Appendix A). All interviews were digitally recorded and all written answers to interview questions were recorded using a digital pen and paper (Livescribe, 2016). The participants in the open-ended interviews were given a code (SS# for student subject followed by a number) to maintain their anonymity.

Study Design

This research was conducted in various steps. The inventory development, test administration, and psychometric analysis constitute the steps in this study. Figure 5.1 gives the general model for the study design.

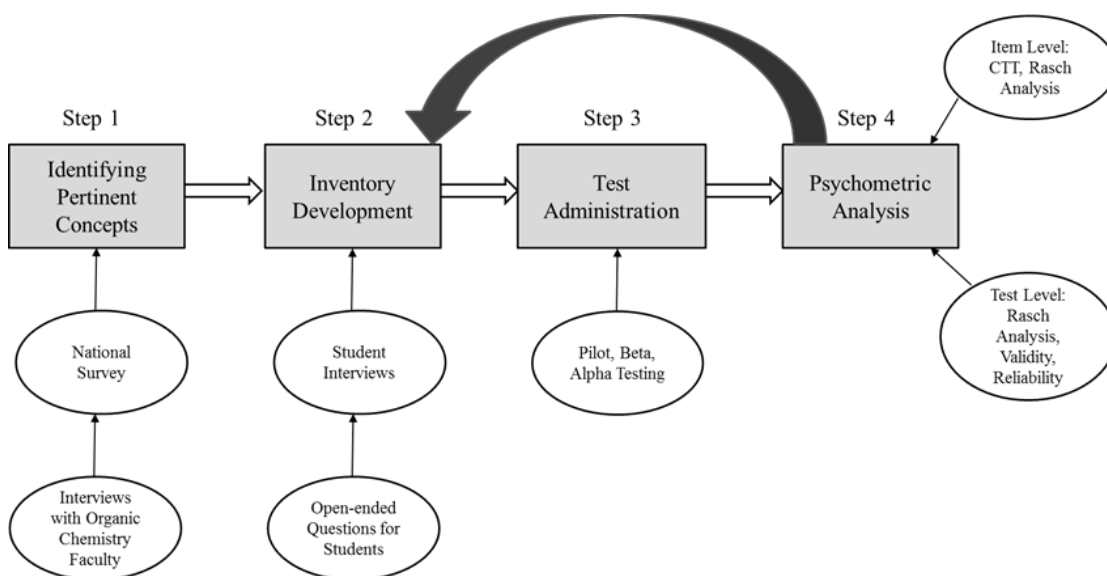


Figure 5.1. General model for study design.

Step 1: Identifying Pertinent Concepts

The concepts pertinent to developing proficiency in organic reaction mechanisms were obtained by conducting interviews with a purposeful sampling of organic chemistry

instructors ($N=11$). The results from the interviews yielded 11 concepts, and these results were generalized by conducting a national survey of organic chemistry instructors ($N=183$). The results from the national survey yielded 10 concepts considered by organic chemistry instructors to be pertinent to developing proficiency in organic reaction mechanisms.

Step 2: Inventory Development

Questions representing each of the 10 concepts (see Appendix D) were administered to 138 first-semester undergraduate organic chemistry students (75% female, 34% chemistry majors) at a D/PU university (doctoral/professional university) in the Rocky Mountain region of the U.S.A. There were approximately three questions representing each concept.

The questions were administered in an open-ended format and asked for an answer and explanation which constituted the two tiers of the inventory. The responses to the questions were analyzed for common alternate conceptions. Some of the most commonly occurring alternate conceptions were subsequently used as distractors for the multiple-choice format of the questions.

Open-ended interviews were conducted with first-semester undergraduate organic chemistry students during the development stages of the inventory. The guiding questions are presented in Appendix E. In this phase of the project a convenient sample of 22 students volunteered to participate of which 82% were female, and 14% were chemistry majors. Students were presented with the items in both open-ended formats and multiple-choice formats. The interviews gave information on students' thought processes and their

use of conceptual knowledge while answering the questions which further assisted in the development of the items.

Step 3: Test Administration

The pilot version of the inventory containing 50 items (see Appendix F) was administered to 105 first-semester undergraduate organic chemistry students at a D/PU university in the Rocky Mountain region of the U.S.A. Among the participants, 71% were female, 48% were sophomores, 24% were chemistry majors, and 12% were repeating the course.

The beta version of the inventory containing 27 items (see Appendix G) was administered to 359 first-semester undergraduate organic chemistry students of which 264 participants were from two different R1 universities (doctoral university: very high research activity) and 95 participants were from an M1 university (masters colleges and universities: larger programs) in the Rocky Mountain region of the U.S.A. Among the participants, 59% were female, 35% were sophomores, 18% were chemistry majors, and 14% were repeating the course.

The alpha version of the inventory containing 26 items (see Appendix H) was administered to 753 first-semester undergraduate organic chemistry students at 14 different universities in the U.S.A. Of the 753 participants, 66% were female, 21% were chemistry majors, 43% were sophomore, 41% graduated high school in 2018, and 90% were taking the organic chemistry course for the first time. The list of schools and the number of students from each school are shown in Table 5.1.

Table 5.1.

List of Schools and Number of Students for Alpha Administration

School	Region in the U.S.	Carnegie Classification	Number of Students
A	West North Central	Baccalaureate Colleges: Diverse Fields	21
B	Mountain	M1: Master's Colleges and Universities – Larger Programs	53
C	Mountain	R1: Doctoral Universities – Very High Research Activity	70
D	Mountain	D/PU: Doctoral/ Professional Universities	121
E	Mountain	Associate's Colleges: High Transfer-Mixed Traditional/Nontraditional	44
F	South Atlantic	D/PU: Doctoral/ Professional Universities	42
G	Mountain	R2: Doctoral Universities – High Research Activity	161
H	Middle Atlantic	Baccalaureate Colleges: Arts & Science Focus	13
I	East North Central	Baccalaureate Colleges: Arts & Science Focus	31
J	West North Central	Baccalaureate Colleges: Arts & Science Focus	38
K	Mountain	D/PU: Doctoral/Professional Universities	51
L	South Atlantic	M3: Master's Colleges and Universities – Smaller Programs	18
M	New England	M1: Master's Colleges and Universities – Larger Programs	48
N	East North Central	D/PU: Doctoral/Professional Universities	42

Note: Region in the U.S. is based on the U.S.A. Census division classification (Census, Regions, and Divisions of the United States, 2013).

The only criterion for participant selection was that the participants had to be in a first-semester organic chemistry class. The test was administered to the participants one month into the semester before they started the study of reaction mechanisms. The participants were provided with a periodic table, and they were not allowed to use any other instructional materials during the test. There was no time limit, but the participants completed the test on a bubble sheet in approximately 45 minutes for the pilot version and 25 minutes for both the beta and alpha versions. The tests were administered in person and participants took it during their regular class period.

The majority of the items in all versions of the RMCPI were based on Treagust's (1988) two-tier design with an answer tier followed by a response tier. The items on the pilot and beta versions were organized under 10 concepts pertinent to developing

proficiency in organic reaction mechanisms namely valence electrons, Lewis structures, hybridization, molecular geometry, bonding, polarity, acids/bases, electrophiles/nucleophiles, resonance/inductive effects, and stability of intermediates. The items on the alpha version were organized under nine concepts since the concept of valence electrons was eliminated after the beta administration.

Step 4: Psychometric Analysis

The psychometric analysis of the RMCPI at the item level was conducted using CTT and Rasch analysis to obtain information regarding the functioning of the items. Item difficulty, item discrimination, and distractor analysis in CTT were used. Item difficulty (P) represents the proportion of participants responding correctly (Doran, 1980). Items that have difficulty values between 0.3 and 0.8 for a criterion-referenced test are said to be acceptable with very easy items being above 0.8 and very difficult items being below 0.3 (Kaplan & Saccuzzo, 1997). Item discrimination indices (D) are measures of the degree to which an item distinguishes between the high performers and low performers (Doran, 1980). For larger samples ($N > 200$), the high performing and low performing groups for calculating discrimination indices are created from the top and bottom 27% of respondents and for smaller samples from the top and bottom 50% of respondents (Kelley, 1939). Discrimination values greater than or equal to 0.3 are deemed acceptable and those below 0.3 may require further investigation (Ebel & Frisbie, 2006).

In Rasch analysis, fit statistics were used to analyze item fit to the Rasch model, and a Wright map was used to compare item difficulty and person ability. The responses were scored as correct or incorrect and aggregated to yield the total score for item

analysis in CTT. For Rasch analysis one assumption is unidimensionality and to satisfy this assumption, local independence must be met (Bond & Fox, 2015). Local independence of the items suggests that how a participant answers one item is not dependent on how the participant answers another item (Bond & Fox, 2015). Therefore for Rasch analysis, the items that are linked pairs were scored as 1 if both tiers were answered correctly and 0 if one or both of the tiers were answered incorrectly.

The psychometric analysis at the test level was conducted by assessing the validity and reliability of the data obtained using the RMCPI. The validity of the data obtained using the instrument was established at various stages during the development process using construct validity and employed the subjective measures of face validity and, content validity. Additionally, the construct validity was also established using Rasch analysis. Cronbach's alpha was used to assess reliability. A high alpha value indicates a high correlation among items and an acceptable Cronbach's alpha value is 0.70-1.00 (Nunnally & Bernstein, 1994). The reliability was also evaluated using person separation and item separation reliability (Bond & Fox, 2015).

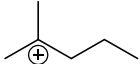
Results and Discussion

Inventory Development

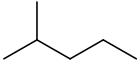
Identifying alternate conceptions. The responses of the participants to the open-ended questions were analyzed to identify common alternate conceptions. The most commonly occurring alternate conceptions were used as distractors when designing the items for the pilot version of the RMCPI. The full list of open-ended questions is presented in Appendix D.

Student interviews. The open-ended interviews with students helped to understand their thought process while answering the questions and gave further information on alternate conceptions they possess. An example of an item where students were choosing the correct option for the answer tier but the incorrect option for the response tier is presented in Figure 5.2.

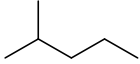
Which is most stable?



1



2



3

(a) 1
(b) 2
(c) 3

What is the reason for your answer to the above question?

(a) Induction
(b) Charge is centralized
(c) It is the most symmetrical
(d) Positive charge is at the end

Figure 5.2. Item assessing stability of intermediates used in student interviews.

When the question was presented in an open-ended format, 14 out of 15 students who were given the question chose option (a) for the answer tier. This participant's (SS008) response for why 1 is the most stable indicates a fragmented understanding:

It's because a positive charge is most stable around the most amount of offshoots.

I don't know what that is called. The higher the degree is the more stable it is so the positive charge would want to move towards that because it's more stable.

SS008

When presented with the above question the same 14 students chose option (a) for the answer tier but they were not sure about the response tier. These results suggest that students know that tertiary carbocations are the most stable but their reasoning is flawed.

Of the 14 participants, seven chose the correct answer for the reason tier but they were not confident about it as seen by this participant's (SS014) comment:

Probably induction just because my professor has said it so many times in lecture.

SS014

These results indicate that students have difficulty understanding fundamental concepts that are important for organic reaction mechanisms. Students seem to remember certain details due to either memorization or repeated exposure to the concept but they have difficulty with providing reasoning.

The alternate conceptions developed by students identified from administration of the open-ended questions and student interviews is given in Table 5.2. These identified alternate conceptions were used to develop items for the pilot version of the RMCPI.

Table 5.2.

List of Concepts and Alternate Conceptions Identified

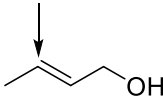
Concepts	Alternate Conceptions
Valence Electrons	Valence electrons equal the number of protons Valence electrons are the number of unpaired electrons in the outermost shell
Lewis Structures Hybridization	Nitrogen atoms always form 3 bonds and carbon atoms form 4 bonds Hybridization depends on the type of bond - single, double, triple 3 electron groups indicate sp^3 hybridization
Molecular Geometry	Double bond affects the geometry Lone pairs on carbon affect the geometry
Bonding Electron Density/Polarity Acids/Bases	All bonds close to triple bonds are strong All electronegative atoms are electrophilic More electronegative leads to higher acidity Lewis base is a proton acceptor
Electrophiles/Nucleophiles	Electrons flow from region of deficiency to region of density Sodium is positive and wants electrons so it is the electrophile The direction of electron flow
Resonance/Induction Effects	Best contributor to an overall resonance hybrid is the one that shows the movement of electrons and charges are spread out Double bonds in the middle make more resonance structures Fluorine atoms contribute more to resonance
Stability of Intermediates	When the charge is on a central atom it stabilizes the carbocation When the carbocation is symmetrical it is stable In a carbonyl group, electrons can go to the carbon and oxygen atoms want to donate electrons

Pilot Administration

The pilot version of the RMCPI contained 50 items. The difficulty and discrimination values for all items in the pilot version were computed (Appendix I). The results indicated that only seven items (9, 19, 20, 21, 29, 44, and 46) had adequate difficulty and discrimination indices and could be retained without modification.

The remaining items were further analyzed by distractor analysis. For a distractor to be effective it should represent a plausible alternate conception and if a distractor does not attract any respondents then it may be implausible and not a good distractor (Bandalos, 2018). The data were analyzed in terms of the percentage each option was selected by the participants. An example of an item with a questionable distractor is shown in Figure 5.3.

Which statement best describes the geometry of the indicated atom?



(a) Trigonal planar
 (b) Trigonal pyramidal
 (c) Bent
 (d) Linear
 (e) Tetrahedral

Figure 5.3. Item assessing molecular geometry with a questionable distractor.

The distribution of the choices for this item were: (a) (52.3%), (b) (18.3%), (c) (12.8%), (d) (2.8%), and (e) (13.8%). The correct option for this item is (a). The option (d) was under-utilized and hence was eliminated, since it is not plausible and therefore not a good distractor. Similarly, distractor analysis was conducted for all the other items to help

modify the items. The poorly performing items on the pilot version were modified or omitted based on results from the pilot administration to create the beta version of the RMCPI.

Beta Administration

The difficulty and discrimination indices for the 27 items on the beta version of the RMCPI were computed (see Appendix J). The results indicate that 16 out of the 27 items have adequate difficulty and discrimination values. The remaining items were further analyzed and either modified or omitted.

Items 1 and 2 are a linked pair and both have difficulty values of 0.71 and 0.6, respectively, suggesting that they are relatively easy items and hence their discrimination indices are only 0.16 and 0.13, respectively. Items 1 and 2 are related to the concept of valence electrons and during the process of establishing content validity, experts suggested that the concept and item were not pertinent to developing proficiency in organic reaction mechanisms. Three other items assessing the concept of valence electrons present on the pilot version of the RMCPI were also found to be easy items suggesting that this is a concept that students are understanding. The item analysis for items 1 and 2 and the item analysis for other items assessing the concept of valence electrons together with the opinion of experts was enough evidence to eliminate the items and hence the concept itself.

Distractor analysis was utilized to further analyze the items and the problematic items were modified or deleted based on item analysis to give the alpha version of the RMCPI. The alpha version contains 26 items.

Alpha Administration

Psychometrics at the test level. The difficulty and discrimination indices for the 26 items on the alpha version of the RMCPI were computed (Appendix K). The scatter plot depicting the difficulty and discrimination values for the 26 items is presented in Figure 5.4.

