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A Process Model for the Comprehension of Organic Chemistry Notation

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A Process Model for the Comprehension of Organic Chemistry Notation

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This dissertation examines the cognitive processes individuals use when reading organic chemistry equations and factors that affect these processes, namely, visual complexity of chemical equations and participant characteristics (expertise, spatial ability, and working memory capacity). A six stage process model for the comprehension of organic chemistry notation was proposed that accounts for the movement of the eyes across the chemical equation (get next); the search of a chemical structure for key features (search); the encoding of features to create an internal representation (encoding and access lexicon); the assignments of relationships among features in the same molecule (intramolecular relationship) and between molecules (intermolecular relationship); and a check of the internal representation for inconsistencies (reaction wrap-up). Two studies were conducted in this investigation. The first study assessed the validity and ability of the *Complexity Rubric for Organic Chemistry Notation* to quantify visual complexity of structural formulas. A three-part investigation examined the content of the rubric, its capacity to measure visual

complexity, and its ability to predict visual complexity as perceived by novices. The results suggest that the rubric differentiates structural formulas with high visual complexity from those with medium-low visual complexity. A follow-up study examined the effect of prior knowledge on the encoding of organic formulas and suggests that knowledge from domains outside chemistry plays a role in the perceived complexity of structural formulas.

In the second study, eye tracking methodology was used to validate the proposed process model for the comprehension of organic chemistry notation and examine factors that affect these processes. Eight instructors and 19 students were eye tracked while reading five high/low complexity pairs of organic chemistry equations for comprehension. The frequency, duration, and sequence of participants' eye fixations were examined. The results provide evidence for each stage of the proposed process model and suggest that visual complexity of the equation, as measured by the rubric, significantly affects the viewing patterns of participants. Expertise of the participant was also shown to play a significant role in viewing patterns. The effects of working memory capacity and spatial ability were shown to be less consistent and may be topic dependent.

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Table of Contents

List of Tables

List of Figures

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Chapter 1 - Introduction

This research focuses on the processes that govern the reading comprehension of the unique chemical representational system used in organic chemistry. The research proposes a novel process model for the comprehension of organic chemistry notation and uses eye-tracking methodology to further develop and validate the model. Careful consideration of the effects of the complexity of the notation on the reading comprehension process is central to this study. This chapter will present background information, the significance of this study, and the research questions to be addressed.

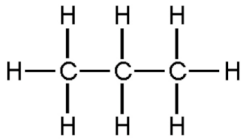
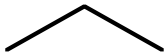
Background

Organic Chemistry Notation

Organic chemistry is a branch of chemistry that involves the scientific study of compounds that contain carbon. Organic chemists study the structure, properties, reactions, and preparation of organic compounds. To convey information to the international community of organic chemists, a unique symbolic representation system has been developed that uses alphanumeric characters, Greek symbols, lines, and/or geometric shapes to convey the number and types of atoms present in the smallest single unit of an organic compound (molecule). These representations can also illustrate how atoms present in the molecule are interconnected (see Table 1 for examples of representations for propane).

Table 1

Examples of Representations for Propane

Representation	Name
C_3H_8	Molecular formula
	Complete structural formula
$CH_3 – CH_2 – CH_3$	Condensed structural formula
	Bond-line formula

Although the representations in Table 1 each convey a different amount of visual information, all of the representations presented are understood by the organic chemistry community to represent propane. Although there are conventions governing these representations, organic chemists and chemical educators often combine aspects of these representations creating hybrid representations. As Weininger (1998) points out, "the fact that while chemists were increasingly adopting a realist stand vis-à-vis molecular structure they could not avoid representations of those structures that were inherently ambiguous." For example, the complete structural formula of propane is very explicit, showing all the bonds in the molecule; however, it does not provide information about how the bonds are arranged in three-dimensional space.

In fact, all of the representations in Table 1 are ambiguous about the spatial arrangement of atoms and do not accurately show the atoms as they exist in the real world. For some

organic compounds, the three-dimensional relationships between specific groups in the molecule are important to understanding the molecule's chemical properties and reactivity. Stereochemistry is the name given to the study of these three dimensional relationship. To relate how atoms or groups of atoms in the molecule are arranged in three-dimensional space, wedges and broken wedges are often used to show spatial relationships (see Figure 1).

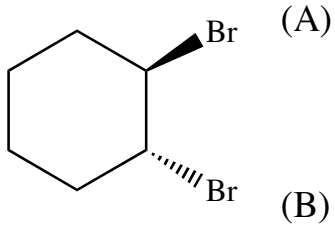


Figure 1. Spatial notation used in the structural formula of 1,2-dibromocyclohexane.

To interpret this representation, the reader must visualize the six-member hexagon ring in the plane of the paper. The solid wedge (A) indicates that the bromine (Br) is up, coming out of the plane of the paper. The broken wedge (B) indicates that a second Br is down, going behind the plane of the paper.

Once the representations of compounds, including all necessary stereochemistry, are produced, they can be combined in a chemical equation that illustrates a chemical reaction. In a chemical equation, under specific conditions one or more organic compounds or reactant(s) are transformed into one or more new compounds or product(s).

Figure 2 illustrates an example of a chemical equation. Bromine and cyclohexene are the reactants (left side of the arrow) and trans-1,2-dibromocyclohexane is the product (right

side of the arrow). Conditions under which the chemical reaction takes place (solvents, temperature, ultraviolet light, etc.) are found written above and/or below the arrow. In this case the reaction uses the solvent carbon tetrachloride, CCl_4.

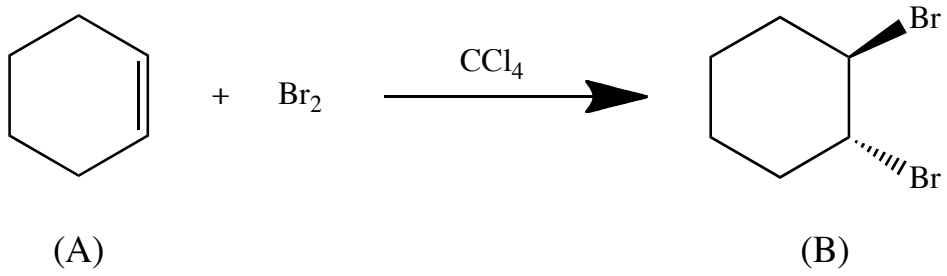


Figure 2. Chemical equation for the reaction of bromine (Br_2) and cyclohexene.

The reaction diagrammed in Figure 2 can be understood as a sentence: bromine (Br_2) is added to cyclohexene (A) in the presence of carbon tetrachloride, a solvent, to produce trans-1,2-dibromocyclohexane (B). The ability to "read" the information presented by organic chemical notation in natural English and vice versa is an important skill in the learning and practice of organic chemistry.

External Representation

Since different forms of representation can provide the reader with different types of information (for example, diagrams express spatial relationships and sentences express sequential relationships), the comprehension process for external representations depends on the type of representation being considered. Larkin and Simon (1987) identify two types of external representations: *sentential representations* and *diagrammatic representations*. A sentential representation is the formal, written form of the natural-language (e.g. English, German, etc) description of a problem. It is a direct translation, with a one-to-one

relationship between the sentence in natural language and the expression in the sentential representation. Sentential representations include words, phrases, sentences, and paragraphs. In a diagrammatic representation, spatial relationships are expressed, including shape, size, geographic location, and orientation in space. Information is "stored in one locus in the diagram, including information about relations with adjacent loci (Larkin & Simon, 1987, p. 66)."

Some have argued that rather than two distinct groups of representation, there exists a continuum from purely sentential representation to purely diagrammatic representation (Cheng, Lowe, & Scaife, 2001). All representations fall somewhere on this continuum. This research hypothesizes that organic chemistry notation falls somewhere along this continuum as well, displaying the features of both sentential and diagrammatic representations; therefore, a model of comprehension for this notation must share features of the comprehension models for both sentential and diagrammatic representations.

Chemical Equations as Sentential Representation

Consider the overall chemical equation for the addition of bromine to cyclohexene (Figure 2). Following the figure was a sentential representation of the reaction to illustrate how an organic chemist would "read" a chemical reaction. This implies that there exists an underlying language of chemistry. One of the most influential studies of chemistry as a language was Crosland's (2004) historical account of the language of chemistry, tracing the evolution of terms and nomenclature from the beginning of alchemy through modern organic chemistry. Others have approached this topic by using an analogy to illustrate

parallels among natural language (e.g. English, German, etc), the written form of natural language, and chemical language (Hoffmann & Laszlo, 1991; Jacob, 2001). In the written form of natural language, an alphabet of single characters can be combined to form words by following specific rules (orthography). For the chemical language, the symbols for the known elements on the periodic table make up a chemical alphabet that can be used to write chemical words or formulas. Theory and chemical concepts form a "chemical orthography" that provides a set of rules for the combination of elements into formulas. These formulas can then be combined into sentences (chemical equations). Other rules ("chemical grammar"), also based on theory and chemical concepts, provide structure for combining formulas into reactions, just as grammar provides structure for the formation of sentences from words. Chemical grammar also determines the type of arrow used (double headed arrow or unidirectional), reaction conditions (solvents, temperature, time, etc.), and coefficients (numbers used to show the ratio of substances involved in the chemical reactions) (Jacob, 2001).

In this simplest view of chemistry as a language, it assumes that "words" are chemical formulas for each molecule in a "sentence" that is a chemical equation; however, for organic chemistry, what constitutes a "word" is not as well defined. Hoffman and Laszlo (1991) hypothesize that different levels of complexity exist with the less complex units of the chemical language including atoms, structural fragments (i.e. C_6H_5, OH, CH_3, CH_2), simple molecules, or complex molecules. It is likely that, depending on level of expertise in organic chemistry, what constitutes a lower unit (e.g. word or clause) in the chemical

language will be different for different people. Research into expertise supports this idea. Since novices and experts in a given domain process and store information differently, comprehension of chemical equations is influenced by the participants' level of chemical expertise.

Novices are distinguished from experts based primarily on how they organize their knowledge of a domain and use this information to solve problems (Chi, Feltovich, & Glaser, 1981; Chi, Glaser, & Rees, 1982; Glaser & Chi, 1988). Because experts have a good deal of domain-specific information organized around underlying principles, the way in which they "see" a problem is different from the way novices "see" the same problem (Chi et al., 1981, 1982). Experts' organization allows them to notice meaningful features and patterns of information not necessarily noticed by novices. Novices focus on the surface features of problem (Chi et al., 1982). In terms of chemistry, novices handle organic representations as a collection of lines and letters that do not have a physical reality (Bodner & Domin, 2000). For experts, the notation used in the problem activates a highly organized understanding based on principles used in the chemical reaction.

Another consideration for treating chemical equations as a sentential representation is the sequence of "reading". For English, words are read from left to right, across a page. Hoffmann and Lazslo (1991) argue that there likewise exists a "conventional sequence" for reading chemical equations that is learned through training and experience. From the beginning of instruction, students are taught to read reactions from left to right and interpret the symbols in the chemical equation (Brown, LeMay, & Bursten, 2000, p. 68). This

convention is reinforced throughout general chemistry and in subsequent courses, including organic chemistry.

Process Model for Reading Comprehension

Information processing models describe how humans take information from sensory organs (eyes or ears), transform the information, store it, retrieve it, and use it when needed. One of the most influential models for the reading comprehension of sentential representations is the process model put forth by Just and Carpenter (1976, 1980) that is based on a series of studies that use eye movement protocol with college-aged readers.

The Just and Carpenter model (Figure 3) describes the structure and processes involved in reading comprehension. In the left hand column, the process stages of reading are depicted in their usual order of execution. The right hand column depicts long-term memory, where procedural and declarative knowledge needed for the execution of the reading processes is stored. Working memory is in the middle, mediating the long-term memory and the reading processes.

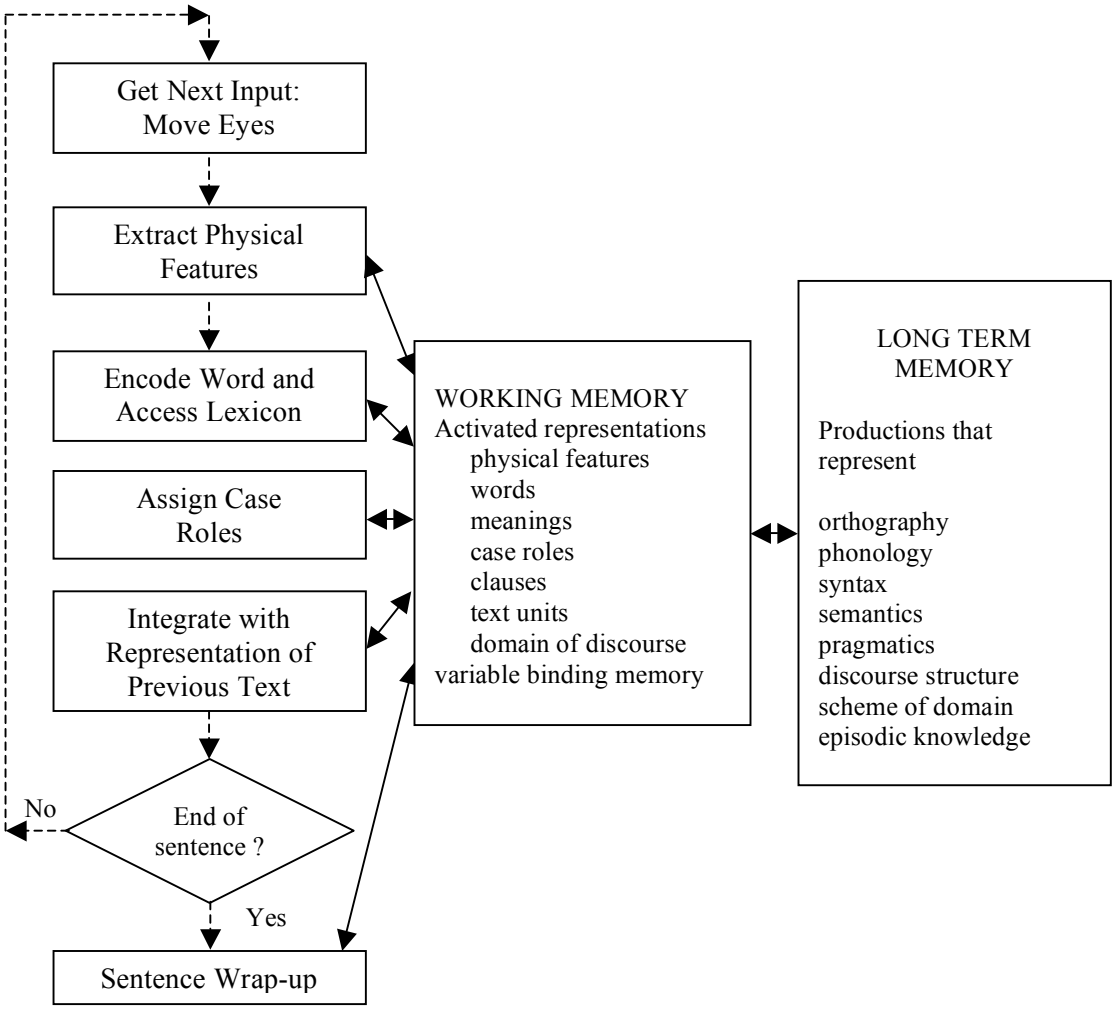


Figure 3. Schematic for Just and Carpenter's (1980) model of reading comprehension. Reprint from *Psychological Review,* 87/4, M.A. Just & P.A. Carpenter, A theory of reading: From eye fixations to comprehension, 329-354, 1980, reprinted with permission from APA (publisher).

Six major processes central to this model include the following: accounting for eye movement from one fixation to the next (G*et next input*); the encoding of the physical shapes of the letters (*Extract physical features);* the formation of an internal representation (*Word encoding and lexical access*); the assignment of relationships among units of text, such as words, clauses, and sentences (*Assigning case roles*); the integration this information

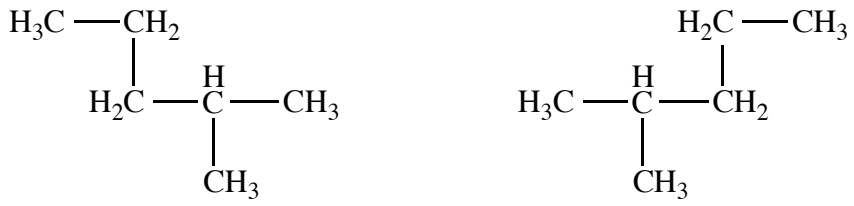
into a new, meaningful representation (*Interclause integration*); and evaluation of a thought or idea that occurs at the end of a sentence (*Sentence wrap-up*).