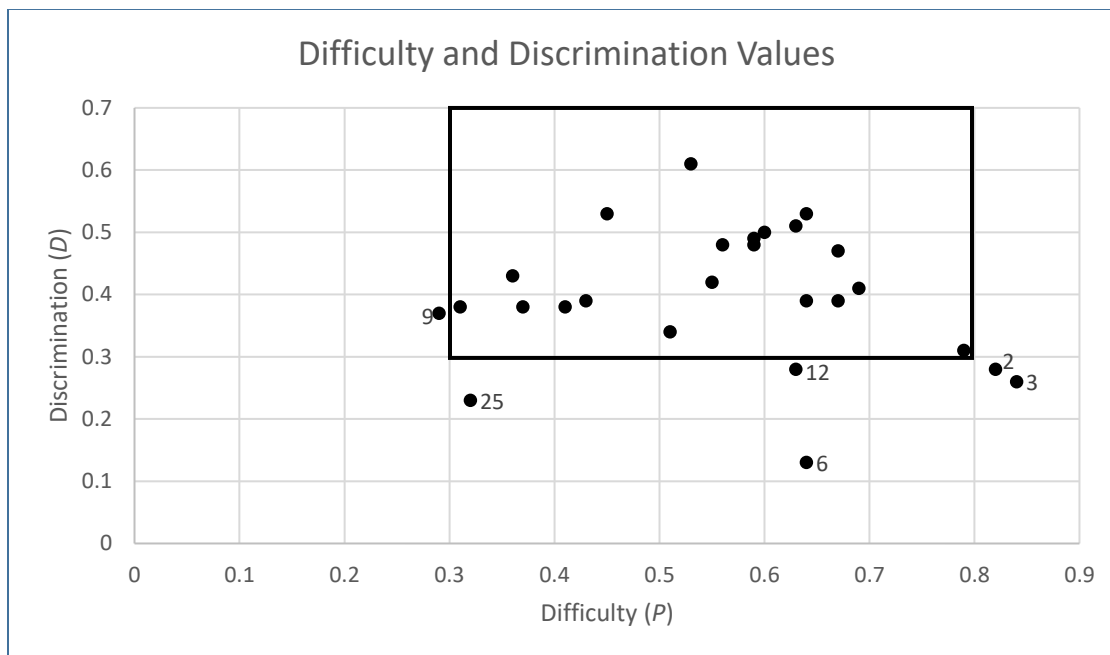


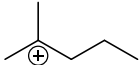
Figure 5.4. Scatter plot showing difficulty (P) and discrimination (D) values for all 26 items on the alpha version of the RMCPI.

Note: Only the poorly-performing items have been labelled. Items 1, 4, 5, 7, 8, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, and 26 are within the rectangle which represents the accepted values of difficulty and discrimination.

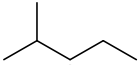
The results indicate that 20 of the 26 items have both difficulty and discrimination indices within the acceptable ranges. The 6 items that are out of the acceptable range for difficulty and discrimination are two-tier items where the linked pair is performing well. Therefore useful information regarding students' alternate conceptions can be obtained from these items.

Item 25 has a discrimination index of 0.23 and a difficulty index of 0.32 which suggests that the item is difficult and not discriminating well. Item 25 is the response tier to item 24; both items are shown in Figure 5.5.

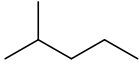
24. Which of the following is the most stable?



1



2



3

(a) 1
(b) 2
(c) 3

25. What is the reason for your answer to question 24?

(a) The alkyl groups are electron-donating.
(b) The carbocation is most symmetrical.
(c) The carbocation can easily grab electrons.

Figure 5.5. Items on the alpha version of the RMCPI assessing the stability of intermediates.

Item 24 is functioning well and 54.4% of the participants chose the correct answer (a). Interestingly, 26.8% of the participants chose (c) which is the least stable carbocation. For item 25 the distribution of answers is: (a) (27%), (b) (32.4%), and (c) (40.6%) with (a) being the correct answer. Items 24 and 25 assess the concept of stability of intermediates. The results from the pilot and beta administrations indicated that this was a concept that students were not understanding thoroughly. These results further indicate that students have a fragmented understanding of carbocation stability and the factors affecting this stability. Even though their psychometric quality is below the acceptable range it can be argued that items 24 and 25 give important information.

Unidimensionality. One assumption made in the Rasch model is that the scale is unidimensional which means that it is measuring a single latent trait which is a hypothetical or unobserved characteristic (Bond & Fox, 2015). In this study, the latent

trait can be defined as the conceptual knowledge required for gaining proficiency in organic reaction mechanisms. Unidimensionality within the Rasch model is analyzed by principal component analysis (PCA) of residuals where if the observed raw variance for measures is greater than 20%, the data are said to be unidimensional (Bond & Fox, 2015). The PCA of residuals for the data obtained using the alpha version of the RMCPI shows that 25.3% of the raw variance was explained by the Rasch model suggesting that the RMCPI is measuring a unidimensional construct.

Item difficulty compared to person ability. The Rasch model places item difficulty and person ability on the same logit scale using a vertical plot called a Wright map. The Wright map for the data obtained using the alpha version of the RMCPI is shown in Figure 5.6.

The Wright map shows that the range of logit measures is from a low of -3 to a high of $+3$. The item difficulties range from about -1.3 logits for the easiest item to about $+2.4$ logits for the most difficult item. This range of logit measures might indicate that the data are not skewed. However, on closer examination it can be seen that some students have ability lower than item I(10.11) which is the easiest item. This indicates that the inventory is marginally difficult and skewed with respect to person ability. Though the inventory is slightly difficult, none of the items were estimated with high imprecision indicating that the items are well targeted to the student population.

Item fit. The fit of the items to the Rasch model was evaluated using infit (weighted) and outfit (unweighted) statistics which help in identifying problematic items. The infit and outfit statistics are shown in Table 5.3.

Table 5.3.

Fit Statistics for the Alpha Version of the RMCPI Data

Item No.	Measure	SE	Infit <i>MNSQ</i>	Infit <i>ZSTD</i>	Outfit <i>MNSQ</i>	Outfit <i>ZSTD</i>
(8.9)	1.64	.11	.93	-1.2	.96	-0.3
(24.25)	1.46	.10	1.01	.2	1.18	1.8
(21.22)	.80	.09	.98	-.5	1.01	.1
(6.7)	.71	.09	1.03	.9	1.00	.0
(18.19)	.56	.09	1.06	1.6	1.09	1.5
(12.13)	.30	.08	1.13	3.7	1.15	3.0
(16.17)	-.11	.08	.93	-2.3	.92	-1.9
(14.15)	-.24	.08	.99	-.2	1.02	.4
20	-.31	.08	1.06	2.2	1.05	1.1
23	-.48	.08	.87	-.48	.82	-4.2
26	-.50	.08	.99	-.2	1.02	.3
5	-.68	.08	1.00	.1	.98	-.4
(3.4)	-.86	.08	.92	-2.7	.86	-2.6
(1.2)	-.94	.08	1.01	.5	1.03	.5
(10.11)	-1.34	.09	1.03	.8	1.20	2.7
<i>M</i>	.00	.09	1.00	-.1	1.02	.1
<i>SD</i>	.85	.01	.06	2.0	.10	1.8

Note: SE = Standard error, MNSQ = Mean square value, ZSTD = Standardized z-score

All the items have mean square (MNSQ) infit and outfit statistics within the acceptable range of 0.70 to 1.30 for a low stakes multiple-choice test (Bond & Fox, 2015). Since the mean squares for all the items are acceptable, the ZSTD values can be ignored (Bond & Fox, 2015). These results suggest that the items fit well to the dichotomous Rasch model and there are no discrepancies between the observations and expectations for the items on the alpha version of the RMCPI.

Psychometrics at the Test Level

Assessment of validity. Several types of validity were assessed. The face validity was established during the developmental stages of the inventory from the input of chemistry graduate students and organic chemistry undergraduate students regarding the

clarity of the items. The items on the inventory were administered to chemistry graduate students ($N=8$) and their feedback was obtained regarding the items (see Appendix L). The input from the graduate students was used to modify the items during the development of the inventory. The undergraduate students who took part in open-ended interviews, were asked to provide their feedback on the items and this feedback was also used to modify the items.

The content validity was established by sending the instrument to organic chemistry faculty ($N=8$) to enable them to revise the content if necessary for clarity, correctness, and relevance. A Qualtrics survey was administered to 50 organic chemistry faculty across the country and eight completed responses were recorded (see Appendix M). One of the items on the inventory assessing the concept of electrophiles and nucleophiles did not have a response tier. The item is presented in Figure 5.7.

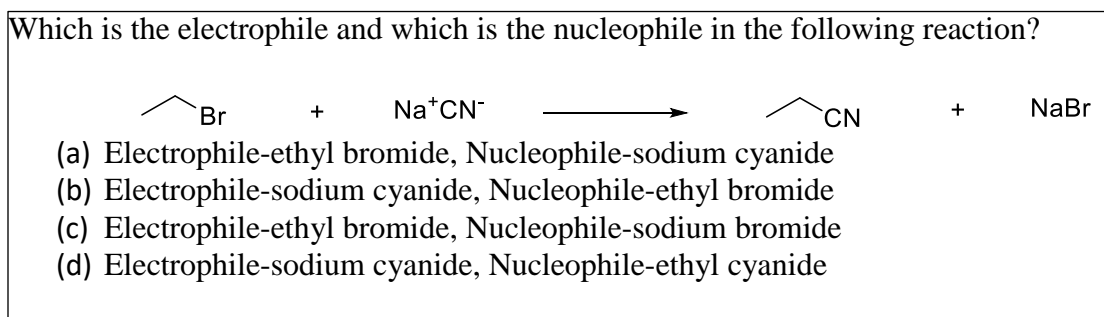


Figure 5.7. Item assessing electrophiles and nucleophiles without a response tier.

The feedback from the experts indicated that labeling the molecules by their names would not be appropriate since that would also test nomenclature, and the use of a simpler nucleophile in place of Na^+CN^- was recommended. Additionally, it was suggested that if the forward reaction was being considered then only the reactants need to be labeled and not the products. This would also help in setting up a response tier to

get further information regarding students' understanding. The item was modified based on these suggestions as shown in Figure 5.8.

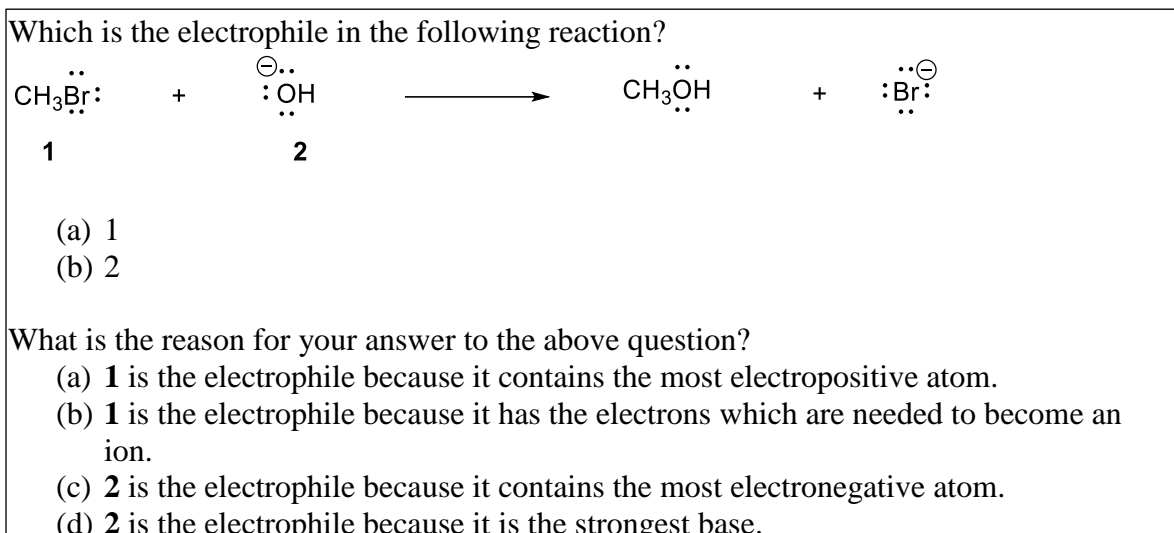


Figure 5.8. Modified item assessing electrophiles and nucleophiles.

The performance of students on the RMCPI items were compared to the performance of students on similar items on the ACS standardized general chemistry and organic chemistry exams. Of the 26 RMCPI items on the alpha version, 15 items had similarities with items on the ACS General Chemistry Exams (Form 2015, Form 2017) and ACS Organic Chemistry Exams (Form 2014, Form 2016). Most of the items on the RMCPI had comparable difficulty and discrimination indices to similar items on the ACS standardized exams. These results suggest that student performance on these items is comparable. For example, item 6 on the RMCPI which had difficulty and discrimination values of 0.64 and 0.13, respectively, was compared to a similar item on an ACS organic chemistry exam which had difficulty and discrimination values of 0.77 and 0.18, respectively. This comparison suggests that even though item 6 on the RMCPI is not discriminating very well, student performance is not different from an item covering the same content area on the ACS exam. The RMCPI items were also compared to the

anchoring concepts content map for undergraduate organic chemistry proposed by the ACS Exams Institute (Raker et al., 2013). It was found that all nine concepts under which the items were grouped are present in the anchoring concepts content map. This indicates that the content coverage of the RMCPI agrees with the national standard.

The PCA of residuals indicated that 25.3% of the raw variance was explained by the Rasch model suggesting the unidimensionality of the instrument. The PCA of residuals together with the item fit to the dichotomous Rasch model, suggests that the alpha version of the RMCPI is measuring the intended construct of students' understanding of concepts that are pertinent to developing proficiency in organic reaction mechanisms. These results further establish the construct validity of the data obtained using the RMCPI.

Assessment of reliability. Several aspects of reliability were assessed. The internal consistency reliability was measured using Cronbach's alpha for the pilot version and beta version and the values obtained were 0.682 and 0.632, respectively, which are slightly lower than the accepted value of 0.7 although Cronbach's alpha is the lower bound of reliability compared to other forms of reliability (Nunnally & Bernstein, 1994). The Cronbach's alpha values were also obtained if items were deleted and this information was used together with results from the pilot and beta versions to eliminate items during the development of the inventory. The Cronbach's alpha value for the 26-item alpha version of the RMCPI was 0.712 which indicates that the items are correlated.

The item separation reliability was found to be 0.99 which is higher than the accepted value of 0.8 (Bond & Fox, 2015), and hence it is adequate. The person separation reliability was found to be only 0.60 which is lower than the accepted value of

0.8. It is difficult to obtain reliability using Rasch analysis within the acceptable range and it is easier to obtain item separation reliability within the acceptable range rather than person separation reliability (Bond & Fox, 2015). The person separation reliability could be improved by increasing the number of items and creating more categories.

Limitations

The pilot version of the RMCPI contained 50 items. The large number of items could have resulted in a higher cognitive load for the participants. Though most of the items in the alpha version of the RMCPI were functioning well, six items did not have adequate difficulty and discrimination. However, important information regarding students' alternate conceptions can still be obtained from these items.

Conclusions

The purpose of this study was to develop and psychometrically assess the Reaction Mechanisms Concept Proficiency Inventory (RMCPI). The validity and reliability of the data obtained using the RMCPI meet the acceptable standards suggesting that the instrument is functioning well to determine students' alternate conceptions of concepts that are pertinent to developing proficiency in organic reaction mechanisms.

Implications for Teaching

The RMCPI could be used as a summative assessment by organic chemistry instructors to detect students' alternate conceptions on these pertinent concepts before they begin the study of organic reaction mechanisms and accordingly modify their course content to help students overcome difficulties with these concepts. Instructions for administration of the RMCPI is included in Appendix N. Alternatively, specific items from the inventory could be used by instructors for formative assessments or as clicker

questions. The information obtained using the RMCPI could also be useful to general chemistry instructors giving them information regarding the utility of general chemistry concepts in organic chemistry.

Additionally, the RMCPI could be useful for establishing the efficacy of instructional materials. Information regarding the type of textbook used for first-semester organic chemistry by the 14 different schools who administered the alpha version of the RMCPI were collected. The type of textbook used by individual schools are presented in Table 5.4 along with the average scores for each school.

Table 5.4

Type of Textbook Used by Schools in Alpha Administration

School	Type of Textbook Used	Average Scores
A	Functional Groups	48.3%
B	Functional Groups	49.7%
C	Functional Groups	46.6%
D	Functional Groups	56.8%
E	Functional Groups	53.9%
F	Reaction Mechanisms	66.8%
G	Functional Groups	51.8%
H	Functional Groups	47.9%
I	Reaction Mechanisms	73.8%
J	Reaction Mechanisms	66.8%
K	Functional Groups	60.3%
L	Functional Groups	40.8%
M	Functional Groups	57.5%
N	Reaction Mechanisms	57.8%

The overall raw average on the alpha version of the RMCPI across 14 different schools was 55.5% with the highest average being 73.8% and the lowest being 40.8%. Four out of the 14 schools (F, I, J, and N) use a textbook that is organized using a mechanistic approach. Schools F, I, and J had the three highest average scores with school I obtaining the highest average of 73.8%. An organic chemistry textbook where the content is organized by reaction mechanisms (Chaloner, 2015; Karty, 2018) is different from the traditional textbooks (Bruice, 2014; Carey, Giuliano, Allison, & Tuttle,

2020; Clayden, Greeves, & Warren, 2012; Klein, 2017; McMurry, 2018; Solomons, Fryhle, & Snyder, 2016, Wade & Simek, 2017) where the content is organized by functional groups. A number of different factors could be responsible for this difference in performance but one of the factors could be the textbook being used and this requires further investigation.

Future Work

The development of a concept inventory is an iterative process and even the alpha version of the RMCPI can be improved in the future. The Rasch analysis indicated that the inventory is marginally difficult for students and this could be addressed by modifying the items. More items for each concept could be added to increase the person separation reliability. Additionally, Differential Item Functioning (DIF) could be used to compare the performance on the RMCPI by gender, or textbook used to gain further information on the factors contributing to student understanding of pertinent concepts.

CHAPTER VI

CONCLUSIONS, IMPLICATIONS, AND FUTURE RESEARCH

The focus of this dissertation was the design, development, and psychometric assessment of the Reaction Mechanisms Concept Proficiency Inventory (RMCPI). The background of the study and the research questions guiding the study were described in Chapter I. A review of the existing literature pertaining to the difficulties students face with organic reaction mechanisms, some pertinent concept inventories developed in chemical education, and the psychometric assessment of concept inventories were presented in Chapter II. The methodology that was utilized for the various stages of this study was described in Chapter III. The results obtained during the design, development, and psychometric analysis of the inventory, were presented in Chapters IV and V. An overall summary of the dissertation study is presented in this chapter including how the research questions were addressed and what the key findings were from this study. Additionally, this chapter includes implications for teaching and practice based on these results and future research directions.

Conclusions

This study was guided by three research questions that were addressed in three different phases. The first phase of the study consisted of obtaining information from organic chemistry instructors regarding concepts that are pertinent to developing proficiency in organic reaction mechanisms to answer the following research question:

Q1 What are the chemistry concepts perceived by experts to be pertinent to developing proficiency in organic reaction mechanisms?

Open-ended interviews were conducted with organic chemistry instructors ($N=11$) from various schools in the Rocky Mountain region of the U.S. The results yielded 11 concepts that were considered to be pertinent to developing proficiency in organic reaction mechanisms.

The second phase of the study consisted of generalizing the results obtained from the first phase by conducting a national survey with organic chemistry instructors. This phase addressed the following research question:

Q2 Is there a consensus at the national level regarding the concepts perceived to be pertinent to developing proficiency in organic reaction mechanisms?

A Qualtrics survey was sent to 1500 organic chemistry instructors across the U.S. of which 183 participated giving a response rate of 12.2%. The instructors were asked to give their opinion on the importance of the concepts obtained in the first phase. The general consensus regarding the concepts was found to be very similar to the first phase. The results yielded a list of 10 concepts that are considered to be pertinent to developing proficiency in organic reaction mechanisms.

The results obtained from the first and second phases indicate a general consensus among organic chemistry instructors regarding the importance of reaction mechanisms for success in organic chemistry. Additionally, instructors are of the opinion that students seem to struggle the most with understanding what the curved-arrow means and therefore resort to rote memorization which could be attributed to a lack of understanding of fundamental general chemistry and organic chemistry concepts.

The third phase of the study was the development and psychometric analysis of the RMCPI. This phase aimed to address the following research question:

- Q3 How can one appropriately assess organic chemistry students' conceptual understanding of the concepts perceived by the experts to be pertinent to developing proficiency in organic reaction mechanisms?

This phase consisted of the assessment instrument development, test administration, and psychometric analysis. During the instrument development, open-ended questions were written addressing each of the concepts identified from the second phase and administered to first-semester undergraduate organic chemistry students to obtain their alternate conceptions as distractors. Open-ended interviews were conducted with students to identify their thought process while answering the questions. The distractors were used to develop a two-tier concept inventory with an answer tier and a response tier. A pilot version and beta version of the inventory were administered to first-semester undergraduate organic chemistry students before the 26-item alpha version of the RMCPI was finalized. The alpha version was administered to 753 first-semester organic chemistry students from 14 different universities across the U.S.A. The alpha version of the inventory consisted of items representing nine pertinent concepts listed in Table 6.1.

Table 6.1.

Final List of Concepts Utilized in the Alpha Version of the RMCPI.

Concepts Identified for Alpha Version of RMCPI
Lewis structures
Hybridization
Molecular geometry
Bonding
Electron density/polarity
Acids/bases
Electrophiles/nucleophiles
Resonance/inductive effects
Stability of intermediates

Psychometric analyses were conducted at both the item level and test level. At the item level, CTT and Rasch analysis were utilized to obtain information on item functioning. This information was utilized to modify items while developing the inventory. For the alpha version of the RMCPI, it was found that only six items were not functioning adequately but they could still be used to obtain useful information regarding students' alternate conceptions. Rasch analysis indicated that the data obtained using the RMCPI were unidimensional and measuring a single construct. The items fit well to the Rasch model and the inventory was found to be marginally difficult for the student population, but the items were being measured with good precision. These results indicate that the RMCPI is psychometrically adequate for measuring the intended construct which is students' conceptual understanding of concepts that are pertinent to developing proficiency in organic reaction mechanisms.

Psychometrics at the test level was computed based on the validity and reliability of the data obtained using the instrument. Face validity was established by obtaining feedback on the items from undergraduate students who took part in open-ended interviews and from chemistry graduate students. Content validity was established by obtaining feedback from organic chemistry instructors regarding the clarity and content of the items. Both the face validity and content validity were utilized to modify or omit items during the development of the inventory. The item analysis results for the RMCPI items were compared to the item analysis results for similar items on the ACS standardized exams, and the results indicated that most of these items function similarly. The concepts were also compared to the ACS Exams Institute anchoring concepts content map for undergraduate organic chemistry (Raker et al., 2013), and it was found that all

the concepts are present in the anchoring concepts content map which suggests adequate content coverage in the RMCPI.

The reliability estimated using the Cronbach's alpha value for the data obtained using the alpha version of the RMCPI was found to be 0.712 suggesting that the items are strongly correlated. The item separation reliability was found to be adequate. However, the person separation reliability was found to be 0.60 which is lower than the accepted value of 0.80 (Bond & Fox, 2015) and could be due to the number of items. These results indicate that the validity and reliability of the data obtained using the RMCPI meet the acceptable standards for concept inventories.

Implications for Teaching

The list of concepts obtained from the first two phases of the study are concepts that are considered pertinent to developing proficiency in organic reaction mechanisms. Organic chemistry instructors can use this information to modify their course content or spend more time reviewing pertinent concepts. This information can help general chemistry instructors identify key concepts that students will need in organic chemistry.

The RMCPI could be used by organic chemistry instructors as a summative assessment to identify alternate conceptions their students have developed. Alternatively, instructors could select items from the RMCPI to use on formative assessments. The instrument could also be used to detect students' learning gains by administering it as a pre-test and a post-test.

Future Research

The development of a concept inventory is an iterative process. Items are developed, tested, and modified before repeating the process. The alpha version of the RMCPI, even though it was the final version used, can still be modified.

The RMCPI was found to be marginally difficult for the student population and modifying the items could help overcome this. More items could be added under each of the concepts to increase the person separation reliability.

Differential Item Functioning (DIF) could be used to compare the performance of students on the RMCPI based on gender or school type. DIF is a statistical characteristic that shows the extent to which an item might be measuring different abilities for members of separate subgroups (Bond & Fox, 2015). This could give useful information regarding the role of gender in performance. This information could also identify the effect of different learning environments on student performance.

Additionally, single topic concept inventories based on the concepts of electron density and polarity, electrophiles and nucleophiles, and stability of intermediates, which are especially challenging to students could be developed. It would be useful to gain further insight into students' difficulties with these concepts by developing such topic-specific concept inventories.

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APPENDIX A

**INSTITUTIONAL REVIEW BOARD
APPROVALS AND INFORMED
CONSENT FORMS**



Institutional Review Board

DATE: February 7, 2018

TO: Sachin Nedungadi
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [1185245-1] Organic Reaction Mechanism Concept Inventory (Open-Ended Interviews of Organic Chemistry Instructors)

SUBMISSION TYPE: New Project

ACTION: APPROVAL/VERIFICATION OF EXEMPT STATUS
DECISION DATE: February 7, 2018
EXPIRATION DATE: February 7, 2022

Thank you for your submission of New Project materials for this project. The University of Northern Colorado (UNCO) IRB approves this project and verifies its status as EXEMPT according to federal IRB regulations.

Sachin -

Thank you for your patience with the UNC IRB process. Your protocols and overall application for this study are clear. Please make the following amendments to your consent form before use in your participant recruitment and data collection:

- 1) **add UNC letterhead; and**
- 2) **update the contact information in the last paragraph as follows, 'If you have any concerns about your selection or treatment as a research participant, please contact Sherry May, IRB Administrator, in the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910.'**

Best wishes with your study.

Sincerely,

Dr. Megan Stellino, UNC IRB Co-Chair

We will retain a copy of this correspondence within our records for a duration of 4 years.

If you have any questions, please contact Sherry May at 970-351-1910 or Sherry.May@unco.edu. Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.



CONSENT FORM FOR HUMAN PARTICIPANTS IN RESEARCH
UNIVERSITY OF NORTHERN COLORADO

Project Title: Organic Reaction Mechanism Concept Inventory (Open-Ended Interviews of Organic Chemistry Instructors)

Researcher: Sachin Nedungadi, M.S. Phone: (650) 201-9909 Email: sachin.nedungadi@unco.edu

Researcher: Michael D. Mosher, Ph.D. Phone: (970) 351-3257

Email: michael.mosher@unco.edu

Researcher: Corina E. Brown, Ph.D. Phone: (970) 351-1285 Email: corina.brown@unco.edu

This research project is aimed at developing an organic reaction mechanism concept inventory to help teachers determine whether students have a good working knowledge of reaction mechanisms and to help identify problem areas in their understanding. The first phase of this process consists of open-ended interviews of organic chemistry professors to discuss their views on the importance of reaction mechanisms in organic chemistry and students' difficulties in this area.

Participants will be asked to complete an interview in person in which they will be asked a series of open-ended questions. The identity of the participants will remain confidential with the use of codes for each participant. Digital audio recordings will be kept locked in my personal office and these will be used to help develop a national survey.

We do not expect you to encounter any risks other than what occurs in a normal day. It will take approximately 45 minutes of your time to interview with me.

Participation is voluntary. You may decide not to participate in this study and if you begin participation, you may still decide to stop and withdraw at any time. Your decision will be respected and will not result in loss of benefits to which you are otherwise entitled. Having read the above and having had an opportunity to ask any questions, please sign below if you would like to participate in this research. A copy of this form will be given to you to retain for future reference. If you have any concerns about your selection or treatment as a research participant, please contact Sherry May, IRB Administrator, in the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910.

Subject's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:



Institutional Review Board

DATE: May 23, 2018

TO: Sachin Nedungadi
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [1245324-1] Organic Reaction Mechanism Concept
Inventory (National Survey for Organic Chemistry
Instructors)

SUBMISSION TYPE: New Project

ACTION: APPROVAL/VERIFICATION OF EXEMPT STATUS

DECISION DATE: May 23, 2018

EXPIRATION DATE: May 23, 2022

Thank you for your submission of New Project materials for this project. The University of Northern Colorado (UNCO) IRB approves this project and verifies its status as EXEMPT according to federal IRB regulations.

Sachin -

Thank you for a clear and thorough IRB application. Your materials and protocols are verified/ approved exempt.

Best wishes with your research.

Sincerely,

Dr. Megan Stellino, UNC IRB Co-Chair

We will retain a copy of this correspondence within our records for a duration of 4 years.

If you have any questions, please contact Sherry May at 970-351-1910 or Sherry.May@unco.edu. Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.



CONSENT FORM FOR HUMAN PARTICIPANTS IN RESEARCH
UNIVERSITY OF NORTHERN COLORADO

Project Title: Organic Reaction Mechanism Concept Inventory (National Survey for Organic Chemistry Instructors)

Researcher: Sachin Nedungadi, M.S. Phone: (650) 201-9909 Email: sachin.nedungadi@unco.edu

Researcher: Michael D. Mosher, Ph.D. Phone: (970) 351-3257
Email: michael.mosher@unco.edu

Researcher: Corina E. Brown, Ph.D. Phone: (970) 351-1285 Email: corina.brown@unco.edu

This research project is aimed at developing an organic reaction mechanism concept inventory to help teachers determine whether students have a good working knowledge of reaction mechanisms and to help identify problem areas in their understanding. This phase of this process consists of a national survey to be completed by organic chemistry instructors to give their opinions on the importance of reaction mechanisms in organic chemistry, concepts that are important for developing proficiency in organic reaction mechanisms and students' difficulties in this area.

Participants will be asked to complete an online survey which should take approximately 10-15 minutes. Although your email addresses are known by the primary researcher, your identity cannot be linked to your survey responses. There are no foreseen potential risks in the study. In no way will your employment be affected by your participation in this study.