There are two major assumptions that Just and Carpenter use to link their model of reading comprehension to eye fixation data. The first is the *immediacy assumption* (Just & Carpenter, 1980). According to this assumption, the reader attempts to interpret each content word as he/she encounters it. Interpretations are made immediately, even if it is a guess that may later be proven incorrect. The second assumption is the *eye-mind assumption*. According to this assumption, as long as the word is being processed, the eye remains fixated on it and that fixation time is a direct measure of processing time (Carpenter & Just, 1977; Just & Carpenter, 1976). These assumptions were used to interpret eye movement data and develop the Just and Carpenter process model for reading comprehension.

Chemical Equations as Diagrammatic Representations

Diagrammatic representations vary widely depending on the topic and function of the representation (For examples, see: Cheng, 1996; Cheng et al., 2001; Just & Carpenter, 1976; Koedinger & Anderson, 1990; Larkin & Simon, 1987; Lowe, 1993). These representations can take a variety of forms, including photographs, maps, three-dimensional arrays, graphs, flow charts, and schematics. Unlike sentential representations, which have rules governing how the representation is constructed (orthography and grammar), diagrammatic representations (diagrams) have no such overarching structure. Instead of using words, diagrams convey information through proximity relationships. Information,

such as size, shape, or orientation, is conveyed by the relationship of one element of the diagram to another (Larkin & Simon, 1987). This is important to consider when looking at chemical notation as a diagram. Consider the structural formulas shown in Figure 4.



(A) (B)

Figure 4. Two representations for 2-methylpentane.

Both representations (A and B) are of 2-methylpentane. In chemical notation, although there are rules governing the inter-connectivity of atoms in the molecule, the orientation of the whole molecule in space is left to the author. To an organic chemist, molecule A and molecule B are identical but may not appear that way to the novice. This presents a challenge to the research, which will be addressed in the methodology section.

Unlike the sentential representations, a diagram does not contain all the information required to comprehend the meaning of the representation (Cheng et al., 2001; Lowe, 1993). The success of the comprehension is dependent on the background and expertise of the participant; therefore, prior knowledge must be considered when studying how individuals comprehend diagrammatic representations.

Process Model for Diagrammatic Comprehension

The process models for diagrammatic comprehension vary as widely as the types of representations themselves (Cheng, 1996). They are based on the task that is to be accomplished and it is unclear whether the model for one type of diagram is applicable to other types of diagrams. For example, Just and Carpenter (1976) developed a process model for a mental rotation task. In the task, participants had to decide "whether two figures were views of the same object or views of different objects" (p. 444). In this process model, three processing stages were suggested: 1) search, 2) transformation and comparison, and 3) confirmation. During the first stage, there is a search for specific elements of the diagram. In the next stage, transformation and comparison, the participants mentally rotate one of the two figures and compare it to the figure that was not rotated. The last stage, confirmation, is a final check to see if the conditions of the task were met. Although the stages 1 and 3 are commonly found in other process models under slightly different names (see Koedinger & Anderson, 1990; Larkin & Simon, 1987), stage 2 (transformation and comparison) is unique to the mental rotation task.

Unfortunately, a process model has not been developed for chemical representations; however, models have been developed for content areas whose diagrams share common features or purpose with chemistry, including physics (e.g. Larkin & Simon, 1987) and mathematics (e.g. Koedinger & Anderson, 1990). Common to these models are the ideas of search and evaluate. In each model, there is a stage where the individual searches for elements of the diagram that meet a specific set of criteria (Search stage). Once the task

dependant processing or manipulation stage is complete, the evaluation stage determines if the new mental representation satisfies the goal of the overall task. If so, then the processing is complete. If not, then the search begins again. Another common feature of process models is the role of prior knowledge. The criteria governing the search and evaluation stages of process models are based on knowledge stored as schema or productions in the participants' long-term memory.

By considering chemical equations as both sentential and diagrammatic representations, I propose a novel model for the comprehension of organic notation that combines the processing models of both. Specific characteristics of the participants and the materials used in this research must be considered in order to fully understand the comprehension of organic chemistry notation. Thus far, this discussion has only touched on the influence of expertise on the understanding of external representations; however, there are other variables related to the individual that can explain differences in reading comprehension. These include, working memory capacity, spatial ability, and representation complexity.

To better understand the comprehension process of organic chemistry notation, it is important to identify individual characteristics that may affect this process. Working memory capacity, expertise, and spatial ability have been identified in the literature as participant characteristics that may affect notation comprehension. Representation complexity has also been shown to affect processing.

Working Memory Capacity

Since Just and Carpenter (1980) believed that "the nature of the comprehension processes depends on a larger issue, namely the architecture of the processing system in which they are embedded" (Just & Carpenter, 1980, p. 332), it is important to look at the cognitive architecture involved in the reading comprehension process. In the Just and Carpenter reading comprehension model (see Figure 4), working memory plays a central role in mediating processes and long-term memory. Working memory refers to "a limited capacity system, which temporarily maintains and stores information, [supporting] human thought processes by providing an interface between perception, long-term memory and action" (Baddeley, 2003a, p. 829), where actions include reading, problem-solving, and learning. Only a limited amount of information can be held in working memory. What is stored in working memory is not only information to be recalled later, but also partial results of information manipulation (Just & Carpenter, 1992a). Some have suggested that there is a maximum amount of resources that working memory has available for storage and processing (working memory capacity), and it is this working memory capacity that accounts for the differences in reading comprehension performance among individuals (Daneman & Carpenter, 1980; Daneman & Merikle, 1996; Just & Carpenter, 1992a).

Stamovlasis and Tsaparlis (2001) found that working memory capacity, as measured by using the backwards digit span test, correlates with achievement on organic synthesis problems. When the problem's mental demands are high enough to strain working memory capacity, persons with lower capacity will experience performance problems. Under these

circumstances, their computations will be slower and the ability to store intermediate answers or interpretations will be hampered (Just & Carpenter, 1992a; Tsaparlis & Angelopoulos, 2000). For example, a correlation has been identified between working memory span and achievement for simple organic synthesis problems (Tsaparlis, Kousathana, & Niaz, 1998). Students with larger working memory capacity had higher achievement than students with lower working memory capacity. Research suggests that errors in solving problems that affect achievement occur not during the execution of the answer but may occur because the individuals do not comprehend the given problem and develop incorrect solution plans (Hegarty, Mayer, & Green, 1992; Lewis & Mayer, 1987; Mayer, 1998). Since achievement is related to the students' ability to read and comprehend the given problem, it is suggested that working memory capacity may affect the way in which individuals view and interpret organic chemistry notation.

Expertise and Prior Knowledge

As was discussed earlier in this chapter, expertise plays an important role in the process models for sentential and diagrammatic representations. The internal representations that experts and novices generate from the same problem are different; experts "virtually 'see' a problem different from the one novices do" (Kozma & Russell, 1997, p. 950). Experts recognize the underlying principles and theories in a problem. They use these principles and theories to build an internal representation that contains both physical features of the problem (such as chemical formulas, structural formulas, and arrows) and concepts related to the problem that are not directly stated (such as electronic properties, reaction

mechanisms, and chemical activity). Novices recognize only the surface features such as lines, letters, and overall shapes (Chi et al., 1981). It is predicted that differences in how a representation is viewed will also affect how organic chemistry notation is viewed and interpreted. Therefore, this study focuses on identifying the differences in viewing patterns of experts (organic chemistry instructors) and novices (undergraduate students) while they study a new chemical reaction.

Spatial Ability

The ability to perceive an object in both two-dimensional and three-dimensional space is known as *spatial ability*. It includes the ability to acquire, store, retrieve, and process spatial properties of an object, including shape and connectivity (Eyal & Tendick, 2001). Since process models for diagrammatic comprehension include the search, acquisition, and processing of spatial relationships of elements in a diagram, spatial ability plays an important role in the processing of organic chemistry notation. Research suggests that spatial ability affects student performance in organic chemistry, especially for problems where participants outline multi-step syntheses, complete a reaction scheme, or manipulate two-dimensional representations (Pribyl & Bodner, 1987). It has been demonstrated that students with high spatial ability are better at "understanding" a problem containing a reaction mechanism than students with low spatial ability.

Representation Complexity

For both sentential and diagrammatic representations, the complexity of the material presented affects processing. Halford, Wilson, and Phillips (1998) argue that the demands

on processing can be traced to the relational complexity of the representation. For example, a sentence that contains a large amount of information requires that a large number of decisions be made during processing including both the determination of relationships within the sentence and the assignment of case roles. This, in turn, slows processing (Just & Carpenter, 1992a; Sweller, 1993). Complexity "can be measured by the dimensionality of the relation, or the number of variables related (Halford et al., 1998, p. 805)." It is predicted that when complex molecules are illustrated using organic chemistry notation, the large number of relationships will affect the way participants view and interpret the chemical equation.

Statement of the Problem

This research focuses on the development and validation of a process model addressing the comprehension of organic chemistry notation and examines the effect of complexity of organic chemistry notation on the comprehension process.

Model for Comprehension of Organic Chemistry Notation

Adapted from the Just and Carpenter model, the proposed model for the comprehension of organic chemistry notation also relies on both the *immediacy* and the *eye-mind assumptions* (Just & Carpenter, 1980). The *immediacy assumption* states that a reader will immediately interpret each visual element (structural formula, element, functional group, etc) as he/she encounters it. The second assumption, the *eye-mind assumption,* states that the eye remains fixated on a visual element during processing. Only when processing is complete will the eye move to the next fixation.

The model for the comprehension of organic chemistry notation is provided in Figure 5. The overall model takes into account the combined characteristics of the processing models for both sentential and diagrammatic representations. Processes are listed in the left-hand column and the long-term memory is listed in the right hand column. Working memory mediates between processes and long-term memory.

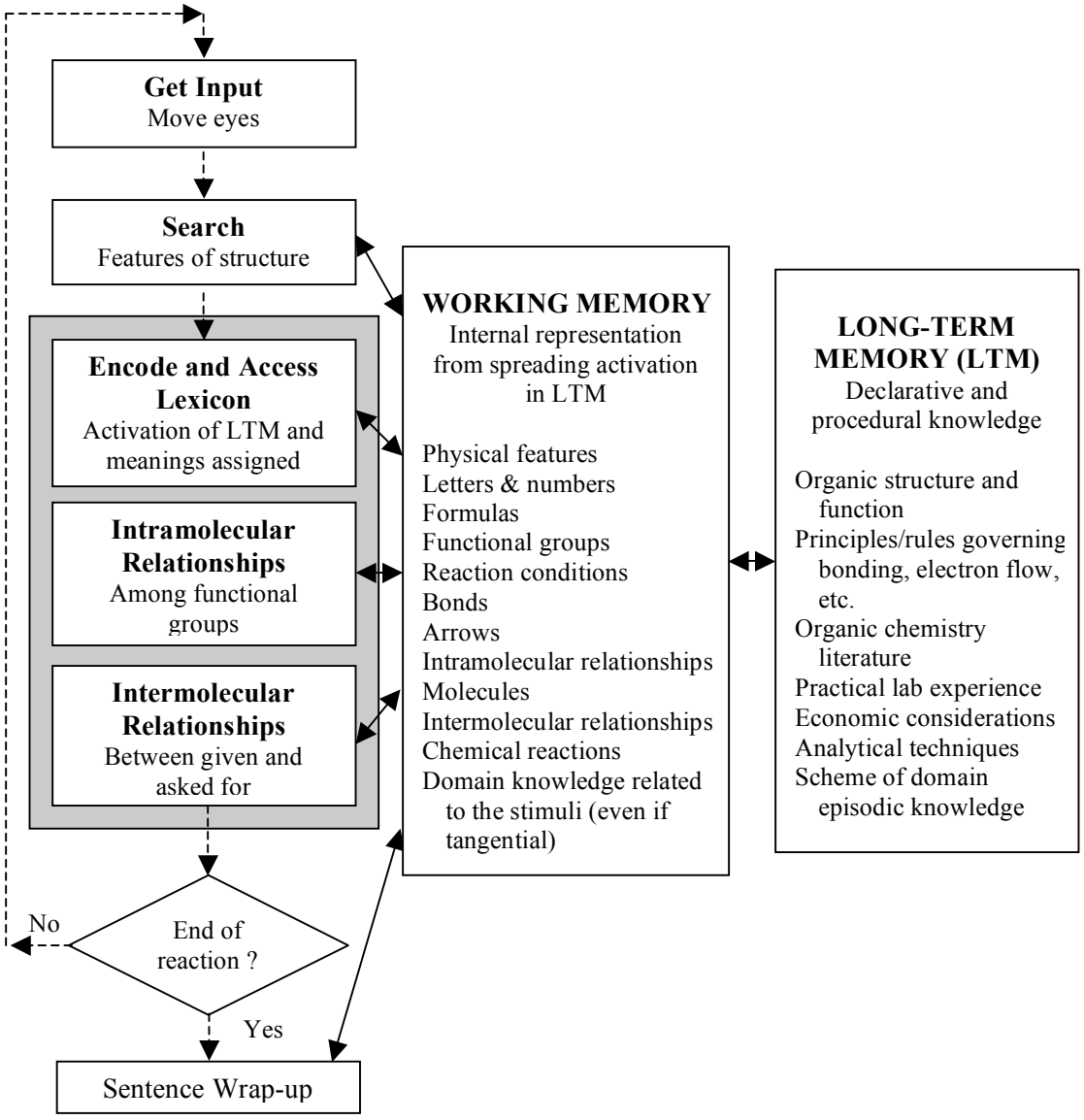


Figure 5. Schematic of the model for the comprehension of organic chemistry notation based on Just and Carpenter (1980) model of reading comprehension.

This model for the comprehension of organic chemistry notation has six major stages. The *Get Input* stage is the first stage in the cycle and governs the movement of the eyes over the chemical reaction. This stage finds information, encodes it, and processes it.

Once the processing is complete, the eye moves to a new place. The progression of movement is hypothesized to be from left to right, similar to reading English text. The participant will start with the reactants, move to the arrow, conditions, and products. The *Search* stage is a systematic intramolecular (within the molecule) search of a given chemical structure. I hypothesize that the participant will search the chemical structure for features that are important to understanding the chemical reaction. This includes functional groups that can be used to aid in classifying the compound in the representation (alcohol, amine, aldehyde, etc.) and features of the site where the reaction takes place. The overall search strategy is hypothesized to start at the reaction center and radiate outward in the given structural drawing for a molecule. Fixations will be on elements that are central to understanding the chemical reaction. During the *Encoding and Access Lexicon* stage, intramolecular features are encoded, creating an internal representation. This representation includes information from long-term memory. Relationships among features in the same molecule are determined in the *Intramolecular relationship* stage. These relationships are governed by chemical principles and theories and include steric effects (size and shape relationships), and electronic effects (electron repulsion, electron attraction, electron donating, and electron withdrawing effects). Relationships between molecules are determined in the *Intermolecular relationship* stage. These include the relationship of two molecules on the same side of the arrow (reactant-reactant or product-product), molecules on opposite sides of the arrow (reactant-product), and reaction conditions for molecules on either side of the arrow (reaction condition-reactant; reaction condition-product). During

this stage a reader may compare similarities and differences between the two molecules or mentally rotate molecules to more favorable orientations (Stieff, 2007). In the last stage, the *Reaction Wrap-up*, the reader completes the viewing of the reaction equation. During this stage, the reader checks for reproduction errors, including the addition or subtraction of a functional group. The reader accounts for any element of the equation that was not assigned a role in the reaction and examines any inconsistencies that cannot be resolved in the reaction when viewed as a whole.

Purpose of the study

The purpose of this study is two-fold: 1) to validate the process model for the comprehension of organic chemistry notation and 2) to address questions directly linked to this validation and analysis process including how participants view specific regions of the reaction equation, as defined by the research.

As part of this research, a rubric was developed to measure the complexity of organic chemistry notation. Since the amount of visual information in chemical equations can vary widely, a means to measure the complexity of the equations used in this research was required. The *Complexity Rubric for Organic Chemistry Notation* was developed to quantify this complexity by identifying the perceptual elements (e.g. bonds, atoms, rings, chiral centers, etc.) in the structural drawing of an organic molecule and assign point values to these elements. A three-part validation plan for the *Complexity Rubric for Organic Chemistry Notation* will describe: 1) Content Validity, 2) Construct Validity, and 3) Predictive Validity (Groth-Marnat, 2009). Once validated, this rubric will be used to

quantify the complexity of equations used in the validation of the process model for the comprehension of organic chemistry notation.

To validate the process model and track how participants view specific regions of the reaction equation, this research project will use eye-tracking methodology. One of the most common eye-tracking metrics is area of interest (AOI) (Jacob & Karn, 2003). This method is a data aggregation technique. Based on some criteria, the researcher defines areas of interest, which are "regions of interest that represent units of information in the visual field (Salvucci & Goldberg, 2000, p. 75)." Consecutive eye fixations that occur within these regions are collapsed into fixation groups. Fixations outside the defined areas of interest are discounted. AOI fixations groups can then be used later for further analysis.