Participation is voluntary. You may decide not to participate in this study and if you begin participation, you may still decide to stop and withdraw at any time. Your decision will be respected and will not result in loss of benefits to which you are otherwise entitled. Having read the above and having had an opportunity to ask any questions, please sign below if you would like to participate in this research. A copy of this form will be given to you to retain for future reference. If you have any concerns about your selection or treatment as a research participant, please contact the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910.



Institutional Review Board

DATE: April 19, 2018

TO: Sachin Nedungadi
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [1227347-1] Organic Reaction Mechanism Concept Inventory (Survey and Interviews with Organic Chemistry Students)

SUBMISSION TYPE: New Project

ACTION: MODIFICATIONS REQUIRED
DECISION DATE: April 19, 2018
EXPIRATION DATE:
REVIEW TYPE: Exempt Review

Thank you for your submission of New Project materials for this project. University of Northern Colorado (UNCO) IRB has determined that the following MODIFICATIONS are REQUIRED in order to secure approval:

Thank you for a succinct and clear IRB application. There are a few items that need to be addressed and submitted for further review. Please highlight these changes/amendments and additions to your materials and protocols and submit according to the instructions provided:

1) the protocol for where, when, how the follow-up interviews will occur is not described. Please provide a step-by-step description and include all materials (additional documents, descriptions, recruitment scripts, etc.) to make it clear how participants will complete the survey and then be recruited and complete the follow-up interview. How will participants indicate they are interested in the follow-up interview? Will this take place immediately after the survey? Will an identifier be used to link the survey and the interview data, how long will the interview take, where will it take place, etc.

Be sure and include any additional relevant information about the interview in the consent form too.

2) The consent form need to include UNCO letter head; and

3) and the information in the last sentence of the last paragraph needs to be updated as follows, "If you have any concerns about your selection or treatment as a research participant, please contact the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910."

I look forward to subsequent review of your amended and additional materials.

Sincerely,

Dr. Megan Stellino, UNC IRB Co-Chair

Research activities in accordance with this submission may not begin until this committee has received a response to these conditions and issued final approval.

This submission has received Exempt Review based on the applicable federal regulations.

If you have any questions, please contact Sherry May at 970-351-1910 or Sherry.May@unco.edu. Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.



Institutional Review Board

DATE: April 27, 2018

TO: Sachin Nedungadi
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [1227347-2] Organic Reaction Mechanism Concept Inventory (Survey and Interviews with Organic Chemistry Students)

SUBMISSION TYPE: Amendment/Modification

ACTION: APPROVAL/VERIFICATION OF EXEMPT STATUS

DECISION DATE: April 26, 2018

EXPIRATION DATE: April 26, 2022

Thank you for your submission of Amendment/Modification materials for this project. The University of Northern Colorado (UNCO) IRB approves this project and verifies its status as EXEMPT according to federal IRB regulations.

Thank you for the thorough amendments to your IRB application. Materials and protocols with the addition of the interviews are verified/approved exempt.

Best wishes with your research.

Sincerely,

Dr. Mgan Stellino, UNC IRB Co-Chair

We will retain a copy of this correspondence within our records for a duration of 4 years.

If you have any questions, please contact Sherry May at 970-351-1910 or Sherry.May@unco.edu. Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.



Institutional Review Board

DATE: September 18, 2019

TO: Sachin Nedungadi
FROM: University of Northern Colorado (UNCO) IRB

PROJECT TITLE: [1227347-3] Organic Reaction Mechanism Concept
Inventory (Survey and Interviews with Organic Chemistry
Students)

SUBMISSION TYPE: Revision

ACTION: MODIFICATION APPROVED/VERIFICATION OF
EXEMPT STATUS

DECISION DATE: September 18, 2019
EXPIRATION DATE: April 26, 2022

Thank you for your submission of Amendment/Modification materials for this project. The University of Northern Colorado (UNCO) IRB approves this project modification and verifies its continued status as EXEMPT according to federal IRB regulations.

Your modification request to add additional data collection sites is approved.

We will retain a copy of this correspondence within our records for a duration of 4 years.

If you have any questions, please contact Nicole Morse at 970-351-1910 or nicole.morse@unco.edu.

Please include your project title and reference number in all correspondence with this committee.

This letter has been electronically signed in accordance with all applicable regulations, and a copy is retained within University of Northern Colorado (UNCO) IRB's records.



CONSENT FORM FOR HUMAN PARTICIPANTS IN RESEARCH
UNIVERSITY OF NORTHERN COLORADO

Project Title: Organic Reaction Mechanism Concept Inventory (Survey and Interviews with Organic Chemistry Students)

Researcher: Sachin Nedungadi, M.S. Phone: (650) 201-9909 Email: sachin.nedungadi@unco.edu

Researcher: Michael D. Mosher, Ph.D. Phone: (970) 351-3257
Email: michael.mosher@unco.edu

Researcher: Corina E. Brown, Ph.D. Phone: (970) 351-1285 Email: corina.brown@unco.edu

This research project is aimed at developing an organic reaction mechanism concept inventory to help teachers determine whether students have a good working knowledge of reaction mechanisms and to help identify problem areas in their understanding. These surveys and interviews will help determine some of the difficulties students face in the area of organic reaction mechanisms and their opinions about these difficulties.

Participants will be asked to complete a survey with 20 short, free-response organic reaction mechanism problems. This should take approximately 30 minutes. At the end of the survey participants will be asked to indicate if they want to take part in a follow up interview which will be conducted in ROSS 3620 at a time convenient to the participant and will last approximately 30 minutes. The identity of the participants will remain confidential with the use of codes for each participant. Digital audio recordings will be kept locked in my personal office and this data will be used to design and develop a concept inventory.

We do not expect you to encounter any risks other than what occurs in a normal day. Your participation in this study will have no bearing on the grade you receive in this course as your instructor will have no knowledge of who did or did not participate in the study.

Participation is voluntary. You may decide not to participate in this study and if you begin participation, you may still decide to stop and withdraw at any time. Your decision will be respected and will not result in loss of benefits to which you are otherwise entitled. Having read the above and having had an opportunity to ask any questions, please sign below if you would like to participate in this research. A copy of this form will be given to you to retain for future reference. If you have any concerns about your selection or treatment as a research participant, please contact the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910.

Subject's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:



CONSENT FORM FOR HUMAN PARTICIPANTS IN RESEARCH
UNIVERSITY OF NORTHERN COLORADO

Project Title: Organic Reaction Mechanism Concept Inventory (Survey and Interviews with Organic Chemistry Students)

Researcher: Sachin Nedungadi, M.S. Phone: (650) 201-9909 Email: sachin.nedungadi@unco.edu

Researcher: Michael D. Mosher, Ph.D. Phone: (970) 351-3257
Email: michael.mosher@unco.edu

Researcher: Corina E. Brown, Ph.D. Phone: (970) 351-1285 Email: corina.brown@unco.edu

This research project is aimed at developing an organic reaction mechanism concept inventory to help teachers determine whether students have a good working knowledge of reaction mechanisms and to help identify problem areas in their understanding. These surveys and interviews will help determine some of the difficulties students face in the area of organic reaction mechanisms and their opinions about these difficulties.

Participants will be asked to complete a survey with 26 free response and multiple-choice conceptual questions regarding organic reaction mechanisms and 5 demographic questions. This should take approximately 15 minutes. At the end of the survey participants may be asked to indicate if they want to take part in a follow up interview which will be conducted in ROSS 3620 at a time convenient to the participant and will last approximately 30 minutes. The identity of the participants will remain confidential with the use of codes for each participant. Digital audio recordings will be kept locked in my personal office and this data will be used to design and develop a concept inventory.

We do not expect you to encounter any risks other than what occurs in a normal day. Your participation in this study will have no bearing on the grade you receive in this course as your instructor will have no knowledge of who did or did not participate in the study.

Participation is voluntary. You may decide not to participate in this study and if you begin participation, you may still decide to stop and withdraw at any time. Your decision will be respected and will not result in loss of benefits to which you are otherwise entitled. Having read the above and having had an opportunity to ask any questions, please sign below if you would like to participate in this research. A copy of this form will be given to you to retain for future reference. If you have any concerns about your selection or treatment as a research participant, please contact the Office of Research, 25 Kepner Hall, University of Northern Colorado Greeley, CO 80639; 970-351-1910.

Subject's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:

Researcher's Signature:

Date:

APPENDIX B**QUESTIONS FOR INTERVIEWS WITH ORGANIC
CHEMISTRY INSTRUCTORS**

Open-Ended Interviews Experts – Questions

1. How would you define a mechanism of a reaction?
2. Describe what one means by the arrow (electron)-pushing formalism in organic reaction mechanisms?
3. What types of problems in organic chemistry can be solved using this arrow (electron) pushing formalism?
4. What is your approach to teaching the course? Is it based on functional groups or mechanisms of reactions?
5. How do you introduce the topic of organic reaction mechanisms to your students?
6. How are organic reaction mechanisms important to the success of students in your organic chemistry courses?
7. What are the main chemistry concepts necessary to understand and apply for a student to be proficient in presenting a reaction mechanism? Can you please provide an example for each concept you identified.
8. What are some of the barriers to understanding reaction mechanisms that your students face? Please provide written examples.
9. What are some of the areas that students do not have difficulties with in organic reaction mechanisms?
10. Anything else that you may like to add?

Demographic Questions

1. At what institution are you a faculty member?
2. What is the highest degree or level of school you have completed?
 - Bachelor's degree
 - Master's degree
 - Professional degree
 - Doctorate degree
3. How many years of teaching experience do you have?
4. Is the organic class you teach one- or two- semester course?

5. What classes have you taught?

6. What classes do you currently teach?

7. Do you use the ACS standardized exam for your classes?

8. Ethnicity origin (or Race): Please specify your ethnicity.
 - White
 - Hispanic or Latino
 - Black or African American
 - Native American or American Indian
 - Asian/Pacific Islander
 - Other

9. What is your gender? _____

APPENDIX C

SAMPLE OF NATIONAL SURVEY FORMAT

Below you are presented with a set of concepts and example questions for each concept. Please classify the concepts in terms of their relevance to developing proficiency in organic reaction mechanisms using the following scale:

Important - concepts that are *critical* for proficiency in organic reaction mechanisms

Foundational - concepts that facilitate the understanding of the important concepts, so in that respect they are *moderately critical*

Not important - concepts that do not have a direct application to the understanding of reaction mechanisms, *not critical*

Are the questions relevant to assess the specific concept?

Please make comments or add additional concepts if you wish.

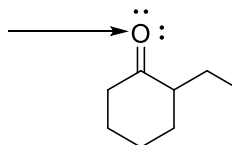
Q50 Hybridization

- Important
- Foundational
- Not important

Q51 Please provide any other comments/suggestions on the above concept.

Q52 Is this a relevant question to assess the concept of hybridization?

What is the hybridization of the indicated atom in the following molecule? Why?



- Yes
- No

Q53 Please provide any other comments/suggestions on the above question.

Q 75 What is your approach to teaching the organic chemistry course? Is it based on functional groups or mechanisms of reactions?

- Functional groups
- Mechanisms of reactions
- Both

Q76 Please provide any other comments on the above question.

Q77 How do you introduce the topic of reaction mechanisms to your students?

- Acid-base chemistry
- Alkene reactions
- Electronic configuration, line drawings, and fundamental general chemistry concepts

Q78 Please provide any other comments/suggestions on the above question.

Q79 How are organic reaction mechanisms important to the success of students in your organic chemistry course?

- Critical
- Moderately critical
- Not important

Q80 Please provide any other comments/suggestions on the above question.

Q81 What are some of the barriers/difficulties to understanding reaction mechanisms that your students face?

Q82 What is the highest chemistry degree you have earned?

- Bachelor's degree
- Master's degree
- Professional degree
- Doctorate degree

Q83 What area of chemistry/organic chemistry would you say is your speciality?

Q84 For how many years have you taught the organic chemistry course?

- 0-2 years
- 2-5 years

>5 years

Q85 Which best describes your university?

Doctoral University: Highest Research Activity (R1)

Doctoral University: Higher Research Activity (R2)

Master's College or University: Larger Programs (M1)

Master's College or University: Medium Programs (M2)

Primarily Undergraduate Institution

Community College

Other (please specify)

Q86 How many semesters is the organic chemistry course you teach or have taught?

One semester

Two semester

Q87 Do you use the ACS standardized exam for your organic chemistry course?

Yes

No

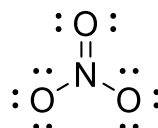
Q88 What is your gender?

APPENDIX D**OPEN-ENDED QUESTIONS FOR
INSTRUMENT DEVELOPMENT**

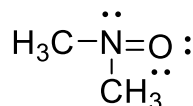
- How many electrons are in $^{14}_7\text{N}^{-3}$? Explain your answer.
- Fill in the orbitals with electrons to give the ground state configuration of $^{13}_6\text{C}$. Explain your reasoning.



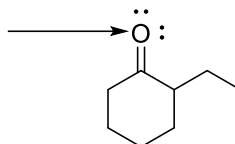
- How many valence electrons does $^{16}_8\text{O}$ have? Why?
- Complete the following Lewis structure by assigning the correct formal charges. Explain your reasoning.



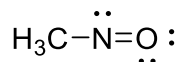
- Are there any mistakes in the following Lewis structure? If yes, then identify them and explain.



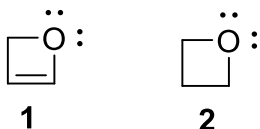
- What is the hybridization of the indicated atom in the following molecule? Why?



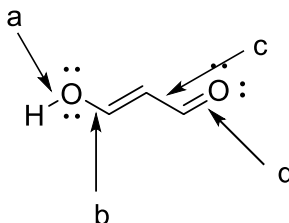
- Describe the orbital overlap between N and O in the following molecule's π bond.



- Which is more stable? Why?

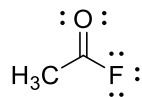


- Which is the shortest bond in the following molecule? Why?



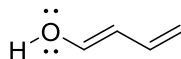
- How many σ and π bonds does the above molecule have?

11. Which atom in the following molecule is most electrophilic and why?

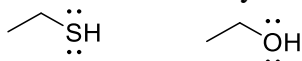


12. Is BCl_3 a polar or non-polar molecule? Explain.

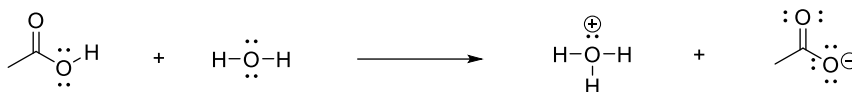
13. Pick the area of most and least electron density in the following molecule. Explain your choice.



14. Which is more acidic and why?

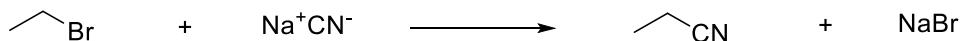


15. Choose the Lewis base in the following reaction. Explain your choice.

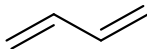


16. Draw curved arrows to show the formation of the products in the above reaction. Explain your answer.

17. Which is the electrophile and the nucleophile in the following reaction? Explain your choice.



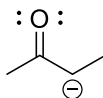
18. Draw one valid resonance structure for the following molecule and explain why your drawing represents a valid resonance structure.



19. Trifluoroacetic acid is more acidic than acetic acid. Why?



20. Why is the following ion stable? Explain.



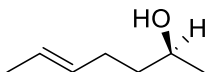
21. Which is more stable and why?