I used two separate methods for defining areas of interest for the chemical equation, yielding two separate levels of specificity. The first level of specificity focuses on each molecule participating in the chemical reaction as a whole. These are the intermolecular areas of interest (AOIs). AOIs are researcher-defined regions of the chemical equation that contain 3 distinct features of the chemical equation: reactant(s), conditions, and products. In the case of bimolecular equations, each reactant has a separate AOI. All other notational features (including arrows and plus signs) were ignored for this portion of the experiment.

The second level of specificity is the intramolecular areas of interest. These are atoms or groups of atoms that share common characteristics. To define these regions, I used an automated data-mining technique called cluster analysis to reveal patterns or "clusters" of fixations. These irregular shaped clusters, called regions of interest (ROIs), contain either

white space or portions of the equation. ROIs were coded as informative, distractor, or off content. Informative ROI (iROI) contain information necessary to understand the chemical reaction. Distractor ROI (dROI) contain information that is not necessary to understand the chemical reaction. Off content ROI (ocROI) are regions of white space that have statistically significant patterns of fixations. It is important to note these ROIs just described do not cover the entire chemical equation, and some features of the chemical equations are not contained in an ROI. This does not mean that these features were not viewed, but only that there was not enough viewing in that region to make the fixations significant.

Once defined, AOIs and ROIs were used to determine if fixations and transitions characteristic of specific stages in the process model occur. They were also used to determine if there are differences in viewing patterns based on expertise, working memory capacity, and spatial ability.

Research Questions

The following questions will be addressed by this research:

Study 1: Validation of *Complexity Rubric for Organic Chemistry Notation*

1. To what extent is the rubric consistent with expert opinion on visual information processing?
2. To what extent does the rubric complexity score measure the visual complexity of the chemical notation?
3. To what extent does the rubric complexity score predict the visual complexity of a molecule?

Study 2: Validation of the process model

4. To what extent does the process model for the comprehension of organic chemistry notation account for eye fixations (frequency and duration) of participants reading organic chemistry equations?
5. For high versus low complexity chemical equations, what are the effects of different participant variables (working memory capacity, expertise, and spatial ability) on the frequency and duration of eye fixations as measured by the eye tracker for:
    a. Informative regions of interest, iROIs, versus distractor regions of interest, dROIs?
    b. Intermolecular areas of interest - AOIs (reactant, condition, product)?
6. For high versus low complexity chemical equations, is there a difference in the sequence of fixations between areas and regions of interest (AOIs and ROIs) as participants "read" organic chemistry equations for:
    a. Participants of differing working memory capacity?
    b. Experts versus novices?
    c. Participants of differing spatial ability?

Hypothesized Data

Study 1: Validation of Complexity Rubric for Organic Chemistry Notation

Part 1 of this study was to determine the extent to which the rubric is consistent with expert opinion on visual information processing (Question 1). Two experts performed an external review of the rubric, assessing each rubric item based on their knowledge of visual

processing. Interviews with the experts focused on whether the rubric adequately identifies and quantifies perceptual elements in molecular structures.

Table 2

Hypothesized Results for Study 1: Parts 2 and 3

Research Question	Research Hypothesis
2) To what extent does the rubric complexity score measure the visual complexity of the chemical notation?	As the rubric complexity score increases, the ability of the participants to accurately reproduce the image of a single molecule or a chemical equation will significantly decrease.
3) To what extent does the rubric complexity score predict the visual complexity of a molecule?	When six molecules are arranged from least complex to most complex, there will be no significant difference between the linear order produced by participants and that predicted by the rubric. If discrepancies are found in the position of two or more molecules, modifications will be made to either the rubric scoring or surveying procedures. Modifications will be based on written justifications provided by participants.

Study 2: Validation of the process model

This study was based on two assumptions found in the literature (Just & Carpenter, 1980). The first assumption, immediacy, states that objects are interpreted as they are encountered and that these interpretations are made immediately. The second assumption is the eye-mind assumption that states that the eye will remain fixed on an object while it is being processed. How long the eye remains fixed on an object (fixation time) is a direct measure of processing time. Accordingly, distinct eye movements will verify each stage of

the process model. In order to capture where the participant is looking to test the comprehension model, eye-tracking methodology was used. Table 3 details the eye-tracking data that was used to address question 4: to what extent does the process model for the comprehension of organic chemistry notation account for eye fixations (frequency and duration) of participants reading organic chemistry equations?

Table 3

Proposed Eye-Tracking Data for Process Model Stages

Stage	Description	Level of Specificity	Data	Analysis
Get Input	Move they eyes from one fixation to another across the reaction equation	AOI	Patterns of first fixations across the AOIs for each equation	Frequency of fixations Heat map visualization Levenshtein Distances
Search	Search of molecular structures for features that are key to understanding the chemical reaction	AOI[a]	Three-fixation patterns within AOIs for the reactant(s) and products	Frequency of fixations
Encoding and Access Lexicon	Encode features of the molecules and retrieve information from LTM to create an internal representation. The meaning of molecular features is activated in LTM during the access of the organic chemistry lexicon.	ROI[b]	Fixation durations in two or more ROIs that contain the same molecular feature in an equation.	Paired sample t-test to determine if the duration of the first fixation is significantly different from the average fixation duration for subsequent fixations.
Intramolecular Relationships	Identify relationships between features within a molecule.	ROI[c]	1. Regression patterns of first fixations across the ROIs within the same molecule. 2. Fixation durations in iROIs and dROIs.	1. Paired sample t-test to determine if the fixation durations in iROIs are significantly longer than fixation durations in dROIs within each molecule. 2. Counts of regressive patterns and percentage of overall fixations within the same molecule.

(continued)

Stage	Description	Level of Specificity	Data	Analysis
Intermolecular Relationships	Identify relationships between molecules in the reaction equation	ROI[d]	1. Regression patterns of first fixations across the ROIs within the equation. 2. Fixation durations for iROIs and dROIs.	1. Paired sample t-test to determine if the fixation durations in iROIs are significantly longer than fixation durations in dROIs for the entire equation. 2. Counts of regressive patterns and percentage of overall fixations for the equation.
Reaction Wrap-up	Integrate new information with existing knowledge and check for inconsistencies and reproduction error	ROI[e]	1. Final fixation duration and average fixation duration for all fixations, excluding final fixation. 2. Classification of the ROIs for the last fixation.	1. Paired sample t-test to determine if the final fixation duration is significantly different from the average duration for all other fixation. 2. Classification of final fixation

Notes. [a] This excludes AOIs for conditions. [b] ROIs for a subset of equations. These ROIs contain the same molecular feature. Eye fixation data from three separate equations were used for this analysis. [c] This includes iROIs and dROIs. [d] This includes iROIs and dROIs. [e] This includes iROIs, dROIs, and ocROIs.

The eye-tracking data will also be used to address the following research questions:

5. For high versus low complexity chemical equations, what are the effects of different participant variables (working memory capacity, expertise, and spatial ability) on the frequency and duration of eye fixations as measured by the eye tracker for:
    a. Informative regions of interest, iROIs, versus distractor regions of interest, dROIs?
    b. Intermolecular areas of interest - AOIs (reactant, condition, product)?
6. For high versus low complexity chemical equations, is there a difference in the sequence of fixations between areas and regions of interest (AOIs and ROIs) as participants "read" organic chemistry equations for:
    a. Participants of differing working memory capacity?
    b. Experts versus novices?
    c. Participants of differing spatial ability?

Table 4. details the hypothesized results for each participant variable in question 5.

Table 4

Hypothesized Results for Question 5

Research Question	Research Hypothesis
For high versus low complexity chemical equations, what are the effects of different participant variables [working memory capacity (WMC), expertise, and spatial ability (SA)] on the frequency and duration of eye fixations as measured by the eye tracker for:	
a. iROIs versus dROIs?	Working memory capacity (WMC) - Participants with larger WMCs will exhibit shorter overall fixations when compared with participants with smaller WMCs. Participants with larger WMCs will exhibit fewer fixations in both iROIs and dROIs when compared with participants with smaller WMCs. Expertise – Experts will have overall shorter fixations than novices. Experts will have greater frequency of fixations in iROIs and a lower frequency of fixations in dROIs. Spatial Ability (SA) - Participants with high SA will exhibit shorter overall fixations when compared with participants with a low spatial ability. Participants with high SA will exhibit fewer fixations in both iROIs and dROIs when compared with participants with low spatial ability.
b. A OIs (reactant, condition, product)?	Working memory capacity (WMC) - Participants with larger WMCs will exhibit shorter overall fixations when compared with participants with smaller WMCs. Participants with smaller WMCs will have higher frequencies of fixations for AOIs than participants with larger WMCs. Expertise – Experts will exhibit shorter overall fixation times than novices. Experts will have lower frequency of fixations than novices. Spatial ability (SA) - Participants with high SA will exhibit overall shorter fixation times than participants with low SA. Participants with high SA spatial ability will exhibit fewer fixations than participants with low SA.

The final portion of this study compares the fixation sequences for each chemical equation to characterize the viewing patterns for different populations. Table 5 details the hypothesized results for each participant variable in question 6.

Table 5

Hypothesized Results for Question 6

Research Question	Research Hypothesis
Is there a difference in the transitions between areas of interest as participants "read" organic chemistry equations:	
a. Between participants of differing working memory capacity?	There will be a significant difference in the sequences of fixations for participants with high vs. low working memory capacity. The literature suggests that participants with a larger working memory span will show more repetition of previously viewed regions (regression) than participants with a smaller working memory span.
b. Between experts and novices?	There will be a significant difference in the sequences of fixations for experts vs., novices. The literature suggests that experts will display a conventional sequence for reading an organic chemistry equation; the sequence of novices will be less predictable and will show more regressions than those of experts.
c. Between participants of differing spatial ability?	There will be a significant difference in the sequences of fixations for participants with high vs. low spatial ability (SA). The literature suggests that participants with greater SAs will show fewer regressions than participants with smaller SAs.

Significance

The significance of this research is three-fold. First, this research provides the organic chemical education community with a validated measure of chemical notation complexity.

In previous research, no systematic approach has been available to classify structures in terms of their complexity. Previously, the choice of compounds to be studied relied on the researchers' instincts regarding what constituted easy and challenging problems. Tsaparlis and Angelopoulos (2000) hinted at the need for such a classification when they focused their study on organic chemical structures with "no noise", meaning low chemical notation complexity, however, currently there is no standard way to quantify the idea of complexity. Second, this research proposes the first process model specifically for the comprehension of chemical notation used in organic chemistry that accounts for the eye fixations of participants as they attempt to understand a chemical reaction. Finally, the effects of the complexity of notation used in the presentation of chemical equations, expertise, working memory capacity, and spatial ability on the way participants view and interpret the chemical equation will be studied.

Limitations

Study 1: Validation of the Rubric

This study use participants from a mid-sized post-secondary institution in the Mid-Atlantic region of the United States. The rubric is not directly generalized to other populations, including community colleges and high school students.

Study 2: Eye-tracking

This study used eye-tracking methodology with a small group of novices and experts. An inherent limitation of eye-tracking methodology is that it shows where the participant is focusing attention but not why the attention is focused at that location. The

interpretation of eye fixations must be inferred using the immediacy assumption and eye-mind assumption. It is these assumptions that introduce a degree of speculation into this research.

Novice participants for this study were drawn from the student population at a mid-Atlantic R1 university. Expert participants were drawn from the same institution and/or neighboring colleges and universities. Since participation in this study was voluntary, the population for this study was self-selected. The modest sample size and the self-selected population cannot be considered random sampling.

Chapter 2 will review the process model for reading chemical notation in the context of the Just and Carpenter model and other models for the comprehension of diagrammatic representations. Included in this discussion will be the research from chemical education that supports the proposed model. Cognitive architecture, forms of representation, expertise, and eye-tracking methodology will also be explored in Chapter 2.

Definition of Terms

The following are terms will be used throughout this study. These definitions are provided as an aid to understanding the subsequent chapters of this dissertation.

Eye-tracking

Eye-tracking methodology – a research method that measures eye movement and eye position relative to the head position of a participant.

Eye movement behavior – generic term for all types of eye movements, including fixations, saccades, look-look away, and smooth pursuits.

Fixations – pauses in eye movements over an area of interest.

Saccade – fast movements of both eyes between fixations.

Areas of Interest (AOI) – square or rectangular region of the visual field that is defined by the researcher. AOIs in this study encompass a single feature of the equation: reactant, condition, or product. AOI includes the line drawing with a 30 pixel buffer region.

Cluster analysis – automated fixation analysis tool in Tobii Studio (version 2.0) software that statistically identifies patterns, or clusters, of fixations with similar characteristics.

Eye fixation sequence – participant's sequence of fixations among AOIs/ROIs. AOIs/ROIs are given single letter codes. The sequence of fixations is converted into a string of letters corresponding to the sequence that the participant fixates in the AOIs/ROIs.

Gaze duration – also known as fixation duration, is the amount of time a particular area of interest is viewed.

Region of Interest (ROI) – irregularly shaped region of the visual field that is defined by cluster analysis of the fixations and has a 50 pixel resolution.

> *Informative Region of Interest (iROI)* – a region of interest that contains visual information necessary to understand the chemical reaction presented.
>
> *Distractor Region of Interest (dROI)* – a region of interest that contains visual information that is not necessary to understand the chemical reaction presented.
>
> *Off Content Region of Interest (ocROI)* – a region of interest that contains only white space.

Regression – also known as *regressive eye movement,* where participant looks back at a previously viewed AOI.

Scan path - repeating series of fixations and saccades that occur when a participant is re-exposed to a visual object. Scan path theory states that these repeating sequences facilitate recognition of the object.

Transition - shifts in attention (transitions) between areas of fixations.

Organic Chemistry

Chemical equation – the written form of a chemical reaction.

Chemical reaction – process by which a chemical substance is transformed into a different substance.

Conditions – specified environment under which a chemical reaction takes place (solvent, temperature, pressure, etc.) written above or below the arrow in a chemical equation.

Organic compound – substance containing carbon.

Organic molecule – two or more carbon atoms chemically joined by a covalent (shared pair(s) of electrons) bond. Most organic molecules also contain hydrogen and many contain other nonmetal elements such as nitrogen, oxygen, and sulfur.

Products – substance(s) that are formed as a result of a chemical reaction (head of the arrow).

Reactants – substance(s) that are present at the start of a chemical reaction (tail of the arrow).

Structural formula – a diagram that uses chemical notation to show the arrangement of atoms and bonds in an organic molecule.

Chapter 2 – Review of the Literature

The learning of organic chemistry and organic chemical notation are inextricably intertwined. Open any organic chemistry textbook and there are hundreds of organic molecules each represented using a systematic notation comprised of lines, geometric shapes, Greek and alphanumeric symbols, mathematical symbols, and arrows. To illustrate this point, an informal survey was conducted using a single chapter from John McMurry's textbook *Organic Chemistry, 6th edition* (2004, pp. 68–102). The chapter introducing the first family of organic compounds, alkanes and cycloalkanes, was chosen because it is one of the chapters taught in the first semester of a year-long organic chemistry course. There were a total of 416 formulas (111 molecular formulas, 206 structural formulas, and 99 incomplete structural formulas) that used organic chemistry notation in the chapter. There were also a total of 40 references to atoms according to their symbol and 7 chemical equations presented in these pages. Looking at other chapters in the same text, it is clear that this chapter is not unique in its use of organic chemical notation. With hundreds of formulas per chapter in a thirty-one chapter textbook, it is easy to see how a student's reading comprehension of organic chemistry notation becomes important to understanding student learning in this subject.

In this chapter, when talking about the reading comprehension of organic chemistry notation, two different perspectives will be considered, namely, chemistry and cognitive psychology. From the chemistry perspective, the development and standardization of this unique form of notation will be discussed. From the cognitive psychology perspective, the

concept of organic chemistry notation as a form of external representation and how different forms of these representations are processed in the mind of the learner will be examined. Process models for the comprehension of sentential and diagrammatic representations will be discussed and, based on these models, a new process model for the comprehension of organic chemistry notation will be presented. In this discussion, factors affecting reading comprehension will be highlighted, including those that are inherent in the test being read (word frequency and complexity) and those that are reader specific (working memory capacity, expertise, and spatial ability).

Organic Chemistry Notation: A Chemical Perspective

History

Although chemical formulas for inorganic compounds have been published since the early 1600s, the first two-dimensional diagrammatic organic formula is credited to William Higgins in 1789 (Mason, 1943). In his article "History of the use of graphic formulas in organic chemistry", Howard Mason (1943) writes that this primitive structure's "resemblance to modern formulas is striking". Higgins used a vector diagram to show the force of "gravity" that holds smaller particles to larger particle (see Figure 6). In this diagram the smaller particles (a-e) are attracted to particle P with a given force of 3 3/5 (no units).

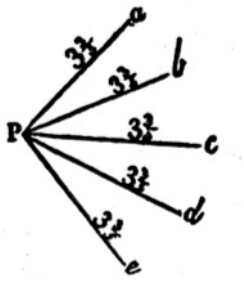


Figure 6. Higgins vector diagram of atomic structure (Mason, 1943).

Over the next forty years, Mason (1943) argues, that developments in the understanding of how atoms combine to form compounds (Dalton, 2009; Thomson, 1804) and the number of bonds each elements can form (Frankland, 1852) sparked a revolution in how chemists viewed organic molecules. This in turn triggered the development of a wide array of different organic chemistry notations. Some examples of the different types of representation follow.

Couper (1858) and Kekulé (1857, 1858) independently proposed the first modern organic chemical structures, centered on two ideas: 1) carbon forms four bonds and 2) carbon can bond to itself. Both works used a unique chemical notation to describe organic molecules. Couper developed a system of alphanumeric characters, dotted lines, and dashes to express the structure of organic compounds (see Figure 7). Couper drew the structure of ethanol, which today has the accepted formula of C_2H_6O ($CH_3– CH_2 – OH$) and oxalic acid, $C_2H_2O_4$.

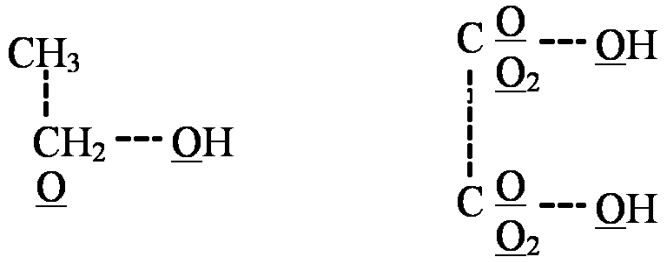


Figure 7. Structures for ethanol and oxalic acid (Couper, 1858).

Kekulé created a system called "sausage formulas" that neither expressed the size or position in space of a given atom (Figure 8). A six member cyclic system was represented by a linear arrangement of six atoms (circles) held together by some affinity (represented by the length of the oval, or "sausage") between atoms (Meinel, 2004). Kekulé chose to note the strength of attraction between the atoms but no bonds are expressly drawn in this representation.

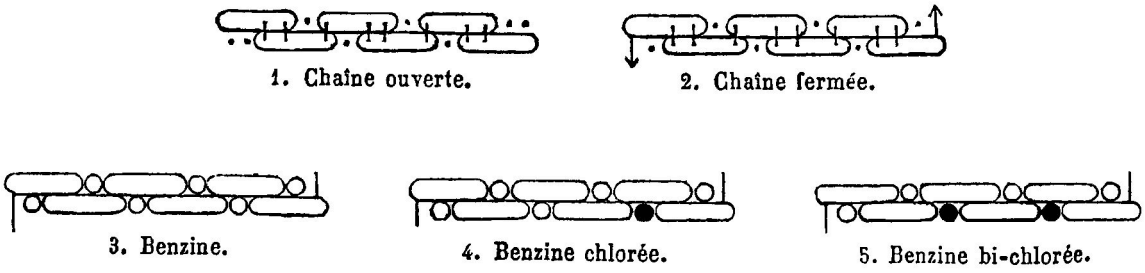


Figure 8. Sausage structures proposed by Kekulé (1857).

Emil Erlenmeyer and Alexander Crum Brown further expanded Kekulé ideas by proposing the carbon-carbon triple bond in acetylene and the carbon-carbon double bond in ethylene, respectively (Leicester, 1971). Brown (1864) used a series of circles connected by

straight lines to represent atoms and bonds in his published work (Figure 9). The relative position of atoms and the bond arrangement connecting the atoms were detailed in the structure. This notation is very similar to the notation in use today.

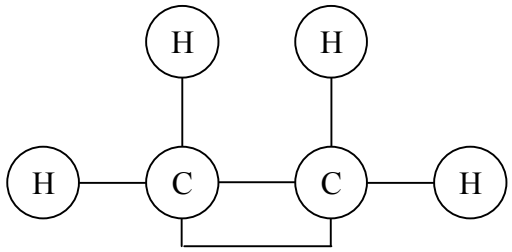


Figure 9. Structure of ethene ($H_2C = CH_2$) proposed by Brown (1864).

In 1865, Kekulé made another major contribution to chemical notation by proposing that a carbon chain can double-back on itself to form a ring. He proposed the structure for a ring containing six carbons and six hydrogens, which today we know as benzene (Figure 10). In this figure, six carbons are depicted as gray circles labeled "C". Lines depict bonds. Note that there are two bonds between the two carbon atoms at the top of the ring, the two atoms on the lower right and the two atoms on the lower left. Although hydrogens are not explicitly drawn, it is understood that they are attached to each carbon on the lines pointing away from the ring.

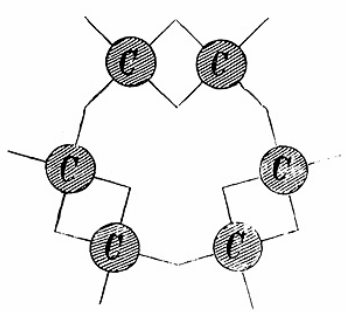


Figure 10. Structure of benzene proposed by Kekule (1867).

In 1874, organic chemists Jacobus van't Hoff and Joseph Le Bel proposed the arrangement of carbon's four bonds evenly distributed in three-dimensional space (Leicester, 1971). This was the first time that the three dimensional nature of organic molecules was depicted (see Figure 11). In this figure, the center of each pyramidal shape is a carbon. The type of carbon-carbon bond is indicated by how the two pyramidal shapes meet. The pyramidal shapes in Figure 11 meet at the tip. This indicates the carbon – carbon bond is a single bond in tartaric acid molecule shown.

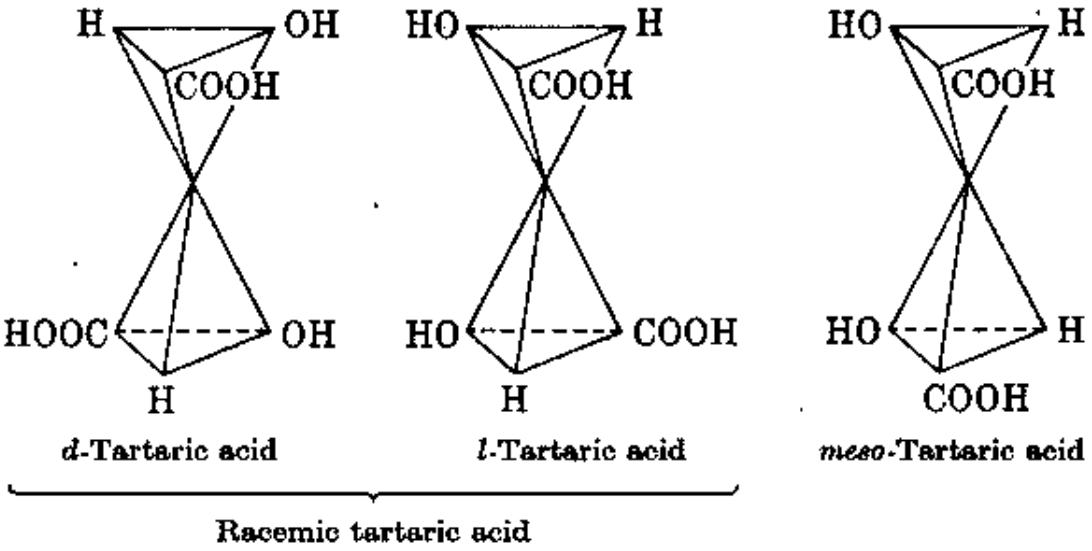


Figure 11. Structures of tartaric acid proposed by van't Hoff and Bel (1874).

Figures 6 - 11 represent some of the major advances in organic chemistry during this time period; however, they also are a good representation of the variability of chemical notation that existed in the chemistry literature during this time period. These very different approaches to illustrating chemical composition led chemists of the time to call for a standardization of notation and nomenclature. In 1882, *Nomenclature and Notation* was published by the English Chemical Society to provide guidelines for a systematic approach to chemical notation and naming, which was followed by the American Chemical Society establishing a Committee of Nomenclature and Notation in 1886 (Breneman, Moore, Leeds, Stebbins, & Rupp, 1886). Finally, in 1919, the International Union of Pure and Applied Chemistry (IUPAC) was founded. Among other accomplishments, IUPAC standardized the naming of organic compounds using a system that is still in use today. In addition, IUPAC created a system by which every compound discovered has a unique name from which a

single correct structure can be drawn. It is this idea of a one-to-one-to-one relationship between a chemical substance, the chemical's name, and the chemical's structure that is crucial to the research presented here.

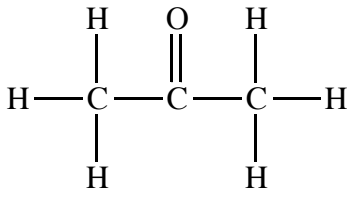
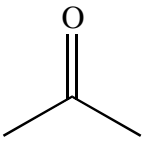
Current Notation

Like its previous forms of notation used throughout the history of organic chemistry, the modern symbolic notation accounts for our current understanding of carbon and how it bonds to other elements. It also includes the insight we have gained from analytical techniques that reveal features of the submicroscopic structures of organic compounds.

The modern standard notation has four distinct forms that are used to write the formula of an organic compound, namely: molecular, condensed, expanded, and the bond-line (also called the geometric) formula (Table 6).

Table 6

Four Forms of Organic Chemistry Notation for 2-propanone

Type of formula	Example
Molecular formula	C_3H_6O
Expanded formula	
Condensed formula	$CH_3 – CO – CH_3$ or CH_3COCH_3
Bond-line formula	

Before discussing the features that differentiate each type of formula, it is important to discuss the features that are common to all forms. The four examples given in Table 6 all contain a compound with three carbon atoms, eight hydrogen atoms, and one oxygen atom. In its own way, each formula also represents the idea that carbon can form only four bonds with itself or other elements. The use of letter symbols to represent some or all of the elements in the formula is also common to all of these representations.

The major difference among the formulas given in Table 6 is how explicitly each formula shows the arrangement of atoms in a molecule of 2-propanone. The first formula, called the *molecular formula*, is the least explicit. It provides the smallest ratio of elements in a single molecule of a compound but does not show how the elements are bonded together. This ratio is fixed for all molecules of 2-propanone and is dependent on the fact

that carbon is tetravalent, forming four bonds. The most explicit formula is the *expanded formula*, which shows the arrangement of every bond in the molecule. Here, bonds are depicted as lines connecting the symbols of every element in the molecule. For every carbon, there are four lines radiating out, depicting the idea that carbon always forms four bonds. The *condensed* and *line formulas* are often referred to as "short-hand" forms of notation and are the major notation formats used in textbooks and journals. In the *condensed formula,* elements bonded to a carbon are grouped together and written as one unit. The lines representing the bonds between carbons are optional. The *bond-line* formula is the least explicit form of notation. When two or more lines intersect or a line terminates without a connecting element, the notation implies that there is a carbon atom. Attached to each of the implied carbon atoms are implied hydrogens, enough to satisfy the need for four bonds to each carbon. Reading and understanding this form of notation requires prior experience with organic chemistry and its notation. It is important to note that these notation are not used exclusively, but are sometimes combined to create a structural formula like Figure 12. In the formula for 2,3-dimethylpentane, the condensed formula is used for all the terminal carbons, CH_3. The other carbons in the molecule are drawn using the bond-line formula.

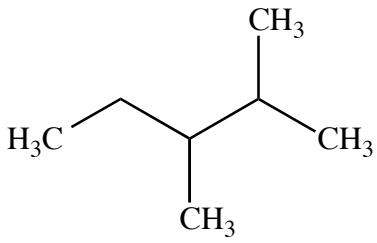


Figure 12. Combined Formula for 2,3-dimethylpentane.

Combination formulas, like Figure 12, are often used to remove ambiguity in structures or to illustrate a specific relationship. This research will focus on the notation most commonly used in organic chemistry literature and textbooks – condensed formula, bond-line formula, and the combination of these two formulas.

There are situations when the three-dimensional nature of a molecule becomes important in describing its chemistry. In these instances, organic chemists will use additional notation to illustrate three-dimensional relationships (Figure 13).

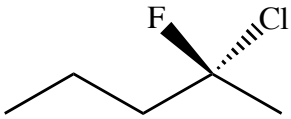


Figure 13. Bond-line formula for 2-chloro-2-fluoropentane.

In this bond-line formula, the wedge connecting fluorine (F) to the carbon chain is used to illustrate that the bond is coming out of the plane of the paper towards the reader. The broken wedge connecting chlorine (Cl) and the carbon chain shows that the bond is going out of the plane of the paper away from the reader.

The wedge and broken wedge notation is most commonly used to illustrate three-dimensional relationships in bond-line formulas (e.g., Figure 13) and expanded formula. In

cases where the three-dimensional relationships are not central to the chemistry of the molecule, formulas are written using the two dimensional format.

Once a style of notation is chosen, formulas for organic compounds can be used to provide a written description of how a compound is transformed during a chemical reaction. This description is called a chemical equation. Chemical equations in organic chemistry follow a specific format. Figure 14 is an example of a chemical equation where the structures are written using expanded formula notation.

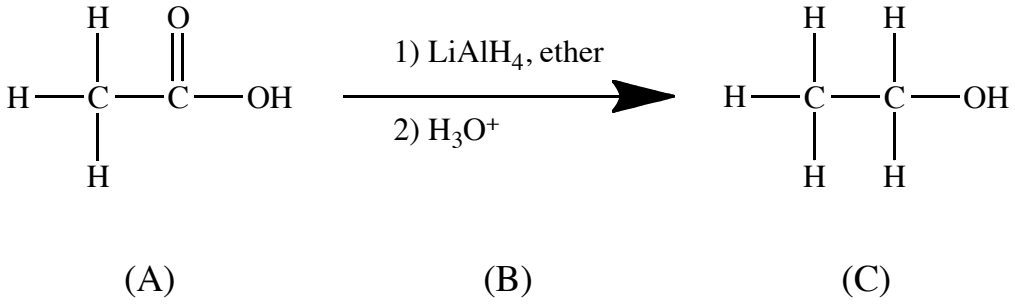


Figure 14. Reduction of acetic acid (A) to produce ethanol (C).

By convention, the reaction equation given in Figure 14 is read from left to right. The compound on the left (A) is called the reactant, the compound on the right (C) is called the product, and the words above and below the arrow (B) are called the conditions. In this chemical equation, the reactant is acetic acid and the product is ethanol. For acetic acid to be transformed into ethanol, the reactant is exposed to two separate conditions - lithium aluminum hydride in ether [(1) $LiAlH_4$, ether] followed by the addition of aqueous acid [(2) H_3O^+]. The chemical equation can be read as a sentence: "acetic acid is reacted with lithium aluminum hydroxide in ether, followed by aqueous acid, to produce ethanol." Understanding

how students read and comprehend chemical equations such as this one is one of the goals of this research.

From a chemical standpoint, organic chemistry notation not only conveys the structure of organic compounds, but also can be used to show how organic compounds are transformed through chemical reactions. These transformations are detailed in written chemical equations that follow a specific format. Those with the prerequisite knowledge of organic chemistry can decipher the formulas into words and translate chemical equations into sentences. In order to understand how the formulas are deciphered and the chemical equation translated into a sentence, it is important to look at the comprehension of organic notation from a cognitive psychology perspective.

Organic Chemistry Notation: A Cognitive Psychology Perspective

External Representations

All figures presented in this chapter are considered *external representations*. According to Zhang (1997), an external representation provides a physical configuration of "symbols, objects, or dimensions (e.g., written symbols, beads of abacuses, dimensions of a graph, etc.)" (p. 179) that contains relationships which can be processed by the reader. These relationships include spatial arrangements, layouts, and sizes. Organic chemists use organic chemistry notation to: 1) describe the structure of molecules and 2) define the relationships that exist between atoms in a molecule and among molecules in a chemical reaction. As we have seen, the notation uses a uniquely written symbolic representation consisting of alphanumeric characters, Greek symbols, lines, and/or geometric shapes to

convey the structure of organic compounds. By combining structures and reaction symbols, chemists propose how substances undergo change in the environment by writing reaction equations. The entire chemical equation can be "read" by interpreting the relationships among the symbols in the chemical equation, including the plus sign ("reacts with" or "and") and the arrow ("to produce"). (Figure 15).

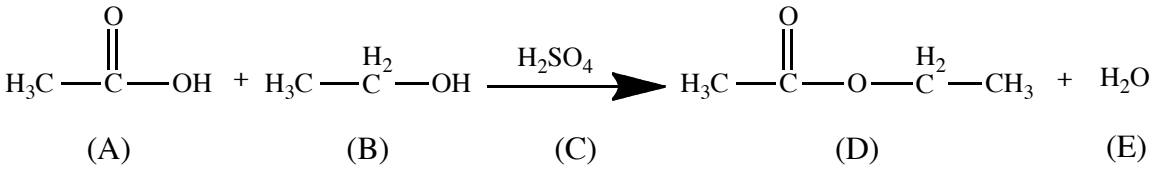


Figure 15. Esterification of acetic acid.