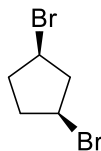
22. Which is a better resonance structure? Why?



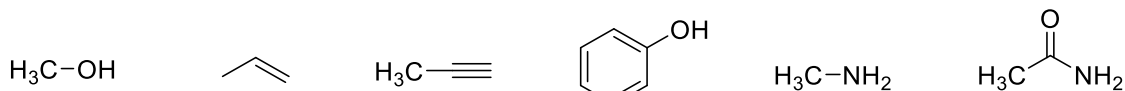
23. Identify the stereocenters in the following molecule. Explain your choice.



24. The following molecule is achiral. Explain why the molecule is achiral.



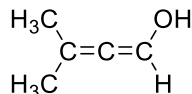
25. Which is the most basic? Explain why you selected the molecule you did.



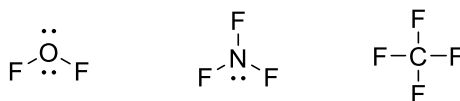
26. Which orbital do the highest energy electrons in a ground state sulfur atom occupy? Explain.

27. Give an acceptable Lewis structure for methyl azide (CH_3N_3). Explain.

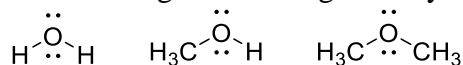
28. How many sp hybridized atoms are in the following structure? Explain.



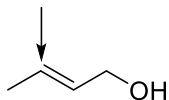
29. Which has the smallest bond angle? Why?



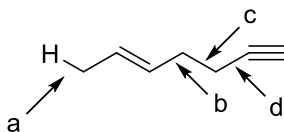
30. Which has the largest bond angle? Why?



31. What is the geometry around the indicated atom? Explain.



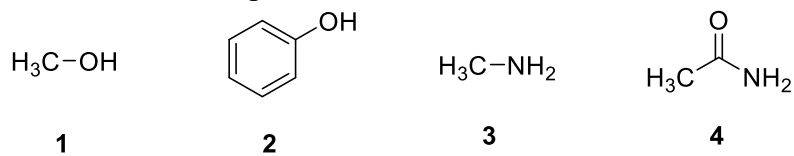
32. Which is the longest bond in the following molecule? Explain.



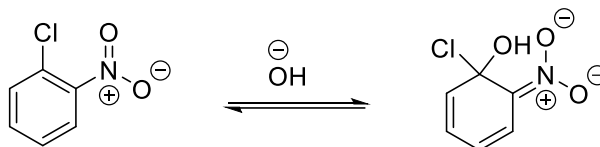
33. How many sigma bonds does the above molecule possess?

34. How many pi bonds does the above molecule possess?

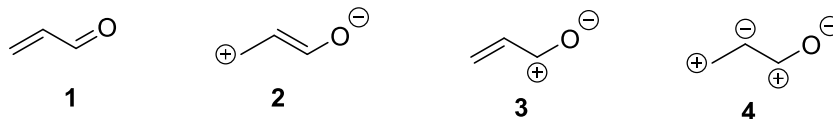
35. Which is the most acidic? Explain.



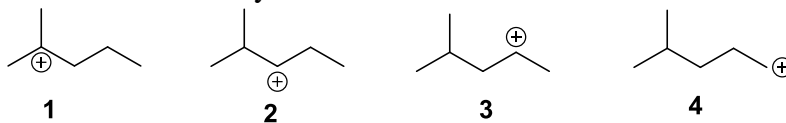
36. Identify the electrophile and nucleophile in the following reaction and give a suitable curved arrow mechanism to show the formation of the product.



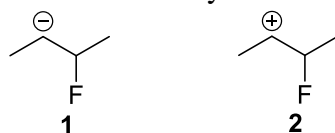
37. Which of the following is the major contributor to the overall resonance hybrid? Explain.



38. Which is more stable and why?



39. Which is more stable? Why?



Demographic Questions

Gender:

Major: Chemistry major

Chemistry non-major

Year of study: Freshman

Sophomore Junior

Senior

APPENDIX E**QUESTIONS FOR INTERVIEWS WITH ORGANIC
CHEMISTRY STUDENTS**

Open-Ended Interviews Students – Questions

1. How would you assess your understanding of the material in the course?
2. Are the terms of the question familiar? Is the question clear? How can it be made clearer?
3. What is your answer to the question? (write down)
4. Please would you explain your thought process?

APPENDIX F

PILOT VERSION OF THE INVENTORY

Pilot Version
50 Items

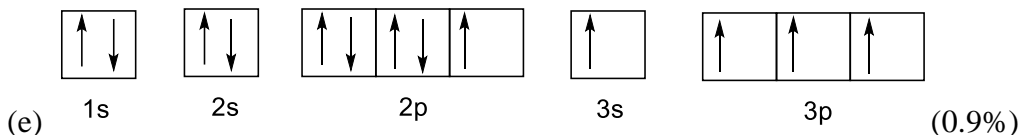
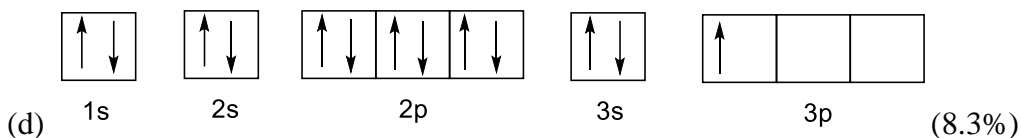
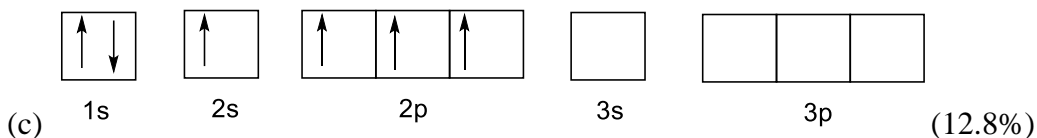
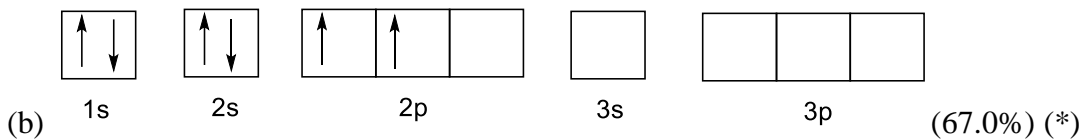
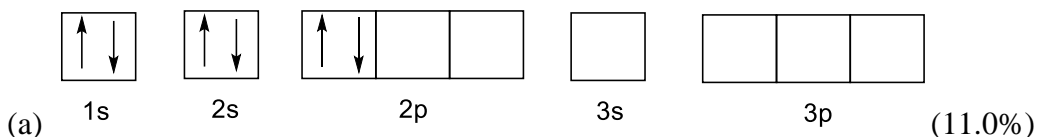
(*) indicates the correct answer

Please answer the following multiple-choice and demographic questions on the scantron.

1. Which orbital do the highest energy electrons in a ground state sulfur atom occupy?

- (a) 2p (15.6%)
(b) 3s (2.8%)
(c) 3p (76.1%) (*)
(d) 4p (5.5%)

2. Which is the correct representation for the ground state configuration of ^{13}C ?



3. What is the reason for your answer to question 2?

- (a) Lower energy orbitals are filled first with one electron before pairing (90.8%) (*)
(b) All the empty orbitals have to be filled with electrons (3.7%)
(c) The mass number gives the total number of electrons present (4.6%)
(d) The electrons in the orbitals have to always be paired (0.9%)

4. How many valence electrons does ^{18}O have?

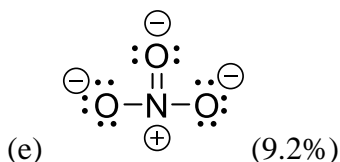
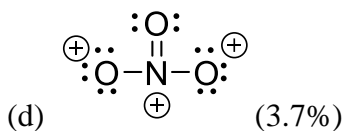
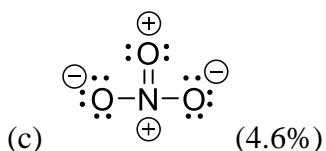
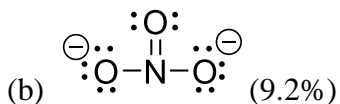
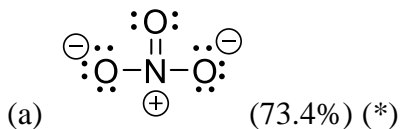
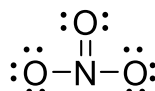
- (a) 10 valence electrons (9.2%)

- (b) 8 valence electrons (12.8%)
- (c) 6 valence electrons (67.9%) (*)
- (d) 4 valence electrons (4.6%)
- (e) 2 valence electrons (5.5%)

5. What is the reason for your answer to question 4?

- (a) The mass number minus the atomic number is the number of valence electrons (9.2%)
- (b) The valence electrons are the number of electrons in the outermost shell (46.8%) (*)
- (c) Oxygen is in the 6th row of the Periodic Table (38.5%)
- (d) There are two unpaired electrons in the outermost shell (6.4%)

6. Which of the following is the correct representation of formal charges for the following Lewis structure?

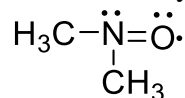


7. What is the reason for your answer to question 6?

- (a) Oxygen atoms without a double bond have negative charge (20.2%)
- (b) Oxygen atoms have an extra electron pair and nitrogen atom does not have an electron pair (62.4%) (*)

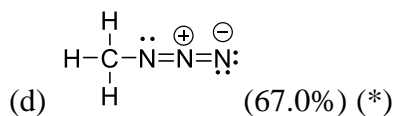
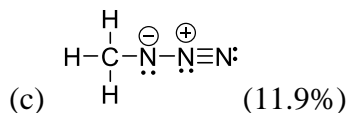
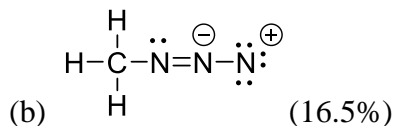
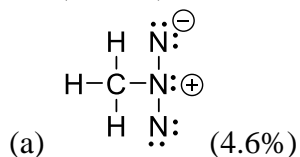
- (c) Oxygen atoms need a charge to eliminate strain (3.7%)
 (d) Oxygen and nitrogen atoms need charges to increase the stability (14.7%)

8. Which of the following best describes what is wrong with the given Lewis structure for a compound with the molecular formula C_2H_6NO ? (All formal charges have been omitted for clarity)



- (a) Oxygen atoms should not have an unpaired electron (38.5%)
 (b) Oxygen atoms should not have any lone pairs (6.4%)
 (c) There are too many electrons around oxygen atom (1.8%)
 (d) There are too many electrons around nitrogen atom (53.2%) (*)

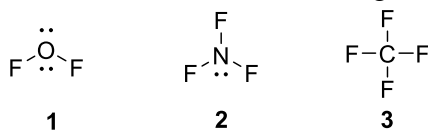
9. Which one of the following is an acceptable Lewis structure for methyl azide (CH_3N_3).



10. What is the reason for your answer to question 9?
- (a) Methyl group is connected to a single nitrogen atom and forms a chain (3.7%)
 (b) Each atom in the structure fully satisfies the octet rule (24.8%)
 (c) Each atom has a complete octet and formal charges are assigned correctly (64.2%) (*)
 (d) Nitrogen atoms always form three bonds and carbon atoms form four bonds (8.3%)

11. What is the hybridization of the labelled atom in the following molecule?

17. Which molecule has the smallest bond angle?

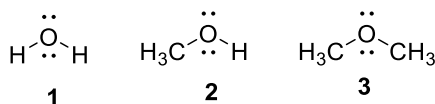


- (a) 1 (19.3%) (*)
 (b) 2 (12.8%)
 (c) 3 (67.9%)

18. What is the reason for your answer to question 17?

- (a) The lone pairs repel each other (35.8%) (*)
 (b) The lone pairs pull the fluorine atoms away (14.7%)
 (c) There are no lone pairs present (50.5%)

19. Which molecule has the largest bond angle?

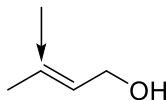


- (a) 1 (54.1%)
 (b) 2 (7.3%)
 (c) 3 (39.4%) (*)

20. What is the reason for your answer to question 19?

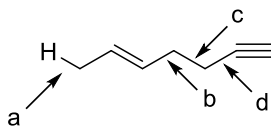
- (a) It has the least number of atoms (16.5%)
 (b) The hydrogen atom occupies less space (35.8%)
 (c) The methyl groups are bulky (47.7%) (*)

21. Which statement best describes the geometry of the indicated atom?



- (a) Trigonal planar (52.3%) (*)
 (b) Trigonal pyramidal (18.3%)
 (c) Bent (12.8%)
 (d) Linear (2.8%)
 (e) Tetrahedral (13.8%)

22. Which is the longest bond in the following molecule?



- (a) a (34.0%)
 (b) b (6.4%)
 (c) c (33.0%) (*)

(d) d (27.5%)

23. What is the reason for your answer to question 22?

- (a) Presence of the triple bond (31.2%)
- (b) Greatest amount of s character (30.3%)
- (c) The rest are carbon atoms (14.7%)
- (d) Least amount of s character (24.8%) (*)

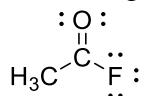
24. How many sigma bonds does the molecule in question 22 possess?

- (a) 6 (6.4%)
- (b) 7 (59.6%)
- (c) 10 (17.4%)
- (d) 15 (9.2%)
- (e) 16 (8.3%) (*)

25. How many pi bonds does the molecule in question 22 possess?

- (a) 1 (4.6%)
- (b) 2 (27.5%)
- (c) 3 (67.9%) (*)
- (d) 4 (0.9%)

26. Which atom in the following molecule is most electrophilic?



- (a) Oxygen atom (11.0%)
- (b) Fluorine atom (67.9%)
- (c) Hydrogen atom (4.6%)
- (d) Carbon atom that is part of the C=O group (6.4%) (*)
- (e) Carbon atom that is part of the CH₃ group (10.1%)

27. What is the reason for your answer to question 26?

- (a) Attached to two electron withdrawing groups (13.8%) (*)
- (b) Has lone pair of electrons to donate (24.8%)
- (c) It has less electronegativity (19.3%)
- (d) It is to the right in the Periodic Table (43.1%)

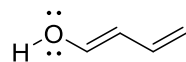
28. Which of the following best describes the BCl₃ molecule?