Figure 15 can be interpreted as follows: acetic acid (A) reacts with ethanol (B) in the presence of the acid catalyst H_2SO_4 (C) to produce methyl ethyl acetate (D) and water (E).

Each molecule in this reaction equation has a unique name from which a single correct structure can be drawn using organic chemical notation. To understand how to translate the chemical equation given in Figure 15 into a sentence, we need to look at how different types of external representations are processed.

Types of External Representations

Larkin and Simon (1987) divide all external representations into two categories: *sentential* representations and *diagrammatic* representations. *Sentential* representations are defined as the written form of a "natural language sentence" and share a one-to-one relationship between elements of the spoken (natural) form of the language and the written expression (Larkin & Simon, 1987, p. 66). *Diagrammatic* representations are two-

dimensional representations of the environment where there also exists a one-to-one relationship between elements in the environment and elements in the diagram. These relationships are preserved through the spatial arrangement of points and elements in the diagram. By analyzing block and pulley problems from physics and theorem proofs from geometry, Larkin and Simon developed theoretical models that compare the processing of sentential and diagrammatic representations of the same problem. The key distinction that Larkin and Simon make about these two types of representations is that while diagrammatic representation preserves location, "topical, and geometric relations", sentential representation preserve linear and temporal relationships. Larkin and Simon are quick to point out that diagrams are explicit, making the search for information more efficient, while relationships in sentential representations are implicit, making the search process more difficult.

The property that Larkin and Simon (1987) use to distinguish sentential representations from diagrammatic representations is the way in which the data is structured. In sentential representations, "elements appear in a single sequence" (p. 68). A given word is adjacent only to the next word in the sentence. Relationships are defined by an element's position in the sequence. In diagrammatic representations, a given "element may be 'adjacent' to any number of other elements (Larkin & Simon, 1987, p. 98)." Information is stored as a location in two-dimensional space rather than sequentially, and relationships are give by proximity in space.

Shimojima (2001) argues that these definitions of sentential and diagrammatic representations are flawed and points to linear diagrams as counterexamples. In the example cited, Shimojima has the reader consider a seating chart with a linear arrangement of chairs. If letters are used to represent names of people sitting in the chairs, we can create a seating chart: L S _ B X (where "L" is Lydia, "S" is Samantha, "B" is Bill, "_" is an empty seat, and "X "may or may not be an empty seat). According to the Larkin and Simon definition, the seating chart would be considered a sentential representation. However, since it is a linear arrangement of symbols that does not have grammatical or semantic relationships, "there seems no reason not to call this a diagrammatic, [or] graphical, representation (2001, p. 317)."

According to Shimojima, what separates diagrammatic representations from sentential is geometric or physical relationships, or *nomic constraints*. In his interpretation, graphical representations are governed by nomic constraints, which involve geometric or physical relationships that exist in the real world. Diagrammatic representations illustrate relationships between objects, as they exist in the real world. Sentential representations are governed by orthography and grammar rules. Therefore, relationships in sentential representation are more implicit and based on the rules of natural language. It is this difference between the explicit nature of the relationships in a diagram and the implicit relationships in a sentence that may account for the proverb "a picture is worth a thousand words".

While the difference between a diagrammatic representation (picture, image, diagram, map, etc) and a sentential representation (symbol, word, phrase, sentence, paragraph, etc) seem obvious, some would argue that the distinction is not clear. Consider the premise that diagrammatic representations preserve spatial information (geometric or physical relationships) while sentential representations preserve sequential and temporal information governed by the rules of natural language. Consider a math equation 2 + 2 = 4. It has both sentential characteristics and diagrammatic characteristics (Cheng et al., 2001). There is a sequence to the given equation that is governed by rules for the use of the equals (=) and plus (+) signs. This equation could also be considered a diagram, showing the spatial arrangements of the graphical elements (e.g., "2", "+", "=") in the equation. Another example is the diagram given in Figure 16.

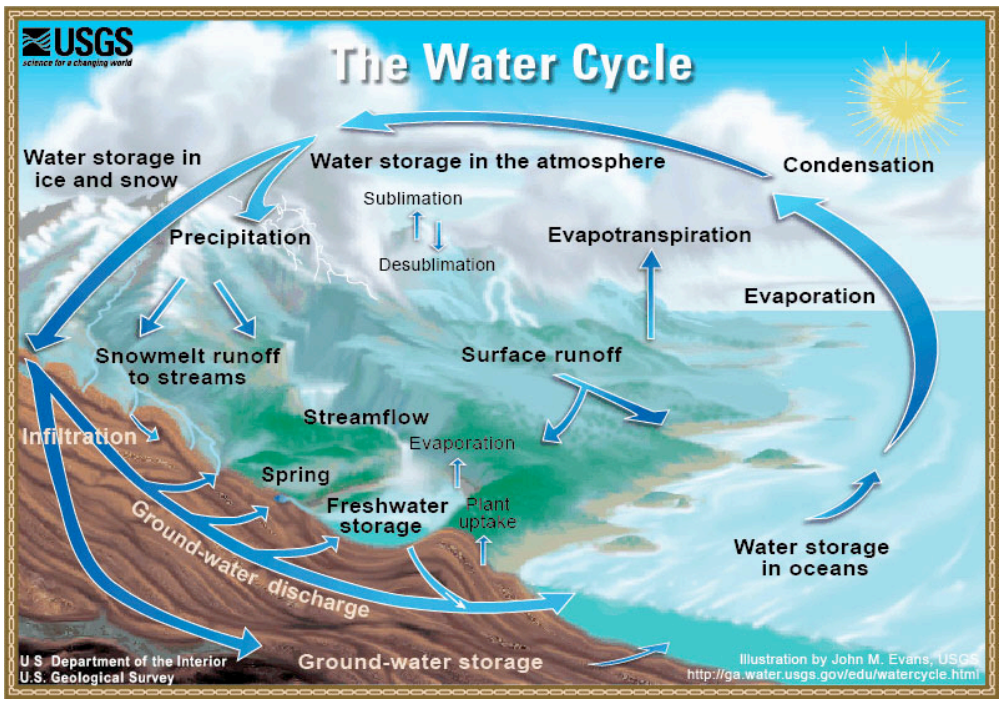


Figure 16. The water cycle. Evans, L. M. The water cycle. Retrieved October 20, 2009 from U.S. Department of the Interior | U.S. Geological Survey website: http://ga.water.usgs.gov/edu/watercycle.html.

Although most would classify this representation as a diagram, it clearly uses words and phrases from the English language to express how water changes states and cycles from the atmosphere to the land to the bodies of water and back to the atmosphere. Using the arrows, the words and phrases can be sequenced and translated into sentences, implying that this diagram also has sentential features characterizing the sequential relationship among elements in the diagram. Examples such as these lead the Cheng and his colleagues (2001) to caution against the use of the diagrammatic-sentential representation dichotomy.

Organic chemistry notation is in the continuum between purely diagrammatic and purely sentential representations. It has features of both a diagrammatic and sentential representation. Consider the following reaction (Figure 17).

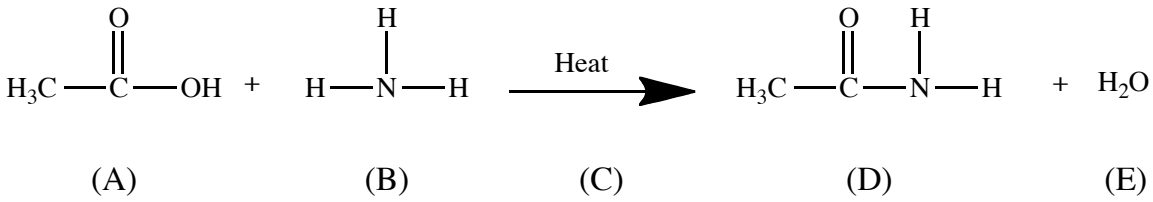


Figure 17. Amide formation

In molecule A, acetic acid, the structure shows a carbon with three hydrogens attached to an adjacent carbon that has a double bond to oxygen (O) and a single bond to a hydroxyl group (-OH). The relationships between the atoms in acetic acid are explicit, showing a spatial or geometric relationship among all the elements within molecule A. When we look at the relationship of one molecule to another in the equation and consider the reaction as a whole, the equation can be considered a sentential representation. According to Larkin and Simon, this representation has a sequential relationship among the molecules in the equation. The equation can be read as: acetic acid (A) reacts with ammonia (B) when heated (C) to produce ethanamide (D) and water (E). Many relationships that are important for the reaction to take place are not defined by the equation as written. These include the reason for the reaction to be heated and the orientation of the molecules to one another during the reaction. It is up to the reader to search the chemical equation for clues to these implied relationships.

According to Shimojima's work, in order for this representation to be considered sentential, the relationships between elements need to be governed by rules of orthography and grammar. Jacob (2001) argues that a reaction equation is governed by "chemical grammar" that includes the use of symbols such as the plus sign (+) and the single-headed arrow (→). Some of the rules used to write the equation above include the following: 1) the reactants are to the left of the arrow; 2) conditions are written on top of the arrow; 3) the products are written to the right of the arrow so that the arrow head points towards the products; 4) the smallest ratio of A to B to D to E is used to write the reaction equation; and 5) the order of the molecules on the reactant side and on the product side of the equation does not correspond to the order in which the reactants are consumed or products formed in the real world. The condensed formulas for A, B, D, and E above translate into real chemicals, but how these real chemicals interact with one another is only implied by the chemical equation. Information such as orientation of the molecules in space, interactions between molecules, and reaction rate are also implied by the chemical equation. The only relationships explicitly expressed in the chemical equation are those governed by the chemical grammar used to write the equation. Once the rules for the chemical grammar are known, the relationships among the molecules in the given chemical equation are interpretable, and the reader learns how to create a desired product using specified starting materials and reaction conditions.

It has been argued that chemical equations have characteristics of both sentential and diagrammatic representations. Condensed and bond-line formulas preserve the geometric

and spatial arrangement of atoms in the molecules involved in the reaction, while the "chemical grammar' of the chemical equation provides the sequential representation of the chemical reaction. Since chemical equations have the characteristics both of a sentential representation and a diagrammatic representation, understanding how this notation is read and comprehended by the reader requires an investigation of how both types of representations are processed and the factors that affect comprehension. From a study of the process models for both sentential and diagrammatic representations, a new process model will be proposed for the reading comprehension of organic chemistry notation.

Process Models

To understand how sentential and diagrammatic representations are understood, researchers have developed process models that rely on human information processing to explain how external representations are processed stepwise into meaning. To better understand what a process model is, Samuels and Kamil (1984) suggest a parallel example from manufacturing. In a factory, raw materials are transformed into finished products through a series of discrete steps. Schematic drawings are developed to show explicitly how this transformation takes place, including, when and where raw materials enter the manufacturing process, how machines transform materials, how materials are stored during various phases of manufacturing, and what form the final product will take.

Human information processing can be likened to this manufacturing process. Consider the processes involved in reading this sentence. We can write a schematic where an external sentential representation, the raw material of the reading process, is transformed

into the final product, reading comprehension. In this analogy, the machines that carry out the transformation are the eyes and the brain. The storage facilities are long-term memory and working memory. Information processing theorists show the movement of data through this system using flow diagrams.

According to Samuels and Kamil, there are three characteristics that make a good process model: 1) the model accounts for the past, 2) it explains the present, and 3) it can predict the future (Samuels & Kamil, 1984, pp. 191–192). Key to this idea is that the model allows us to formulate hypotheses about the process that can be tested.

The process for the reading comprehension of organic notation is based on what is known about human information processing. This newly proposed model relies on the small body of literature on problem solving and students' understanding of organic chemistry problems; explains the eye movements of students as they read chemical equations; and predicts how changes to the notation used in chemical equations will affect reading comprehension. Since chemical equations share features of both sentential and diagrammatic representations, the proposed model acknowledges how both types of representations are processed.

Sentential Representations

According to our understanding of reading comprehension, sentential representations, like the ones on this page, are processed as the eye scans over the sentences. Since chemical equations share characteristics of sentential representations, a process model for comprehension of organic chemistry notation must share characteristics with process

models for reading comprehension. Several process models for reading comprehension have been published (for examples, see: Gough, 1984; Just & Carpenter, 1980; Rumelhart, 1977; Stanovich, 1980). These attempts to explain reading comprehension all focus on two key elements, namely, how information is processed and how this information is represented in the mind of the reader. One such model is Just and Carpenter's (1980) process model of reading comprehension. In this work, Just and Carpenter use eye-movement data from college-age readers to develop a model for reading comprehension.

Process Model for Reading Comprehension

In order to translate eye movements into a process model of a complex task like reading, Just and Carpenter make two assumptions. The first assumption is the *immediacy assumption* (Just & Carpenter, 1980) that says that the reader attempts to interpret each word as he/she encounters it. These interpretations are made immediately and prior to when the reader moves on to the next word. The second assumption is the *eye-mind assumption*. According to this assumption, as long as the word is being processed, the eye remains fixated on it and that fixation time is a direct measure of processing time (Carpenter & Just, 1977; Just & Carpenter, 1976). The typical eye fixation is between 200 and 300 ms (Rayner, 1998), which is directly related to the time it takes to extract, encode, and process the information (Goldberg & Kotval, 1999; Just & Carpenter, 1976). It is these assumptions that are key to Just and Carpenter using eye fixation data to develop a model that accounts for the entire reading process, from the moment when the reader's eyes encounter a written passage to the final comprehension of the text (Figure 18).

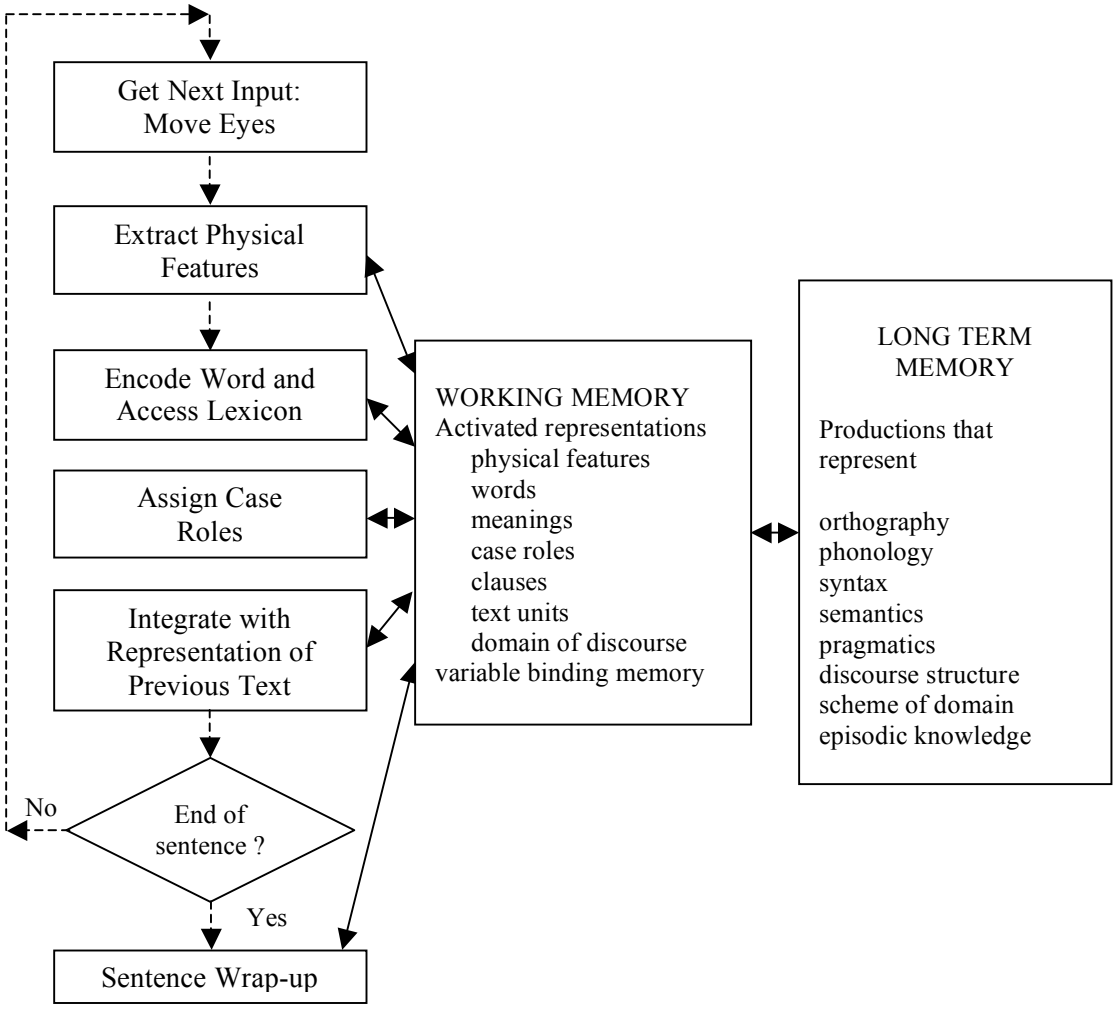


Figure 18. Schematic for Just and Carpenter's (1980) model of reading comprehension. Reprint from Psychological Review, 87/4, M.A. Just & P.A. Carpenter, A theory of reading: From eye fixations to comprehension, 329-354, 1980, reprinted with permission from APA (publisher).