- (a) Polar (38.5%)
- (b) Non-polar (58.7%) (*)
- (c) Apolar (2.8%)

29. What is the reason for your answer to question 28?

- (a) All atoms have equal formal charge (12.8%)
- (b) Chlorine atoms pull electrons towards themselves (45.0%)
- (c) Electronegativity difference is too small (10.1%)
- (d) The molecule is symmetrical (32.1%) (*)

30. Which are the areas of greatest and least electron density in the following molecule?

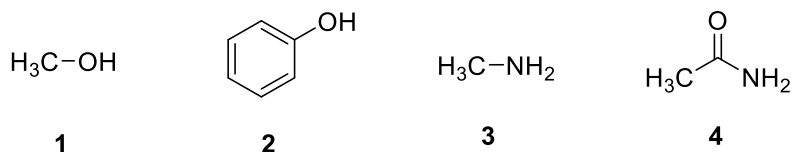


- (a) Greatest electron density is centered on the oxygen atom and the least is centered on the hydrogen atom attached to the oxygen atom (50.5%) (*)
- (b) Greatest electron density is centered on the oxygen atom and the least is centered on the internal double bond (15.6%)
- (c) Greatest electron density is centered on the internal double bond and the least is centered on the terminal double bond (14.7%)
- (d) Greatest electron density is centered on the oxygen atom and least is centered on the terminal double bond (19.3%)

31. What is the reason for your answer to question 30?

- (a) No lone pairs are present (11.9%)
- (b) Double bonds are harder to break (30.3%)
- (c) The least electronegative atom has the least electron density (52.3%) (*)
- (d) Too many bonds present (5.5%)

32. Which is the most acidic?



- (a) 1 (11.9%)
- (b) 2 (46.8%) (*)
- (c) 3 (17.4%)
- (d) 4 (23.9%)

33. What is the reason for your answer to question 32?

- (a) Possibility for hydrogen bonding (28.4%)
- (b) Most number of protons available to donate (16.5%)
- (c) Conjugate base stabilized by resonance (40.4%) (*)
- (d) Most electronegative atoms present (14.8%)

34. Which is more acidic?

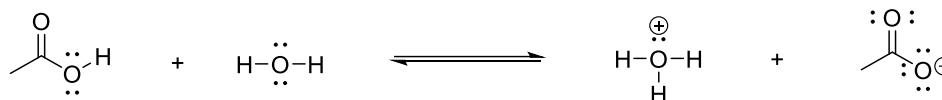


- (a) 1 (40.4%) (*)
- (b) 2 (59.6%)

35. What is the reason for your answer to question 34?

- (a) Sulfur is more polarizable (24.8%) (*)
- (b) The O-H bond is stronger than the S-H bond (26.6%)
- (c) The product is more stable with a positive charge (9.2%)
- (d) Oxygen atoms are more electronegative (32.1%)
- (e) It is able to hold the charge better (7.3%)

36. Which molecule is the Lewis base for the forward reaction?

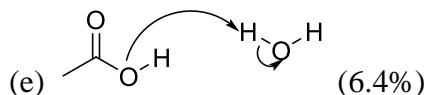
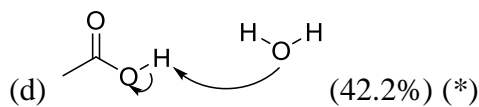
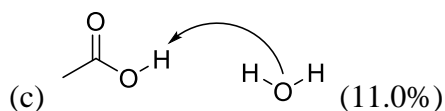
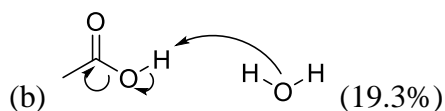
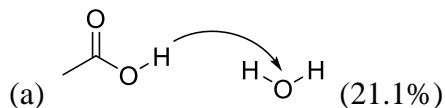


- (a) Acetic acid (17.4%)
- (b) Water (69.7%) (*)
- (c) Hydronium ion (5.5%)
- (d) Acetate ion (7.3%)

37. What is the reason for your answer to question 36?

- (a) It donates the hydrogen atom (2.3%)
- (b) It is a proton acceptor (52.3%) (*)
- (c) It is an electron-pair donor (14.7%)
- (d) It becomes a conjugate acid (10.1%)

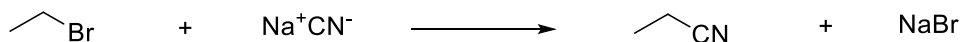
38. Which of the following best depicts the curved arrows to show the formation of the products in the above reaction? (All lone pairs have been omitted for clarity)



39. What is the reason for your answer to question 38?

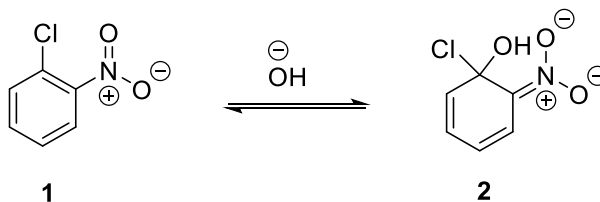
- (a) Lone pair on water forms a bond to a proton and the electrons go to the oxygen atom (38.5%) (*)
- (b) The water molecule pulls the proton off of the acetic acid molecule (33.0%)
- (c) Electrons flow from the hydrogen atom to make the bond (22.0%)
- (d) Oxygen atom of acetic acid is most susceptible to protonation from a water molecule (6.4%)

40. Which is the electrophile and which is the nucleophile in the following reaction?



- (a) Electrophile-ethyl bromide, Nucleophile-sodium cyanide (38.5%) (*)
- (b) Electrophile-sodium cyanide, Nucleophile-ethyl bromide (31.2%)
- (c) Electrophile-ethyl bromide, Nucleophile-sodium bromide (18.3%)
- (d) Electrophile-sodium cyanide, Nucleophile-ethyl cyanide (11.9%)

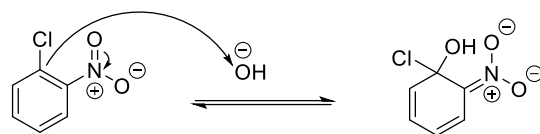
41. Which one of the following gives the correct curved arrow notation for the formation of the product and correctly identifies the electrophile and the nucleophile?



- (a) Nucelophile-1, Electrophile-2 (20.2%)

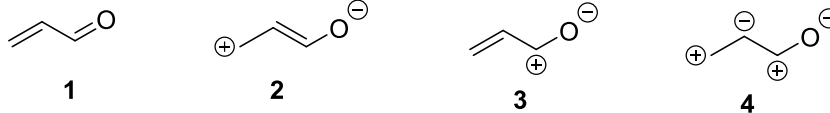
- (b) Nucleophile-OH⁻, Electrophile-1 (43.1%)

- (c) Nucleophile-OH⁻, Electrophile-1 (32.1%) (*)



(d) 1 2 Nucleophile-1, Electrophile-OH⁻ (4.6%)

42. Which of the following is the major contributor to the overall resonance hybrid?



- (a) 1 (23.9%) (*)
 (b) 2 (36.7%)
 (c) 3 (24.8%)
 (d) 4 (14.7%)

43. What is the reason for your answer to question 42?

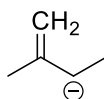
- (a) It has the most number of bonds (22.9%) (*)
 (b) It shows the movement of electrons (34.9%)
 (c) The charges are next to each other (18.3%)
 (d) The charges are alternating (23.9%)

44. Trifluoroacetic acid is more acidic than acetic acid. Why?



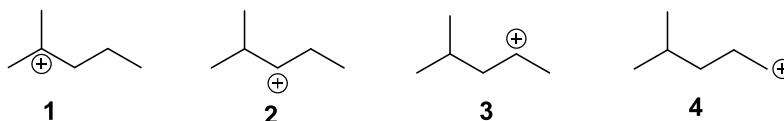
- (a) Because trifluoroacetic acid is tertiary (6.4%)
 (b) Because fluorine is more acidic than OH (24.8%)
 (c) It has more hydrogen bonding capability (9.2%)
 (d) Additional resonance from the three fluorine atoms (18.3%)
 (e) The inductive effect of the fluorine atoms stabilizes the anion (41.3%) (*)

45. Why is the following ion stable?



- (a) Resonance (61.5%) (*)
 (b) Induction (24.8%)
 (c) Position of the electrons (6.4%)
 (d) Hydride shift (1.8%)
 (e) Stable electron density (5.5%)

46. Which is most stable?

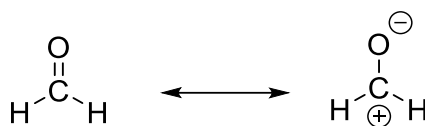


- (a) 1 (50.5%) (*)
- (b) 2 (27.5%)
- (c) 3 (7.3%)
- (d) 4 (14.7%)

47. What is the reason for your answer to question 46?

- (a) Induction (45.0%) (*)
- (b) Charge is centralized (30.3%)
- (c) It is the most symmetrical (10.1%)
- (d) Positive charge is at the end (14.7%)

48. Why is the following molecule an acceptable resonance structure of formaldehyde?



- (a) Electrons can go to the carbon atom (19.3%)
- (b) The oxygen atom wants to donate electrons (17.4%)
- (c) The oxygen atom can leave easier as a leaving group (11.9%)
- (d) The oxygen atom is more electronegative than carbon atoms (51.4%) (*)

49. Which is more stable?



- (a) 1 (56.9%) (*)
- (b) 2 (43.1%)

50. What is the reason for your answer to question 49?

- (a) The fluorine atom can delocalize the electrons (22.0%) (*)
- (b) The ion can attract positively charged compounds (15.6%)
- (c) The fluorine atom is electronegative (50.5%)
- (d) Cations are more stable than anions (11.9%)

Demographic Questions

51. Gender

- (a) Male
- (b) Female
- (c) Other

52. Major

- (a) Chemistry
- (b) Biology

- (c) SES
- (d) Dietetics
- (e) Other

53. Year of study

- (a) Freshman
- (b) Sophomore
- (c) Junior
- (d) Senior
- (e) Other

54. High school graduation year

- (a) 2017 or 2018
- (b) Other

55. Organic Chemistry course information

- (a) I am taking this course for the first time
- (b) I am repeating this course

APPENDIX G

BETA VERSION OF THE INVENTORY

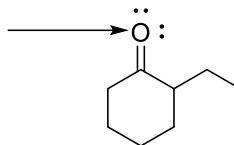
Beta Version
27 Items

(*) indicates the correct answer

Please answer the following multiple-choice and demographic questions on the bubble sheet.

- How many valence electrons does $^{18}_8\text{O}$ have?
 - 10 valence electrons (3.9%)
 - 8 valence electrons (20.3%)
 - 6 valence electrons (71.6%) (*)
 - 2 valence electrons (4.2%)
- What is the reason for your answer to question 1?
 - The mass number minus the atomic number is the number of valence electrons. (4.2%)
 - The valence electrons are equal to the number of protons. (12.5%)
 - Oxygen is in group 6A of the periodic table. (63.5%) (*)
 - The number of unpaired electrons in the outermost shell. (18.9%)
- Which one of the following is an acceptable Lewis structure for methyl azide (CH_3N_3)?
 - $$\begin{array}{c} \text{H} \\ | \\ \text{H}-\text{C}-\text{N}=\text{N}-\ddot{\text{N}} \\ | \\ \text{H} \end{array} \begin{array}{l} \ominus \\ \oplus \end{array}$$
 (21.4%)
 - $$\begin{array}{c} \text{H} \\ | \\ \text{H}-\text{C}-\text{N}^{\ominus}=\text{N}^{\oplus} \\ | \\ \text{H} \end{array} \text{N} \equiv \text{N}:$$
 (11.4%)
 - $$\begin{array}{c} \text{H} \\ | \\ \text{H}-\text{C}-\text{N}^{\oplus}=\text{N}^{\ominus} \\ | \\ \text{H} \end{array} \text{N} \equiv \text{N}:$$
 (66.6%) (*)

- What is the reason for your answer to question 3?
 - The nitrogen atoms furthest away from a carbon atom have a positive charge. (10.0%)
 - Each atom has a complete octet and formal charges are assigned correctly. (79.4%) (*)
 - Nitrogen atoms always form three bonds and carbon atoms form four bonds. (10.6%)
- What is the hybridization of the labelled atom in the following molecule?

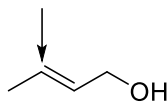


- (a) sp (17.3%)
 (b) sp² (76.6%) (*)
 (c) sp³ (6.1%)

6. What is the reason for your answer to question 5?

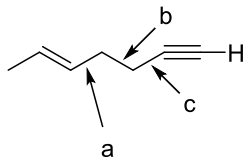
- (a) The oxygen atom has only one connection to a carbon atom. (11.4%)
 (b) The oxygen atom has a π bond. (47.6%)
 (c) The oxygen atom has three electron groups around it. (40.9%) (*)

7. Which statement best describes the geometry of the indicated atom?



- (a) Trigonal planar (63.5%) (*)
 (b) Trigonal pyramidal (11.1%)
 (c) Bent (18.4%)
 (d) Tetrahedral (6.7%)

8. Which is the strongest bond in the following molecule?

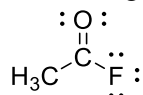


- (a) a (4.5%)
 (b) b (26.7%)
 (c) c (68.2%) (*)

9. What is the reason for your answer to question 8?

- (a) The proximity of the triple bond makes the bond the strongest. (60.7%)
 (b) It has the greatest percentage of s orbitals that make up the hybrids in the bond. (19.8%) (*)
 (c) It is the one that has the overlap of sp³ orbitals from both atoms. (19.5%)

10. Which atom in the following molecule is most electrophilic?

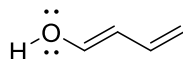


- (a) Oxygen atom (7.0%)
 (b) Fluorine atom (69.1%)
 (c) Carbon atom that is part of the C=O group (14.8%) (*)
 (d) Carbon atom that is part of the CH₃ group (9.2%)

11. What is the reason for your answer to question 10?

- (a) The atom is attached to two electron withdrawing groups. (19.8%) (*)
- (b) The atom has a lone pair of electrons to donate. (8.9%)
- (c) The atom has the least electronegativity. (11.4%)
- (d) The atom is furthest to the right in the Periodic Table. (60.2%)

12. Which is the region of greatest electron density in the following molecule?



- (a) The greatest electron density is centered on the oxygen atom. (74.7%) (*)
- (b) The greatest electron density is centered on the hydrogen atom (2.8%)
- (c) The greatest electron density is centered on the internal double bond (17.8%)
- (d) The greatest electron density is centered on the terminal double bond (4.7%)

13. What is the reason for your answer to question 12?

- (a) There are no lone pairs present in that region. (4.2%)
- (b) The double bonds are harder to break. (12.8%)
- (c) The most electronegative atom has the most electron density. (71.3%) (*)
- (d) The other atoms are stabilized by resonance. (11.4%)

14. Which is more acidic?

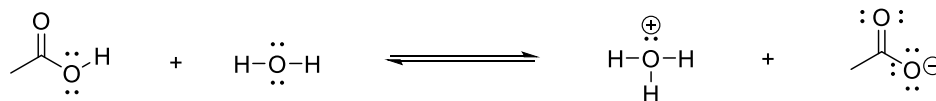


- (a) 1 (62.4%) (*)
- (b) 2 (37.6%)

15. What is the reason for your answer to question 14?

- (a) The sulfur atom is more polarizable thereby stabilizing the conjugate base. (37.6%) (*)
- (b) The S-H bond is stronger than the O-H bond. (13.6%)
- (c) The product is more stable with a positive charge. (6.4%)
- (d) The oxygen atom is more electronegative than the sulfur atom. (42.3%)

16. Which molecule is the Brønsted-Lowry base for the forward reaction?

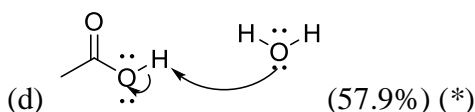
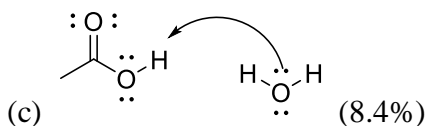
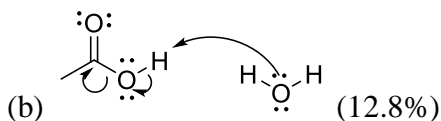
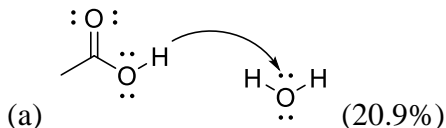


- (a) Acetic acid (13.1%)
- (b) Water (63.2%) (*)
- (c) Hydronium ion (13.4%)
- (d) Acetate ion (9.7%)

17. What is the reason for your answer to question 16?

- (a) The Brønsted-Lowry base donates the hydrogen atom. (17%)
 (b) The Brønsted-Lowry base is a proton acceptor. (66.9%) (*)
 (c) The Brønsted-Lowry base is an electron-pair donor. (12.8%)
 (d) The Brønsted-Lowry base becomes negatively charged. (3.3%)

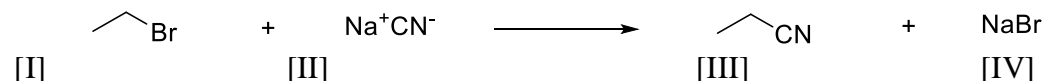
18. Which of the following best depicts the curved arrows to show the formation of the products in the above reaction?



19. What is the reason for your answer to question 18?

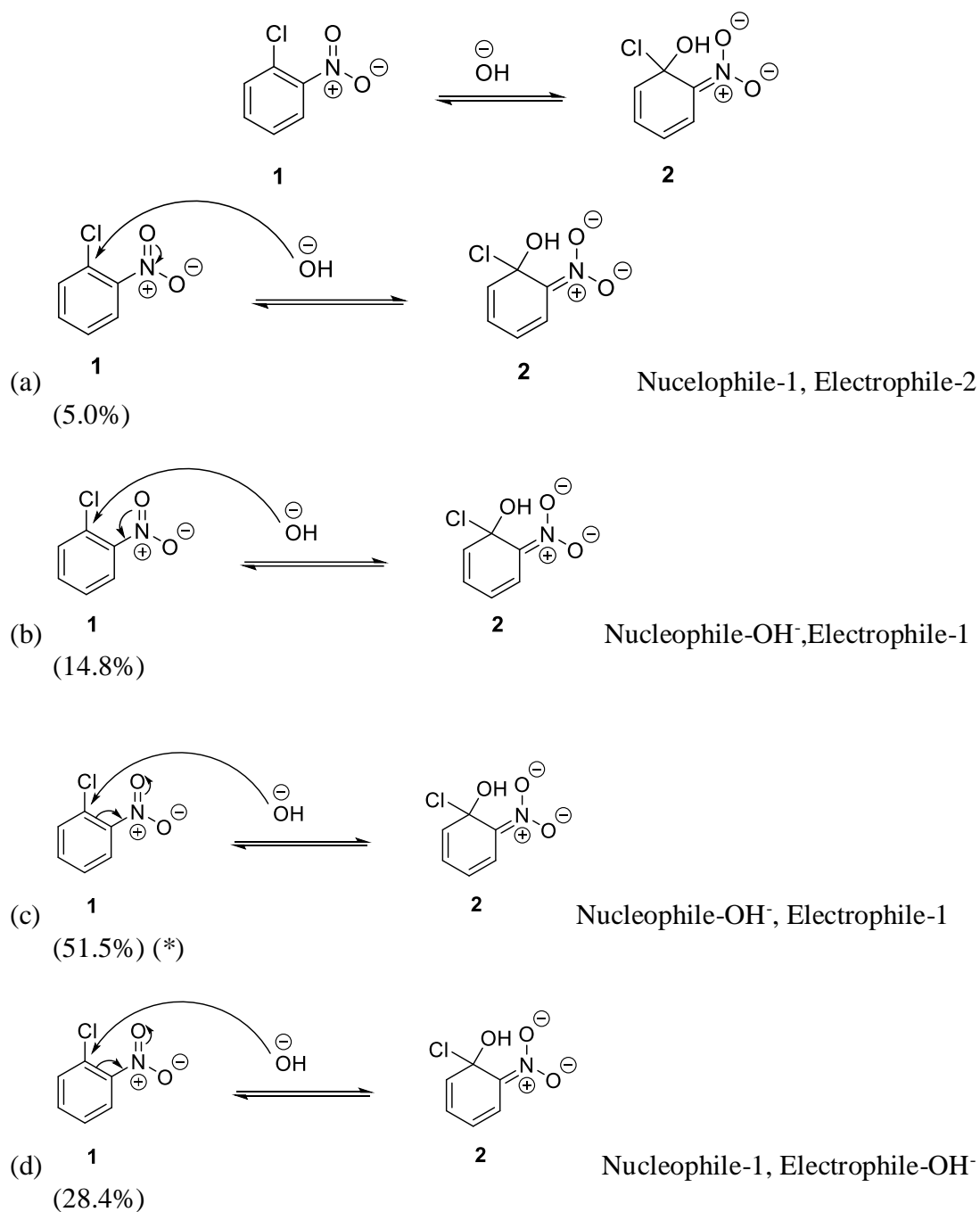
- (a) Lone pair on water forms a bond to a proton and the electrons go to the oxygen atom. (62.1%) (*)
 (b) The water molecule accepts the proton from the acetic acid molecule. (23.4%)
 (c) The electrons flow from the hydrogen atom to make the bond. (7.8%)
 (d) Oxygen atom of acetic acid is most susceptible to protonation from a water molecule. (6.9%)

20. Which is the electrophile and which is the nucleophile in the following reaction?

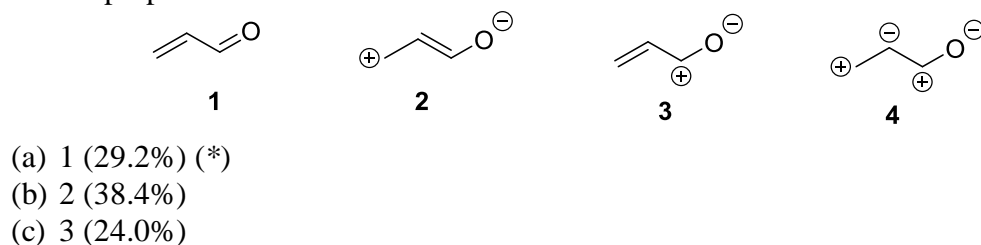


- (a) Electrophile-[I], Nucleophile-[II] (35.4%) (*)
 (b) Electrophile-[II], Nucleophile-[I] (35.9%)
 (c) Electrophile-[I], Nucleophile-[IV] (16.2%)
 (d) Electrophile-[II], Nucleophile-[III] (12.5%)

21. Which one of the following gives the correct curved arrow notation for the formation of the product and correctly identifies the electrophile and the nucleophile?



22. Which of the following is the major contributor to the overall resonance hybrid for prop-2-enal?



(d) 4 (8.4%)

23. What is the reason for your answer to question 22?

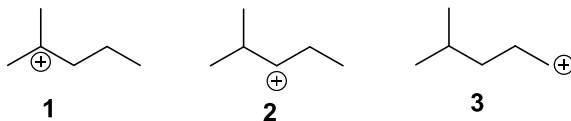
- (a) It has the most number of bonds. (19.2%) (*)
 (b) It shows the movement of electrons. (32.9%)
 (c) The charges are next to each other. (17.8%)
 (d) The charges are alternating. (30.1%)

24. Trifluoroacetic acid is more acidic than acetic acid. Why?



- (a) This is because fluorine is more acidic than OH. (17.3%)
 (b) This is because it has more hydrogen bonding capability. (9.5%)
 (c) There is additional resonance from the three fluorine atoms. (22.0%)
 (d) The inductive effect of the fluorine atoms stabilize the conjugate base. (51.0%)
 (*)

25. Which is most stable?

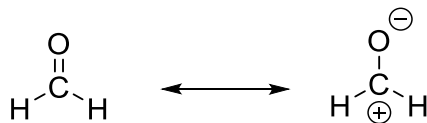


- (a) 1 (67.7%) (*)
 (b) 2 (13.1%)
 (c) 3 (17.0%)

26. What is the reason for your answer to question 25?

- (a) The alkyl groups are electron donating. (20.9%) (*)
 (b) The charge is on the central atom. (40.1%)
 (c) The carbocation is most symmetrical. (20.1%)
 (d) The carbocation has a positive charge at the end. (18.9%)

27. Why is the following molecule an acceptable resonance structure of formaldehyde?



- (a) The electrons can go to the carbon atom. (12.3%)
 (b) The oxygen atom is capable of donating electrons. (19.8%)
 (c) The oxygen atom can leave easier as a leaving group. (4.7%)
 (d) The oxygen atom is more electronegative than the carbon atom. (63.2%) (*)

Demographic Questions

28. Gender

- (a) Male
- (b) Female
- (c) Other

29. Major

- (a) Chemistry
- (b) Biology
- (c) SES
- (d) Dietetics
- (e) Other

30. Year of study

- (a) Freshman
- (b) Sophomore
- (c) Junior
- (d) Senior
- (e) Other

31. High school graduation year

- (a) 2017 or 2018
- (b) Other

32. Organic Chemistry course information

- (a) I am taking this course for the first time
- (b) I am repeating this course

APPENDIX H

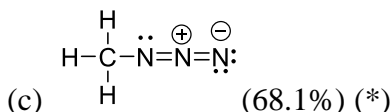
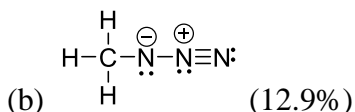
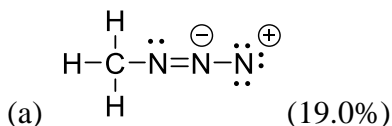
ALPHA VERSION OF THE INVENTORY

Alpha Version
26 Items

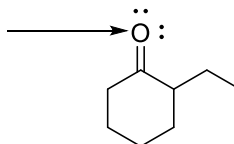
(*) indicates the correct answer

Please answer the following multiple-choice and demographic questions on the bubble sheet.

1. Which of the following is an acceptable Lewis structure for methyl azide (CH_3N_3)?



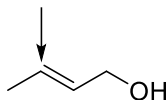
2. What is the reason for your answer to question 1?
- (a) The nitrogen atoms furthest away from a carbon atom have a positive charge. (6.6%)
- (b) Each atom has a complete octet and formal charges are assigned correctly. (81.8%) (*)
- (c) Nitrogen atoms always form three bonds and carbon atoms form four bonds. (11.6%)
3. What is the hybridization of the labelled atom in the following molecule?



- (a) sp (9.8%)
- (b) sp^2 (83.9%) (*)
- (c) sp^3 (6.2%)

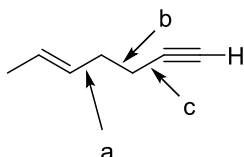
4. What is the reason for your answer to question 3?
- (a) The oxygen atom has only one connection to a carbon atom. (11.3%)
- (b) The oxygen atom has two lone pairs of electrons. (21.5%)
- (c) The oxygen atom has three electron domains around it. (67.2%) (*)

5. Which statement best describes the geometry of the indicated atom?



- (a) Trigonal planar (57.6%) (*)
- (b) Trigonal pyramidal (16.3%)
- (c) Bent (18.5%)
- (d) Tetrahedral (7.6%)

6. Which is the strongest bond in the following molecule?

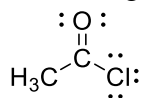


- (a) a (4.9%)
- (b) b (31.7%)
- (c) c (63.3%) (*)

7. What is the reason for your answer to question 6?

- (a) The hybridization of the atoms leads to the longest bond. (23.2%)
- (b) It has the greatest percentage of s orbitals that make up the hybrids in the bond. (39.4%) (*)
- (c) It is the one that has the overlap of sp^3 orbitals from both atoms. (37.3%)

8. Which atom in the following molecule is most electrophilic?

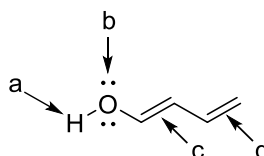


- (a) Oxygen atom (19.1%)
- (b) Chlorine atom (42.5%)
- (c) Carbon atom that is part of the $\text{C}=\text{O}$ group (26.6%) (*)
- (d) Carbon atom that is part of the CH_3 group (11.8%)

9. What is the reason for your answer to question 8?

- (a) The atom is attached to two electron withdrawing groups. (26.3%) (*)
- (b) The atom has a lone pair of electrons to donate. (17.9%)
- (c) The atom has the least electronegativity. (18.5%)
- (d) The atom is furthest to the right in the Periodic Table. (37.3%)

10. Which is the region of greatest electron density in the following molecule?



- (a) The greatest electron density is centered on a. (2.8%)
 (b) The greatest electron density is centered on b. (81.4%) (*)
 (c) The greatest electron density is centered on c. (13.1%)
 (d) The greatest electron density is centered on d. (2.7%)

11. What is the reason for your answer to question 10?

- (a) There are no lone pairs present in that region. (3.7%)
 (b) The double bonds are harder to break. (11.7%)
 (c) The most electronegative atom has the most electron density. (73.2%) (*)
 (d) The other atoms are stabilized by resonance. (11.4%)

12. Which is more acidic?

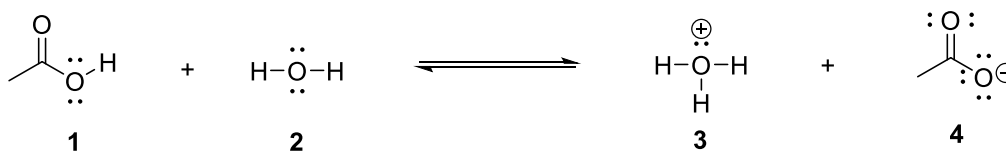


- (a) 1 (62.4%) (*)
 (b) 2 (37.6%)

13. What is the reason for your answer to question 12?

- (a) The sulfur atom is more polarizable thereby stabilizing the conjugate base. (41.2%) (*)
 (b) The S-H bond is stronger than the O-H bond. (15.9%)
 (c) The product is more stable with a positive charge. (6.8%)
 (d) The oxygen atom is more electronegative than the sulfur atom. (36.1%)

14. Which molecule is the Brønsted-Lowry base for the forward reaction?

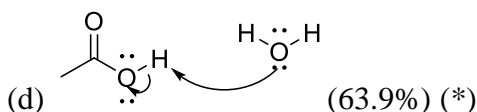
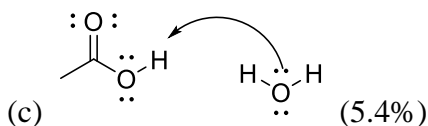
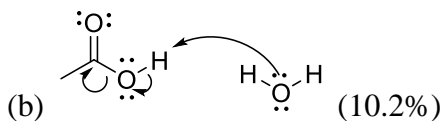
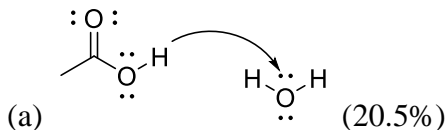


- (a) 1 (15.4%)
 (b) 2 (60.6%) (*)
 (c) 3 (13.3%)
 (d) 4 (10.8%)

15. What is the reason for your answer to question 14?

- (a) The Brønsted-Lowry base donates the hydrogen atom. (19.0%)
 (b) The Brønsted-Lowry base is a proton acceptor. (64.7%) (*)
 (c) The Brønsted-Lowry base is an electron-pair donor. (12.7%)
 (d) The Brønsted-Lowry base becomes negatively charged. (3.6%)

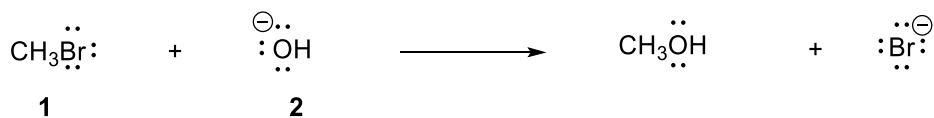
16. Which of the following best depicts the curved arrows to show the formation of the products in the reaction shown in question 14?