The schematic given in Figure 18 is divided into three columns. In the leftmost column are the processes that occur during reading, the center column is working memory, and the rightmost column is long-term memory. The following section begins with a discussion of memory structures (long term memory and working memory) that support

reading comprehension followed by a discussion of each process in the reading comprehension model.

Long-term memory. Long-term memory (LTM) is what most people think of when they are talking about "memory". It is the relatively permanent storage of information that can last for days or even decades. The process model proposed by Just and Carpenter (1980) assumes that the comprehension process involves the interaction of representations from long term memory (LTM) to working memory (WM), as illustrated by the arrow connected LTM and WM. The representations stored in LTM include the meaning of words, rules grammar and syntax, information on the context of the written passage, memories of personally experienced events (episodic knowledge), and processes related to reading comprehension. One specific theory of human cognition, the ACT theory (Anderson et al., 2004), distinguishes two types of knowledge stored in LTM, namely procedural knowledge (knowledge of how perform a task) and declarative knowledge (explicit knowledge of facts).

Procedural knowledge encodes the skills and processes needed to achieve a certain goal in the form of productions. Productions are sets of condition-action pairs (if-then statements). Conditions ("if") are specified by the goal of the task and may require the retrieval of declarative information. The action ("then") can perform a variety of tasks, including altering declarative knowledge, changing the goal, initiating motor response to the environment, or changing the contents of working memory. A production will fire when the condition(s) of the if-then statement are satisfied, carrying out a specific action.

Declarative knowledge, such as water is made of two hydrogen atoms and one oxygen atom, is represented as "chunks" (Anderson et al., 2004). Chunks encode very small, independent patterns of information using a slot structure (Anderson & Lebiere, 1998). Each chunk contains a "type" and some number of "slots" that encode the contents of the chunk. The "type" is a general categorization of the chunk (e.g., a class of compounds, a chemical principle, etc.), and each "slot" contains an attribute of the chunk (e.g., color, size, smell, etc.) (Anderson et al., 2004; Daily, Lovett, & Reder, 2001). Consider the following chunk: "the child threw the ball". In this example, the type of chunk is "threw". There are two slots that encode the contents of the chunk, the agent of threw (ball) and the object of the action (child). In this example, a limited amount of information is encoded. The number of slots for the given type of chunk limits the amount of information encoded. Each slot is filled with units from declarative or procedural knowledge that have a unique role in characterizing the encoded information (e.g., child and ball). The information in the slots contains links to other chunks (chunks for child and ball), creating hierarchical structures, where a given chunk may fill a slot of other chunks. This creates interconnectedness or "schema-like" structures where there are associations among chucks stored in LTM (Daily et al., 2001).

How these chunks are retrieved is controlled by *chunk activation*, a measure of "both the probability and the speed of access to memory" (Anderson, 2005, p. 183). This quantity reflects how relevant a chunk is to the current context; how recently a chunk has been accessed in the past; and how often a chuck is used. Base-level activation, the starting

activation for a chunk, is based on the recency and frequency of access. For example, words that are frequently encountered have higher base-level activation than words that are encountered less frequently. If a low frequency word is re-encountered, its base level of activation increases. Chunk activation is the sum of a base-level activation (starting activation for a chunk) and the spreading activation (association between the current context and the chunk) across all the slots in the chunk. This activation plays a key role in the retrieval of information. "A chunk can only be retrieved if the activation is greater than a fixed retrieval threshold" (Budiu & Anderson, 2004). Once activation reaches this threshold, the chunk can be retrieved into working memory.

Working memory. Central to the Just and Carpenter model of reading comprehension is working memory. Working memory is a brain system, consisting of processes and structures that temporarily maintain task-relevant information to support the manipulation of information needed to complete complex cognitive tasks (Baddeley & Hitch, 1974; Daneman & Carpenter, 1980). Working memory can be considered the "work space" where individuals process information. It is a system that acts as an interface between perception, long-term memory and action (Baddeley, 2003a). In this process model, working memory is described as a limited capacity system that acts as storage for the following: information encoded from processing the text (left column); the intermediate and final products resulting from computations made by the reader; and representations retrieved from long term memory (right column) (Just & Carpenter, 1980, 1992). At the core of Just and Carpenter's process model is a production system, which acts on the information held in

working memory. When specific information from working memory is recognized, a condition is met, and a production rule fires. The production performs an operation on that information, and the resulting new information is inserted into working memory. Then a new cycle begins, where productions assess the contents of working memory. If a condition is met, a production fires and the contents of working memory change again. For each stage proposed by this model, there are specific productions that are responsible for the processing.

Baddeley and Hitch (1974) proposed a Model of Working Memory which is a three-component system that included the *central executive* (attention control) and two specialized subsystems namely, the *phonological loop* (dealing with verbal and acoustic information) and the *visuospatial sketchpad* (dealing with visual information). In 2000, Baddeley incorporated a third subsystem into this model of working memory, namely, the episodic buffer. The role of this new subsystem is to bind "together information from a number of different sources into chunks or episodes, hence the term 'episodic'" (Baddeley, 2000, 2003b). In this model (Figure 19), the central executive acts as a control system, managing the movement of information to and from the subsystems. To do this, it acts as an *attentional control system* with the capacity to focus available attention, divide attention among the subsystems, and, to a lesser degree, switch attention (Baddeley, 2007). This view of the central executive as an attentional control system is similar to the Norman and Shallice's (1980) Supervisory Attentional System (SAS).

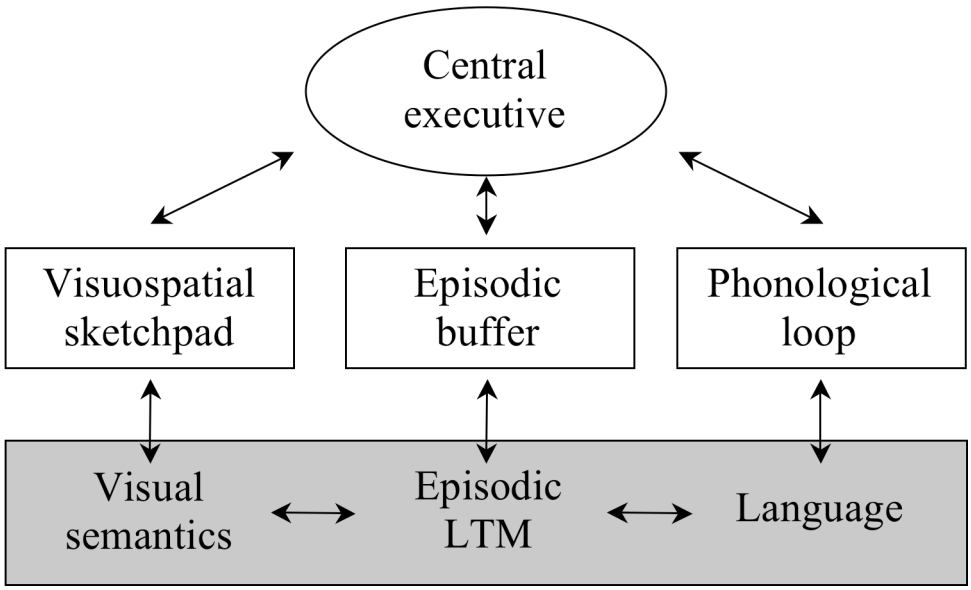


Figure 19. Working memory model (Baddeley, 2000). Reprint from *Trends in Cognitive Sciences*, 4/11, Alan Baddeley, The episodic buffer: a new component of working memory? 421, 2000, with permission from Elsevier.

Processes. The processes of reading comprehension are located in the leftmost column of Just and Carpenter's process model for reading comprehension (Figure 18*)*. When a student is presented with a passage to read, his/her eyes fixate on the first word. Finding the first fixation and subsequent fixations is the *get next input* stage. Once the word has been completely processed, the eye moves to a new fixation. For texts in English, the next fixation is one or two words to the right of the previous fixation. Once the student gets to the end of a line in the text, his/her eyes will sweep to the next line and to a new fixation. Then processing starts with the *extract physical features* stage. Here the physical shape of the letters and words are encoded. During the *word encoding and lexical access* stage, visual features of the words fire productions that activate a mental representation of the

word in working memory. Other productions fire that access information from long-term memory associated with this mental representation. Underlying concepts are activated, creating a representation from various resources and giving a more precise meaning to the word. This stage is best illustrated if we consider a student reading a passage where he/she encounters a word that repeats in the text. The total time that he/she fixates on a word decreases with each new encounter (Rayner, Raney, & Pollatsek, 1995). Once a word has been activated in long-term memory, it is expected to take less time to reactivate it in subsequent encounters.

The next two stages, *assigning case roles* and *interclause integration* deal with the relationship between words and phrases. Once a representation is activated in the student's working memory, relationships between words need to be assigned. These relationships include "agent, recipient, location, time, manner, instrument, or state" (Just & Carpenter, 1980, p. 341). This is the *assigning case roles* stage. As a student reads a passage, he/she will assign semantic roles to the words that have already been encountered. Specific patterns of gazes can be identified for words that are related, and different gaze times are reported for different semantic cases (e.g. verb, adverb/manner, place/time, and agent/instrument). *Interclause integration* identifies the relationships between new phrases or sentences and those that already exist in working memory. During this phase of the reading process, new words and phrases are compared with the current representation of the passage. New information is either added to the current mental representation or the new information replaces old information that needs updating. During this stage, the student's

gaze duration and frequency depends largely on the number of concepts that need to be integrated and the complexity of the relationships in the passage. These gazes are not localized to a particular word, but rather to a specific region of the text.

The final stage in the reading process is the *sentence wrap-up*. Here, the student attempts to resolve inconsistencies within the sentence and integrates the new information with existing knowledge in long-term memory. This is also the time when the reader evaluates a thought or idea that occurs at the end of a sentence. This integration is characterized a pause at the end of a sentence and recorded as longer fixation times on punctuation marks.

All of the stages, except *get next input*, are illustrated with arrows connecting them to working memory in Figure 18. Working memory is shown connected to long-term memory. These connecting arrows represent the flow of information between the stages of reading and the human memory. All of the procedural and declarative knowledge needed for the reading process is stored in long-term memory, including word and sentence structure, pronunciation, grammar, schemas for particular concepts, and propositions. When productions fire, key information located in long-term memory is activated in working memory and becomes available to enrich current representations or provide for the manipulation of the mental representations held there (Daneman & Carpenter, 1980; Just & Carpenter, 1980, 1992). This dual role of working memory in reading comprehension has been supported in the literature (Daneman & Carpenter, 1980; Daneman & Merikle, 1996; Masson & Miller, 1983). By using this idea of working memory and its role as a mediator

between long-term memory and the stages of reading, Just and Carpenter have created a model for reading comprehension that accounts for the processes that occur from the time a person's eyes meet the paper to the final comprehension of a written passage.

Since organic chemistry notation of chemical equations shares many features of sentential representation, a process model for the comprehension of organic chemistry notation will share many features with that of reading comprehension. The Just and Carpenter model of reading comprehension details the process of reading, starting with the eye fixating on a word (*get next input*). The reader encodes the word and its meaning by using prior knowledge from long-term memory (*extract physical features* and *encode word and access lexicon*). Then he/she determines the relationship between the word and the rest of the text (*assign case roles* and *interclause integration*). Finally, the reader has a chance to resolve any inconsistencies with his/her understanding of the text and integrate this new knowledge with what is already known (*sentence wrap-up*).

By adapting the Just and Carpenter model of reading comprehension to account for the unique features of organic chemistry notation (including those that are related to the diagrammatic qualities of the notation), a new process model for the comprehension of organic chemistry notation is proposed. The focus of this research project is the validation of this model, which will employ eye-tracking methodology (to be discussed in Chapter 3).

Process Model for the Comprehension of Organic Chemistry Notation

Adapted from the process model for reading comprehension proposed by Just and Carpenter (1980) and drawing on the research in problem solving in organic chemistry, a

new process model for the comprehension of organic chemistry notation has been developed (*Figure 20*).

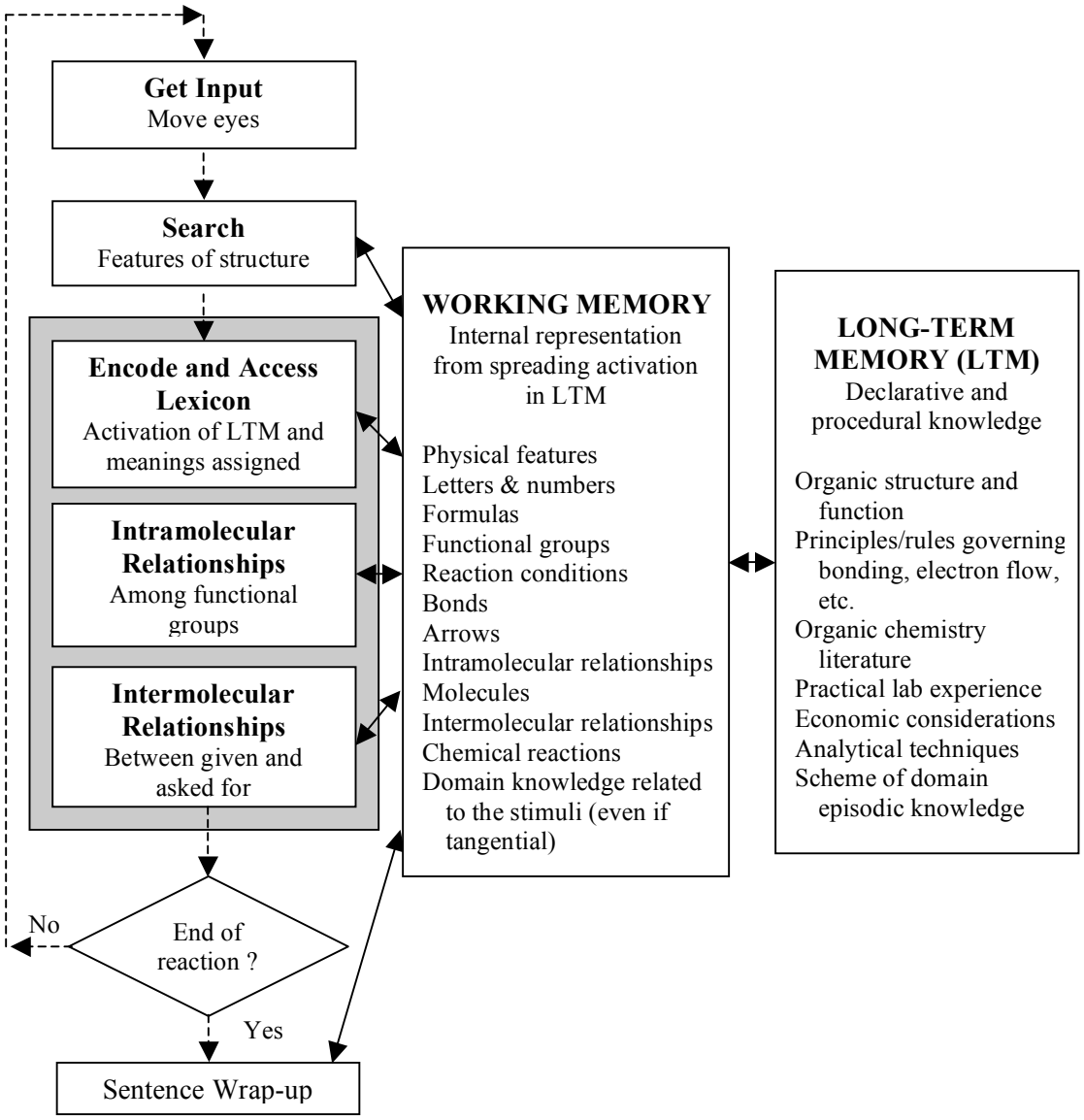


Figure 20. Schematic of the model for the comprehension of organic chemistry notation based on Just and Carpenter (1980) model of reading comprehension.

The resulting model shares a similar structure with the Just and Carpenter model, relying on working memory as the mediator between the processes of reading and long-term memory.

Long term memory (LTM). As in Just and Carpenter's model (1980), LTM encodes both procedural and declarative knowledge. The representations stored in LTM of this model are related to chemical principles and theories, practical lab experiences, analytical techniques related to the identification and separation of organic compounds, and organic chemistry notation (Bowen, 1990).

Working memory (WM). Mediating these stages in the proposed model is working memory. Here, working memory still performs the same dual role of storage and processing as in the reading comprehension model. Now, instead of representations based on syntactic and semantic relationships, the mental representations held in working memory are based on chemical theory and principles.

Processes. Like the six stages in the model proposed by Just and Carpenter, the model for the comprehension of organic chemistry notation also has six major stages.

The *get input* stage is the first stage in this model. Like the model for reading comprehension, the *get input* stage governs the movement of the eyes over the chemical equation. The reader's eyes fixate on a feature of a molecule. Once the processing from later stages is complete, the eye moves to a new region of the molecule. Overall, the progression of eye movements will start with the left most reactant, then move to any subsequent reactants, the arrow, the condition, and finally end at the product.

The *intramolecular search* stage does not have a parallel in the model of Just and Carpenter. This stage will attempt to explain how reading progresses within a given molecule. Consider how we read a given word. The sequence of letters in the word "dog" is read D – O - G. For the reader, this word may create a mental representation of a furry, domesticated mammal of the genus Canis. If the sequence of letters is read in the reverse direction, G – O – D, a different word emerges that creates an entirely different mental representation. This new mental representation may be of a deity. In organic chemistry, there is no directionality to the notation. Organic formulas can be written in a variety of orientations and still represent the same molecule (Figure 21).

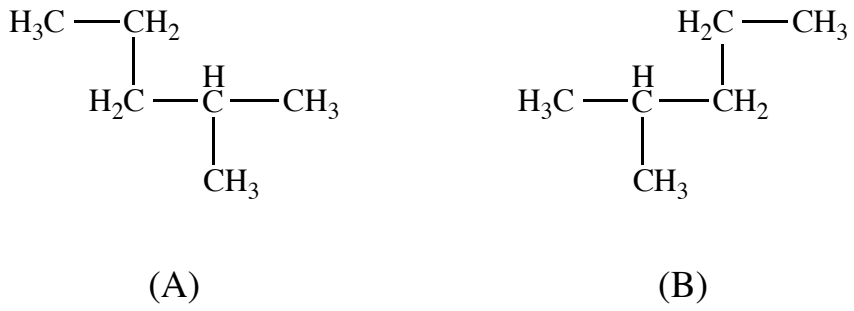


Figure 21. Structures for 2-methylpentane. Structure A is the mirror image of structure B.

To a chemist, these two molecules are identical, separated only by their orientation on the paper. Although they look very different, both A and B are condensed formulas for 2-methylpentane molecule. Without a single accepted orientation for molecules in the written notation, it is necessary to include a step in the comprehension process that systematically searches within a molecule for a particular sequence of atoms. It is hypothesized that the participant will search the chemical structure for features that are key

to understanding the chemical reaction. This includes both functional groups that can be used to aid in classifying the compound in the representation (alcohol, amine, aldehyde, etc.) and features of the site where the reaction takes place. For reactants, the overall search strategy will start left of the arrow and radiate outwards. For products, the search strategy will start closest to the head of the arrow and radiate outwards. Fixations will be on features that are key to understanding the chemical reaction.

During the *encoding and access lexicon* stage, the features of the molecule are encoded, creating a new mental representation of the molecule. During this stage, long-term memory provides other information that enriches the mental representation. There is evidence from the chemistry education literature that students access long-term memory when reading problems in organic chemistry. Using the think aloud protocol, Bowen (1990) found that students draw on a variety of information to read and solve problems, including past experience in the lab, published articles that they read in the chemistry literature, chemical principles and theory, diagrammatic representations that used chemical notation, and other written forms of organic chemistry including IUPAC names for compounds and names for specific reactions. When they read the problems, a variety of information is accessed from long-term memory that is inter-related with the synthesis task students are asked to complete. This information is not explicitly presented in the formulas provided.

Once the students have a mental representation of the molecule, they need to identify the relationships between atoms and groups of atoms in a given molecule (intramolecular relationships) and relationships between molecules in a given chemical

equation (intermolecular relationships). Relationships among features in the same molecule are determined in the *intra-molecular relationship* stage. These relationships are governed by chemical principles and theories, including relationships based on size, shape, attraction, repulsion, electron donating and withdrawing. Relationships between molecules are determined in the *intermolecular relationship* stage. These include the relationship of two molecules on the same side of the arrow (reactant-reactant and product-product); molecules on opposite sides of the arrow (reactant-product); and reaction conditions with all the molecules in the equation (reaction condition-reactant and reaction condition-product). During this stage an individual may compare similarities and differences between two molecules or mentally rotate molecules to more favorable orientations (Stieff, 2007).

The last stage, *reaction wrap-up*, is parallel with the *sentence wrap-up* stage in the Just and Carpenter model. In this stage the student attempts to clear up any confusion in his/her understanding of the chemical equation and integrate the chemical reaction with prior knowledge. The student also checks for reproduction errors, including the addition or subtraction of a functional group. This is a time to account for any element of the equation that was not assigned a role in the reaction and process any inconsistencies that cannot be resolved in the reaction when looked at as a whole. When reading English text, this stage is characterized by a fixation on the punctuation mark for the sentence. Since chemical equations do not have punctuation, it is hypothesized that this step will be characterized by a pause on the rightmost molecule in the equation or in the white space at the end of the equation.

While the proposed model for the comprehension of organic chemistry notation, adapted from the Just and Carpenter model of reading comprehension, has many stages that are parallel to the processing of sentential representations, organic chemical notation also shares features with diagrammatic representation. To more fully understand how chemical notation is read and understood, it is necessary to investigate how diagrammatic representations are comprehended and the factors that affect this comprehension.

Diagrammatic Representations

For the purpose of this proposal, the term "diagrammatic representation" will refer to static images and will not include animations. These images represent a spectrum of types of diagrammatic representations. A commonly used system for categorizing diagrams, developed by Hegarty, Carpenter, and Just (1991), categorizes images into three broad classifications: iconic diagrams, schematic diagrams, and charts/graphs. The type of information and the way it is depicted distinguishes one category from another. In *iconic diagrams,* the image has a concrete spatial relationship to the object that is the referent. This type of representation preserves spatial arrangements that exist in the real world and includes images such as photographs and line drawings of objects. Information such as position in space, orientation, shape and size are preserved in this type of representation

Schematic diagrams depict abstract relationships and concepts. This type of representation relies on the depiction of the organization of abstract components and their interrelationships. This category includes organization charts, electrical circuits, and flow charts. Unlike diagrammatic representations that depict how things exist in the real world,

the components of a schematic diagram do not typically exist in the real world. Therefore, the physical attributes that are assigned to the components do not coincide with real world physical attributes.

The final category that was identified is *charts/graphs*. These images depict a set of related facts and represent their relationship quantitatively. Here again, the physical attributes that are assigned to the components do not coincide with physical attributes in the real world.

Although these classifications make it easy to talk about diagrammatic representations, these three graphical types are not exclusive. Examples can be found that possess shared attributes, as well as counter examples for a range of diagrams that are not easily included within the given system (for example, Blackwell & Engelhardt, 1998). Organic chemical equations are one example that is not easily classified. While the notation for each molecule is like an iconic diagram, preserving some of the spatial relationships among atoms as they exist in the real world, the overall chemical equation is more like a schematic diagram. It illustrates the sequence of chemical change from reactant(s) to product(s) with little regard for how the molecules are positioned in three-dimensional space. The equation also uses notation to show the directionality of the reaction ("+" signs and an arrow). The equations share qualities with sentential representations, such as an overall "grammatical" structure and the use of letter sequences (functional groups) and words (reaction conditions such as "heat"). These factors place chemical equations on the

continuum of representations, somewhere between "little use of diagrammatic properties to encode information through to substantial use of such properties" (Cheng et al., 2001, p. 84).

Use of Diagrams

Much of the research on diagrammatic representations has focused on how diagrams are used by the student. A diagram plays two roles, acting as both as an external organizer of multiple pieces of data that explicitly depicts relationships and as a location for offloading memory load.

External organizer. The diagram can often be "worth a thousand words" providing more information than the sentential representation (Larkin & Simon, 1987; Winn, 1988). Larkin and Simon (1987) argue that diagrams simultaneously offer a variety of relationships between objects in the diagram. This is an advantage over text, which must be sequentially processed. Larkin and Simon also argue that a diagram can convey these relationships in a concise manner, illustrating relationships in less space on a page than a text account of the same situation.

This concise depiction of information afforded by diagrams may help cognitive processing due to the explicit way it represents relationships within a problem (Larkin & Simon, 1987). Larkin and Simon express a fundamental difference between sentential and diagrammatic representations as "the diagrammatic representation preserves explicitly the information about the topological and geometric relations among components of the problem, while the sentential representation does not" (1987, p. 66). Diagrams retain many important features of a problem and display them in a visually explicit manner. This

explicitness aids in the search of a diagram for information and reduces the need for the student to "work out" relationships between component on his/her own.

Working memory offload. Multiple examples of diagrams being used as objects of cognitive offload can be found in the literature. For example, Bauer and Johnson-Laird (1993) found that diagrams help facilitate deductive reasoning. In this study, icons were used to distinguish between relationships that were inclusive and exclusive, making these relationships more explicit than found in the text of the same problem. Participants responded significantly faster on these diagrammatic problems and drew almost 30% more valid conclusions from the diagram than from the text. They theorized that participants could solve problems and make inferences by using an external representation as a cognitive support instead of trying to develop relationships in their head. Hegarty and Kozhevenikov (1999) also found that learners used external diagrammatic symbols to "offload" information, as a strategy to reduce memory load.

Although diagrams have visually explicit properties that can facilitate problem solving, research into the use of diagrams has also shown that diagram use is not always beneficial. For example, Zhang and Norman (1994) found that not all diagrams are created equal. Different diagrams of the same problem were shown to provide differing amounts of diagrammatic offloading. Consider the following equation from organic chemistry (Figure 22):

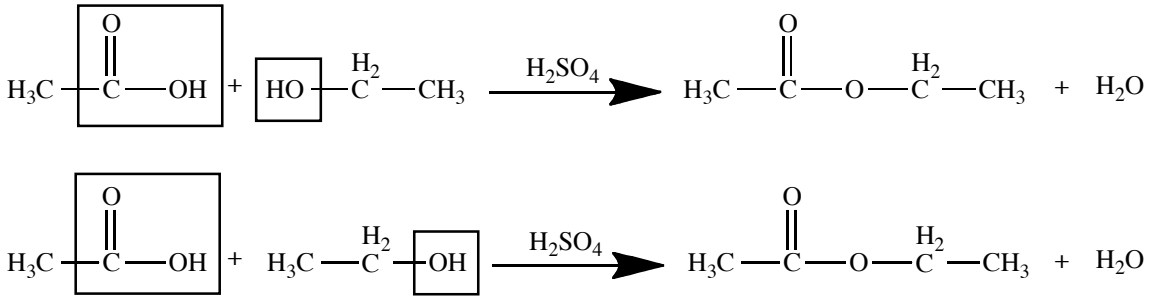


Figure 22. Two examples of esterification of acetic acid.

In the chemical equations presented in Figure 22, the carboxylic acid functional group (-COOH boxed in the first molecule) in acetic acid reacts with the alcohol functional group (-OH boxed in the second molecule) in ethanol to produce an ester, ethyl ethanoate, and water. Although both equations provide the same information about the chemical reaction, the functional groups of the reactant molecules in the first chemical equation are correctly spatially oriented towards one another, making this relationship explicit. In the second equation, the -OH group on the second reactant is pointing away from the carboxylic acid function group. In order to comprehend this reaction, the student typically must mentally rotate the second molecule (ethanol) so that the alcohol functional group (-OH) is oriented towards the carboxylic acid functional group (-COOH) in order to understand how these two molecules react. Although these two proposed chemical equations are of the same esterification reaction, the different orientations of molecules in the equation affects the amount of diagrammatic offloading that occurs. When the diagram is more explicit in the visual information it displays, it can guide the understanding of the relationships between features in the diagram (e.g., -OH and –COOH). Explicit diagrams, like the first equation,

require fewer inferences, guiding and "even [determining] the pattern of cognitive behavior" (Zhang, 1997, p. 184).

Diagrams can make important aspects of information more accessible and facilitate the encoding and processing of key components essential for problem solving and learning (Scaife & Rogers, 1996). They can control the number of inferences necessary for the reader to make in order to answer problems, and allow for working memory offloading.

Diagram Comprehension

There are many process models of diagrammatic comprehension. Difficulty occurs when one tries to compare them for common features. Unlike sentential comprehension, where the goal of the process is usually to read and comprehend the semantic and syntactic relationships governed by rules of grammar and orthography, the goal of diagram comprehension is task specific (Just & Carpenter, 1976; Koedinger & Anderson, 1990). Comparing process models becomes difficult when the steps of comprehension are goal driven. For example, Just and Carpenter (1976) describe a process model for comparing two figures to see if they are the same figure, each having a different orientation in space. This model consists of three steps including *search*, *transformation & comparison*, and *confirmation*. During the *search* step, the viewer searches for a segment that corresponds to the target by looking for a feature that meets certain criteria. The viewer performs a mental rotation task and compares the new mental representation to the original diagram. Finally, the answer is checked for congruence to determine if all the features overlap and the selection of the answer matches the criteria.

In the work done by Koedinger and Anderson (1990), diagrammatic comprehension of geometric figures is also a three-step process, namely, *diagram parsing, statement encoding, and schema search*. Here, the *diagram parsing* is similar to Just and Carpenter's *search* step, where the individual identifies familiar configurations and activates corresponding schema. During the *statement encoding*, the individual attempts to comprehend the given goal statements of the problem and how they relate to the diagram. Finally, the person attempts to solve the task by applying a *schema search* in a forward or backward direction, reducing the distance between the given and the goal statements until the task is complete. Other process models show similar patterns of *search*, *process*, and *answer*, however, the process steps can be different depending on the task.

In the two models of diagrammatic comprehension discussed, the person performs a visual search of the diagram for specific elements that meet a given criteria or that relate to the statement of the problem. For organic chemistry, this search may be to identify specific features that can participate in the chemical reaction. Such specific configuration of atoms is necessary for the reaction to take place. In the proposed model for the comprehension of organic notation (Figure 14), this search is incorporated into a reading stage called *intramolecular search*. During this stage, the student searches the notation for a group of atoms that are key to understanding the chemical reaction. Incorporation of this search step into the proposed model addresses specific questions about the processing of organic chemistry notation that arise due to its diagrammatic qualities, including lack of a standard orientation for each molecule in the chemical equation.

Since the process models for the comprehension of diagrammatic representations are task specific, the purpose of the student viewing a specific chemical equation becomes very important in the research design. Not only will the process model for diagrammatic representations of a chemical reaction be different than the process models for other diagrams like mental rotation exercises, flow charts, and electrical schematics, but it will also differ for each task presented to the learner as he/she views the chemical equation. It is hypothesized that different processes occur if a chemical equation is read for memorization versus conceptual understanding. This idea becomes important when designing studies to validate a model. For this study, the task is explicitly identified in the methodology requiring that the student read the equations for understanding rather than for memorization.

Factors Affecting the Comprehension of Organic Notation

I have argued that organic chemistry notation shares features with both sentential and diagrammatic representations. Comprehension of this notation is a complex cognitive task that requires the coordination of many systems, as illustrated in the proposed model (see Figure 18). I hypothesize that factors affecting the comprehension of each of these types of representation will also affect the comprehension of organic chemistry notation.

The proposed model for comprehension of organic notation is adapted from the work of Just and Carpenter on reading comprehension, and strong parallels between the two models can be seen in the stages of reading comprehension. With both models sharing many similarities, I hypothesize that the factors that affect reading comprehension of text will also affect the comprehension of organic chemistry notation. This section will look at

three factors that have been shown to consistently affect this process, namely, working memory capacity, expertise, and prior knowledge.

When considering the diagrammatic nature of chemical notation, there are also factors that have been shown to affect diagrammatic comprehension apart from type of diagram and the task presented to the viewer. The literature suggests that the spatial ability of the viewer and the complexity of the diagrams influence diagrammatic comprehension. This section will also look at these two factors.

Reading Comprehension and Problem Solving

Any discussion regarding the factors affecting the comprehension of organic chemistry notation must include the current research from the literature. The research in organic chemistry education has focused on problem solving in organic chemistry (e.g., Bhattacharyya & Bodner, 2005; Bowen & Bodner, 1991; Coll & Treagust, 2002). The information processing model for problem solving provides a explanation of how problem solving in organic chemistry is related to reading comprehension.

The information processing model for problem solving describes a cyclic model where the solver searches a problem space consisting of a representation of problem in some degree of solution (Newell & Simon, 1972). Two distinctive, yet interdependent phases of problem solving have been delineated as problem representation and problem solution (Mayer, 1991). In order to solve a problem, the words or picture supplied by the external representation must be converted into an internal mental representation (problem representation). Next, the solver searches the problem space for a solution and uses problem

solving strategies to create a new representation, or state, of the problem for evaluation. The new state is evaluated and the process will either result in an answer or a new search will begin (problem solution). The key to problem solving is the initial formation of the problem representation. Success depends on the accuracy of this internal representation. The ability to form an accurate internal representation depends largely on the how well the solver comprehends the external representation such as the chemical equation.