17. What is the reason for your answer to question 16?

- (a) Lone pair on water forms a bond to a proton and the electrons go to the oxygen atom. (58.4%) (*)
- (b) The water molecule accepts the proton from the acetic acid molecule. (27.0%)
- (c) The electrons flow from the hydrogen atom to make the bond. (8.1%)
- (d) Oxygen atom of acetic acid is most susceptible to protonation from a water molecule. (6.5%)

18. Which is the electrophile in the following reaction?



- (a) 1 (61.1%) (*)
- (b) 2 (38.9%)

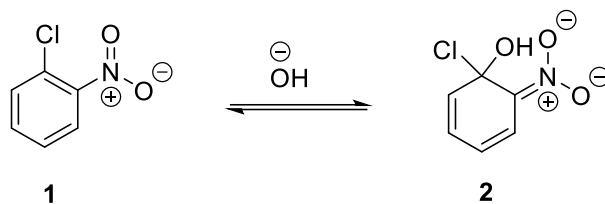
19. What is the reason for your answer to question 18?

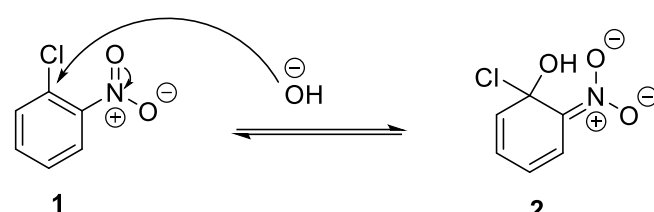
- (a) 1 is the electrophile because it contains the most electropositive atom. (34.8%) (*)
- (b) 1 is the electrophile because it has the electrons which are needed to become an ion. (24.7%)

(c) 2 is the electrophile because it contains the most electronegative atom. (27.1%)

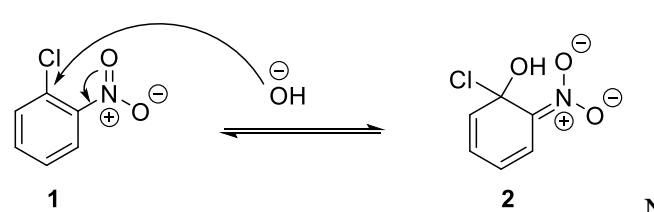
(d) 2 is the electrophile because it is the strongest base. (13.4%)

20. Which one of the following gives the correct curved arrow notation for the formation of the product and correctly identifies the electrophile and the nucleophile?

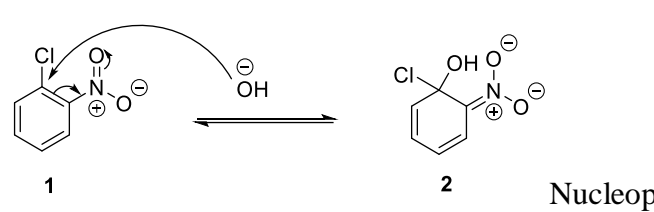
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1 **2**
- (a) 

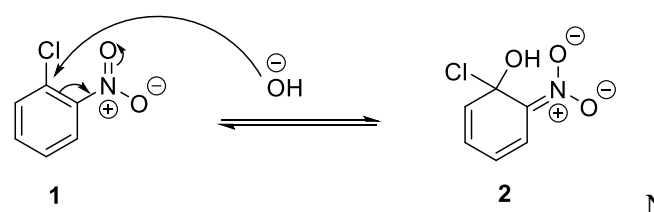
1 **2** Nucleophile-1, Electrophile-2

 (6.6%)
- (b) 

1 **2** Nucleophile-OH⁻, Electrophile-1

 (17.9%)
- (c) 

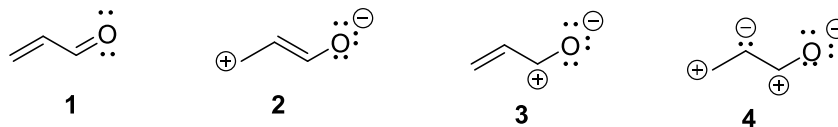
1 **2** Nucleophile-OH⁻, Electrophile-1

 (50.7%) (*)
- (d) 

1 **2** Nucleophile-1, Electrophile-OH⁻

 (24.7%)

21. Which of the following is the major contributor to the overall resonance hybrid?



- (a) 1 (41.0%) (*)
 (b) 2 (23.4%)
 (c) 3 (23.6%)
 (d) 4 (12.0%)

22. What is the reason for your answer to question 21?

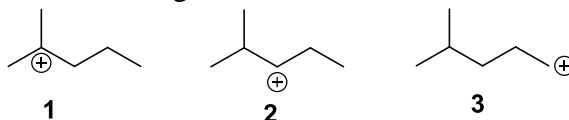
- (a) It has the most number of bonds. (32.0%)
 (b) It shows the movement of electrons. (33.2%)
 (c) The charges are next to each other. (13.8%)
 (d) The charges are alternating. (21.0%)

23. Trifluoroacetic acid is more acidic than acetic acid. Why?



- (a) This is because fluorine is more acidic than OH. (21.1%)
 (b) This is because it has more hydrogen bonding capability. (8.2%)
 (c) There is additional resonance from the three fluorine atoms. (16.3%)
 (d) The inductive effect of the fluorine atoms stabilize the conjugate base. (54.3%)
 (*)

24. Which of the following is the most stable?

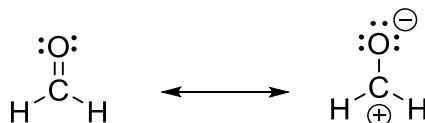


- (a) 1 (54.4%) (*)
 (b) 2 (18.7%)
 (c) 3 (26.8%)

25. What is the reason for your answer to question 24?

- (a) The alkyl groups are electron donating. (27.0%) (*)
 (b) The carbocation is most symmetrical. (32.4%)
 (c) The carbocation can easily grab electrons. (40.6%)

26. Why is the following molecule an acceptable resonance structure of formaldehyde?



- (a) The electrons can go to the carbon atom. (10.0%)

- (b) The oxygen atom is capable of donating electrons. (27.2%)
- (c) The oxygen atom can leave easier as a leaving group. (8.1%)
- (d) The oxygen atom is more electronegative than the carbon atom. (55.1%) (*)

Demographic Questions

27. Gender

- (a) Male
- (b) Female
- (c) Other

28. Major

- (a) Chemistry/Biochemistry
- (b) Biology/Pre-health
- (c) Sports and Exercise Science
- (d) Dietetics
- (e) Other

29. Year of study

- (a) Freshman
- (b) Sophomore
- (c) Junior
- (d) Senior
- (e) Other

30. High school graduation year

- (a) 2016
- (b) 2017
- (c) 2018
- (d) 2019
- (e) Before 2016

31. Organic Chemistry course information

- (a) I am taking this course for the first time
- (b) I am repeating this course

APPENDIX I**DIFFICULTY (*P*) AND DISCRIMINATION (*D*)
VALUES FOR PILOT VERSION ITEMS**

Item	Difficulty (<i>P</i>)	Discrimination (<i>D</i>)
1	0.75	-0.06
2	0.7	0.09
3	0.9	0.06
4	0.68	0.02
5	0.46	0.19
6	0.72	0.23
7	0.62	0.28
8	0.52	0.13
9	0.66	0.32
10	0.6	0.09
11	0.64	0.25
12	0.41	0.21
13	0.16	0.13
14	0.38	0.08
15	0.67	0.04
16	0.51	0.23
17	0.21	0.26
18	0.37	0.25
19	0.42	0.34
20	0.45	0.32
21	0.54	0.4
22	0.35	0.17
23	0.26	-0.02
24	0.09	0.17
25	0.63	0.26
26	0.08	0.08
27	0.14	0.09
28	0.59	0.26
29	0.35	0.47
30	0.51	0.19
31	0.51	0.15
32	0.47	0.02
33	0.37	0.17
34	0.39	0.25
35	0.25	0.15
36	0.69	0.23
37	0.14	0.06
38	0.41	0.17
39	0.38	0.15
40	0.34	0.15
41	0.36	0.11
42	0.26	0.25
43	0.26	0.32
44	0.34	0.34
45	0.57	0.08
46	0.42	0.38
47	0.38	0.23
48	0.45	0.09
49	0.5	0.08
50	0.27	0.08

APPENDIX J**DIFFICULTY (P) AND DISCRIMINATION (D)
VALUES FOR BETA VERSION ITEMS**

Item	Difficulty (<i>P</i>)	Discrimination (<i>D</i>)
1	0.71	0.16
2	0.6	0.13
3	0.63	0.53
4	0.77	0.28
5	0.78	0.1
6	0.46	0.35
7	0.65	0.49
8	0.68	-0.05
9	0.19	0.1
10	0.19	0.21
11	0.22	0.28
12	0.7	0.38
13	0.67	0.35
14	0.65	0.45
15	0.41	0.39
16	0.6	0.47
17	0.61	0.4
18	0.57	0.54
19	0.62	0.62
20	0.34	0.35
21	0.5	0.44
22	0.32	0.29
23	0.2	0.25
24	0.49	0.59
25	0.7	0.43
26	0.26	0.24
27	0.62	0.56

APPENDIX K**DIFFICULTY (P) AND DISCRIMINATION (D)
VALUES FOR ALPHA VERSION ITEMS**

Item	Difficulty (P)	Discrimination (D)
1	0.67	0.39
2	0.82	0.28
3	0.84	0.26
4	0.67	0.47
5	0.59	0.49
6	0.64	0.13
7	0.41	0.38
8	0.31	0.38
9	0.29	0.37
10	0.79	0.31
11	0.69	0.41
12	0.63	0.28
13	0.43	0.39
14	0.63	0.51
15	0.64	0.39
16	0.64	0.53
17	0.59	0.48
18	0.60	0.50
19	0.37	0.38
20	0.51	0.34
21	0.45	0.53
22	0.36	0.43
23	0.53	0.61
24	0.55	0.42
25	0.32	0.23
26	0.56	0.48

APPENDIX L

**PROTOCOL FOR ESTABLISHING
FACE VALIDITY**

General Feedback

1. Is the wording of the questions clear? Please indicate all questions where the wording is not clear to you.
2. Do you understand what the questions are asking you? Please indicate all questions where the meaning is not clear to you.
3. Which questions (if any) were easy?
4. Which questions (if any) were difficult?

Demographic Questions

1. What is the highest degree or level of school you have completed?
2. What is your area of specialization in chemistry?
3. Ethnicity origin (or Race): Please specify your ethnicity.
4. Gender _____

APPENDIX M

**SAMPLE OF CONTENT VALIDITY SURVEY
FORMAT**

Q2 The concept inventory contains multiple-choice questions which fall under ten different concepts identified by experts to be important for developing proficiency in organic reaction mechanisms.

These concepts are:

1. Electronic configuration
2. Lewis structures
3. Hybridization
4. Molecular geometry
5. Bonding
6. Polarity and electron density
7. Acids and bases
8. Electrophiles and nucleophiles
9. Resonance and induction effects
10. Stability of intermediates.

Below you will find a list of questions and their answers developed based on the main concepts derived from our expert's interviews. Some of the questions are linked pairs and they will be presented together. Please rate them as one item and provide any feedback you have regarding them.

Please review each question using the following criteria:

1. Is the question covering the concept?
2. Please rank the relevance of the question towards organic reaction mechanisms (from important to not important)
3. Is the wording of the question appropriate?
4. Do you agree with the proposed answer?
5. Please provide any other comments you may have regarding the question.

Thank you very much for your valuable input and the time devoted to this.

Q3 Electronic Configuration [Correct answers: 1(c), 2(b)]

1. How many valence electrons does ^{18}O have?
 - (a) 10 valence electrons
 - (b) 8 valence electrons
 - (c) 6 valence electrons
 - (d) 2 valence electrons

2. What is the reason for your answer to question 1?
 - (a) The mass number minus the atomic number is the number of valence electrons
 - (b) The valence electrons are the number of electrons in the outermost shell
 - (c) Oxygen is in the 6th row of the Periodic Table

Q4 Is the question appropriately covering the concept?

Yes

No

Q5 Please rank the relevance of the question towards organic reaction mechanisms.

Important

Neutral

Not important

Q6 Is the wording of the question appropriate?

Yes

No

Q7 Do you agree with the proposed answer?

Yes

No

Q8 Please provide any other comments you have regarding the question.

APPENDIX N

**MEMORANDUM TO THE INSTRUCTORS FOR
THE ADMINISTRATION OF THE
INVENTORY**

The Reaction Mechanisms Concept Proficiency Inventory (RMCPI) can be used as a summative assessment to determine students alternate conceptions on concepts that are pertinent to developing proficiency in organic reaction mechanisms. Here are specific instructions needed for administration of the RMCPI.

Number of Questions: 26

Time Duration for Test: 25 minutes

Student Population: First-semester undergraduate organic chemistry students

Testing:

- The test is best administered in week 7 of the semester – results indicate how the students performed after any review of general chemistry material that they should have been exposed to and organic chemistry material that is covered during the first few weeks of the class
- The test is administered in the regular class period
- No instructional materials (class notes, textbook, etc.) are allowed
- A Periodic Table can be provided to the students

Concepts Covered:

Majority of the questions are in linked pairs which is indicated below where students have to first choose their answer and then provide a reason for their choice which gives more information on their thought process while answering the questions.

Concept	Question Numbers	Knowledge Statements (from correct responses)
Lewis structures	1/2	-drawing Lewis structures while satisfying octet rule and assigning correct formal charges
Hybridization	3/4	-identifying state of hybridization based on electron domains around an atom
Molecular geometry	5*	-identifying molecular geometry at specific centers
Bonding	6/7	-determining bond strength based on percentage s character
Electron density & polarity	8/9 10/11	-identifying electrophilic centers based on polarity -identifying regions of electron density based on electronegativity
Acids & bases	12/13 14/15 16/17	-identifying acids based on stability of conjugate bases -determining Brønsted-Lowry bases for a given reaction -recognizing electron-flow for proton-transfer reactions

Electrophiles & nucleophiles	18/19 20*	-choosing electrophiles and nucleophiles for specific reactions
Resonance & inductive effects	21/22 23* 26*	-selecting possible resonance structures and the resonance contributors that contribute most to the resonance hybrid -effect of induction on acidity
Stability of intermediates	24/25	-factors affecting stability of carbocations

*Single questions that are not linked pairs

Results: Instructors should examine the results of the test based on the aggregate score, by determining specific questions where students underperform. For example, if the students do not obtain a satisfactory score on questions 18/19, the instructor may wish to provide additional information/instruction on the concept of electrophiles & nucleophiles before introducing the topic of reaction mechanisms to the students.