Several factors have been identified that affect the comprehension of external representations. The remainder of the section will discuss four of these factors - working memory capacity, expertise and prior knowledge, spatial ability, and diagrammatic complexity.

Working memory capacity (WMC)

Unsworth and Engle (2007) propose that working memory capacity is a measure of both "the ability to actively maintain information [in working memory] and the ability to retrieve task relevant information in the presence of irrelevant information" (p. 105). They argue that working memory maintains a representation for ongoing processing by allocating attention to these representations, similar to the *attentional control system* of the central executive (Baddeley, 2001). Retrieval is accomplished by associative access relying on cuing. Retrieval cues are associated with items that are stored in LTM along. They are based on the context in which the information was processed. During retrieval, cues from the current context are compared with retrieval cues. Information with retrieval cues similar to the context cues is attended to by working memory. Retrieval is constrained by similarity

- based interference and chunk activation (Lewis, Vasishth, & Van Dyke, 2006). If individuals have retrieval cues that activate irrelevant information (interference) or their chuck activation is below the critical threshold for retrieval, differences will be seen in working memory capacity. According to this theory, individuals with lower working memory capacity are "poorer at maintaining items in [WM] and are poorer at using cues to guide the search process of [LTM] " than individuals with higher working memory capacity (Unsworth & Engle, 2007, p. 121). They cannot maintain items in working memory when attention is captured by irrelevant information from the stimuli and their noisier context cues result in the recall of a large set of irrelevant information (Engle & Kane, 2004). This translates into slower response times for individuals with lower working memory capacities due to the extra time required to search for the target information in the large search set.

Working memory capacity and reading. How working memory capacity is measured is the focus of much research. In their work, Danemon and Carpenter (1980) highlighted the importance of working memory to account for individual differences in reading comprehension. For their studies, Just and Carpenter (1992) are careful to define working memory as the "working memory of language" (p. 125). In this view, working memory capacity is task specific. Readers develop strategies that allow for more efficient use of working memory resources. These specific strategies allow them to reduce the demands of processing and devote more resources to storage. Since working memory includes both short and long term storage and processing, Danemon and Carpenter (1980) developed the *reading-span test* where a participant is read aloud three sets of two to six

sentences and immediately asked to recall the final word in each sentence. Not only does the participant have to manipulate the sentence to determine the last word but he/she must also store the last word for each sentence until it is reported back to the tester. The span score is reported as the highest level at which the participant recalls a majority of sentences from the set that is read aloud. The cutoff that Daneman and Carpenter used in their research is the correct recall of 2 out of 3 sets of sentences. Using this complex span score, Daneman and Carpenter (1980) were able to show that short-term memory span correlated with reading comprehension test scores (correlations between 0.5 and 0.9), depending on the comprehension task.

Others have argued that working memory span tasks measures a WMC that is domain general, predicting complex cognitive behaviors across a wide variety of tasks not just reading (Conway et al., 2005; Unsworth & Engle, 2007). This view stresses the role of attention in working memory. In their meta-analysis of 77 studies, Daneman and Merikle (1996) reported a moderate correlation (average correlation = 0.41) between reading span and overall reading comprehension measured by standardized tests such as the verbal SAT. Engle, Carullo, and Collins (1991) found correlations between overall span score and participants ability to follow oral directions (correlations between 0.30 and 0.47). Similar correlations have also been reported for computer programming skills (Shute, 1991) and fluid intelligence (Ackerman, Beier, & Boyle, 2005; Kyllonen & Christal, 1990; Unsworth & Engle, 2006) .

Baddeley (2007) argues that reading span tests are measures of sentence processing rather than working memory capacity. He also points out that there is no standardized reading span test and that most of the research in the literature uses different sentences to test working memory capacity. Variables such as vocabulary affect reading comprehension and, in turn, influence these measures of working memory capacity. For example, consider the effects of word frequency. How often a word appears in printed language (word frequency) can affect the speed with which a reader can comprehend a word. Known as the *word frequency effect*, it has been observed that more frequently used words are "processed faster and more accurately than words that occur infrequently" (Just & Carpenter, 1987, p. 70). This effect can be explained by the ACT-R theory (Anderson et al., 2004). Words that are encountered more frequently have higher chunk activation than words that are encountered less frequently. When encountered in a new context, these words require less activation than their low frequency counterparts and are processed faster. Depending on the words chosen in the reading-span test, it is possible to have significant differences in the measurement of WMC based on the word frequency effect. Baddeley suggests that tests using symbols, such as digit span, do not have the same constraints of language and are better measures of working memory capacity.

Digit span tests. During digit span tests, participants listen/read a sequential string of digits ranging from two to eight numbers, then immediately recall what was heard/read. Scores are assigned based on the number of correct strings that are recalled. The forward digit span (recalling the string of digits in the given order) has been shown not to be a good

measure of working memory (Daneman & Carpenter, 1980; Oberauer, 2005); however, there is evidence that that the digit span backwards (DSB) test (recalling the string of digits in reverse order) correlates positively with other measures of working memory capacity. While it is assumed the forward digit span measures the storage capacity or working memory, the DSB test is a better measurement because it measures both storage and mental transformation without relying on participant's prior knowledge of vocabulary. The DSB includes the additional task of mentally reordering the string of digits making it a measurement of both storage and transformation. This test has been shown to strongly correlate ($r = 0.55$) with working memory span and other measures of working memory capacity (Oberauer, Süβ, Schulze, & Wittman, 2000).

Working memory capacity and eye movement. Working memory is a limited capacity system that provides resources for the temporary manipulation and storage of information (Baddeley, 2000). Subjects with high WMCs have a greater amount of resources to allocate to activities of working memory, which decreases processing time and limits forgetting (Just & Carpenter, 1992). The greater capacity allows these individuals to store more than one representation in working memory, speeding overall processing time. According to the eye mind assumption, eye fixation times are a direct measure of processing time (Just & Carpenter, 1980). This suggests that subjects with high WMCs will exhibit significantly shorter fixations than subjects with low WMCs. King and Just (1991) found that there was a significant difference in the fixation times on more demanding features of a sentence for high WMC and low WMC individuals, with low WMC individuals exhibiting

significantly longer fixation times on critical verbs than their high WMC counterparts. These differences became larger when the structural complexity of the sentence increased.

This difference in fixation times has also been reported for high and low WMC individuals reading Japanese, a logographic language (Osaka & Osaka, 2002). Osaka and Osaka used the moving window method, which restricts the individual's effective visual field by limiting the amount of the amount of information accessible to the reader. They showed that high WMC individuals exhibited significant smaller fixation times and better comprehension then low WMC individuals. With the restricted view, individuals are forced to spend more resources on information storage. Since high WMC individuals have more resources left over for sentence processing than low WMC individuals, they perform better on comprehension measures than their low-span counterparts.

Kemper, Crow, and Kemtes (2004) monitored the eye fixation patterns of high and low WMC individuals as they read sentences containing complex syntactic ambiguities. They found that, when compared to high MWC readers, "low [WMC] readers made many [more] regressions and their total fixation times were longer" (Kemper et al., 2004, p. 157). However, when fixations times were examined during first-pass reading, high WMC readers were reported to have longer initial fixations than low WMC readers (Kaakinen, Hyona, & Keenan, 2003). It has also been shown that, regardless of their prior knowledge, high WMC readers show less regression (look-backs) than low WMC readers (Kaakinen et al., 2003). Kaarkinen, Hyona, and Keenan suggest that high WMC readers are better at allocating attentional resources than low WMC readers. High WMC readers "invest so much

attentional resources to relevant text information already during the first-pass reading that they do not need to reread relevant information to be able to recall it later" (Kaakinen et al., 2003, p. 453). In contrast, low WMC readers have more difficulty attending to relevant information and process information later after they have had time to reread information and encode it. Although low WMC readers have longer total fixations because they need to reread information in order to encode it, high WMC readers show longer initial fixations because they encode information during first-pass reading.

In this study, I hypothesized that there will be a difference in the eye movements of participants based on their WMC. Participants with high WMC will have shorter overall fixations durations than low WMC participants. Participants with high WMC will have less regressive eye movements than low WMC participants, leading to a lower frequency of fixations and less repetitive sequences of fixations.

Working memory capacity and organic chemistry. Research has suggested that, when an organic chemical reaction is read, the information is encoded into working memory. While in working memory, the internal representation that results from the encoding is processed. When the working memory capacity of an individual is overtaxed by the demands on working memory (the amount of information that needs to be stored and processed), achievement on organic synthesis problems significantly decreases (Tsaparlis, 1998; Tsaparlis & Angelopoulos, 2000). It has been suggested that errors on achievement measures are primary caused by a lack of comprehension that leads to the development of an incorrect solution plan rather than resulting from errors in the execution of a solution plan

(Lewis & Mayer, 1987). Working memory is central to the comprehension process, as illustrated by the process model for the comprehension of organic chemical notation (see Figure 20). Since working memory of an individual has limitations, the working memory capacity of an individual will affect reading comprehension in organic chemistry. This link between reading comprehension in organic chemistry and working memory will be further explored in this research.

Domain Expertise and Prior Knowledge

Expertise and prior knowledge are inextricable linked. Experts in a specific domain possess more extensive knowledge of that domain than non-experts and excel in their domain (Glaser & Chi, 1988). Research in expertise suggests that the acquisition of this domain specific knowledge "requires many years of intensive experience" (Mayer, 1991, p. 390). During these years of intensive experience, practice and training facilitates an expert's acquisition of numerous patterns of information in the domain. These patterns store information regarding actions that should be taken when the expert encounters a similar situation (Simon & Chase, 1973). It has been suggested that, for a variety of domains, it takes approximately ten years to attain expert status (Ericsson & Lehmann, 1996). However, Ericsson and Lehman argue that the relationship between years of experience and expertise may not be as important as the amount of time spent performing a task (for example, years teaching organic chemistry or years of research in organic chemistry). For this study, experts will have at least a master's degree in organic chemistry (approximately 7

years of training in chemistry) and three years of experience teaching organic topics to undergraduate students.

The knowledge of experts that is gained through years of experience and performance is effectively organized around principles within the domain, allowing for more efficient access to this prior knowledge and better performance on domain specific tasks (Chi, Glaser, & Farr, 1988; Ericsson & Charness, 1994). In comparison, novices, having little experience in the domain possess far less domain-specific knowledge (patterns). The domain knowledge that they do possess is stored in fragmented sets of information that do not allow for quick access to information.

Since experts and novice differ in the amount and organization of domain specific knowledge, they also differ in the way that they describe problems within the domain (Chi et al., 1982). The prior knowledge of experts is highly organized around central principles. Therefore, experts are able to perceive meaningful patterns in problems and describe them more abstractly. Studying chess players, de Groot (2008) showed that chess masters (experts) were significantly better at recalling meaningful patterns of chess pieces than casual chess players (novices). After a 5 second exposure to chess positions (a possible arrangement of pieces on the chess board that could occur in a game), experts could recall the positions of over 20 pieces while the novice could only recall 4-5 pieces. When presented with an implausible arrangement of chess pieces (chess positions that could not occur in a game), the difference between novice and expert disappeared. de Groot concluded that the expert remembered the overall pattern of the pieces and not the individual

position of each piece because of his/her extensive experience playing chess. This experience exposed the expert to a great number of plausible patterns of chess pieces. It is these patterns that give the expert an advantage over the novice in the recall task. When presented with implausible patterns with which the expert has little experience, the advantage disappears. Chase and Simon (1973) continued this work, showing that as expertise increases from beginner to Class A chess player to Chess Master, the ability to recall plausible chess positions also increases. They attributed this ability to recall patterns to an individual's ability to recognize patterns ("chunks") of information. For the Chess Master, these chunks are larger and consist "of a familiar subconfiguration of pieces. Pieces within a single chunk are bound by relations of mutual defense, proximity, attack over small distances, and common color and type" (Chase & Simon, 1973, p. 80) which are stored in the Chess Master's long term memory. The "chunks" of the novice are smaller, containing less meaningful patterns.

Since identifying meaningful patterns is difficult for novices, their descriptions and internal representations of problems tend to be superficial, relying on surface features and literal translations (Chi et al., 1982). It is theorized that the reason for this is that the schema-like chunks that novices possess in the content domain are also based on superficial similarities and lack the connections between these features and underlying principles (Chi et al., 1981). In contrast, experts have both well-defined schema-like chunks (deep hierarchies of information stored in LTM) that interconnect principles, theory, and

procedural knowledge about applicability and solutions. This allows experts to create more intricate representations and think abstractly about a problem.

The ability to identify meaning patterns also affect the strategies that experts and novices used during complex cognitive tasks such as problem solving and reading. Experts rarely engage in general search processes, but rather use domain specific strategies to solve problems (Gick, 1986; Gick & Holyoak, 1980; Larkin, McDermott, Simon, & Simon, 1980). For the synthetic organic chemist, these strategies may include a retrosynthetic analysis (Corey & Cheng, 1989), where the chemist starts with the products of the reaction and works backwards towards the reactant(s). This is the technique used when a desired product (e.g., a molecule isolated from nature) is known and the researcher wants to develop of scheme to produce the molecule in the lab. Novices describe problems based on surface features such as objects originally stated in the problem. Since they lack the domain specific knowledge to identify meaningful patterns in the problem, novices rely on domain general strategies. Although these strategies are flexible and can be applied to a number of domains, these strategies are weaker and do not always lead to a correct solution. These strategies include reasoning by analogy and brainstorming.

On first glance, it would seem that during the reading process, experts would exceed their WMC when they recall the complex hierarchies of information that are stored in their LTM. However, evidence from the literature suggests that this is not the case. Unsworth and Engles (2007) propose that working memory capacity is the ability to maintain information in working memory and retrieve relevant information from LTM. They point

out that this WMC "is important in a number of domains, [but] working memory as a system is not needed in all cognitive operations" (Unsworth & Engle, 2007, p. 105). They argue that working memory is used when the individual needs to overcome automatic tendencies, especially during an encounter with information in a novel context. Theories on skill acquisition suggest that expert performance is more automatic, requiring fewer processing resources (Anderson, 1993, 1996; Fitts & Posner, 1967). While novices must rehearse facts as they perform a task like reading a chemical equation and attend to every step in the process, the expert automates some of the process, reducing the overall demands on working memory capacity. Experts develop procedures for performing skills that are outside of working memory, thereby increasing the speed by which the expert can perform a skill.

As we have seen, expertise influences how individuals approach a given domain specific task like reading a sentence or a chemical equation. Based on their level of expertise, individuals will apply different strategies and procedures to the problem of comprehending a given representation. According to both the proposed model of reading comprehension and that proposed by Just and Carpenter, there exists a relationship between long-term memory and working memory, as illustrated by the arrows connecting these two memory structures (Figure 18 and Figure 19). Working memory uses information stored in long-term memory for manipulation as well as enrichment of the mental representation. Therefore, the accessibility of information in long-term memory has a direct impact on comprehension processes in both models. Since experts and novices differ in the amount and organization of information in long-term memory regarding a specific content area,

expertise in a specific content area is likely to affect reading comprehension (Bransford, Brown, & Cocking, 2000; Chi et al., 1981; Glaser & Chi, 1988).

Expertise and eye movements. Differences in eye movements for experts and novices have been reported in the literature. Charness, Reingold, Pomplun and Stampe (2001) found that when chess players were asked to predict the next move for a given chess position, chess experts had a higher frequency of fixations on salient pieces. The first five expert fixations were longer in duration than those of novices. This pattern of longer fixations for experts has also been reported for experts during check-detection tasks in chess (Reingold, Charness, Pomplun, & Stampe, 2001). The opposite effect has also been reported in the literature. Chapman and Underwood (1998) found that novice drivers have longer fixations than expert drivers, especially when dangerous situations were presented for viewing. Longer fixations have also been reported for novice versus expert pilots (Kaakinen et al., 2003) and surgeons (Law, Atkins, Kirkpatrick, & Lomax, 2004). The discrepancies between fixation durations in the studies of chess players and the other studies mentioned might be due in part to the number of fixations that were analyzed. In both chess studies, the first five fixations were analyzed, while in the other studies longer sequences of fixations were studied. It is theorized that during first pass reading (in this case, the first five fixations) experts have longer fixations. It is during the first-pass that they encode information about the image because they are able to quickly identify meaningful patterns in the information. Novices have difficulty identifying meaningful patterns and are less efficient at allocating attentional resources. This means that novices often need to reread

relevant information to encode it into memory. Since encoding requires processing time, initial fixations are longer in duration for the expert than the novice. However, because novices must reread information, they exhibit longer total fixation times than their expert counterparts.

Another difference in expertise-based differences in eye movements is the visual search. Overall, eye movement data showed that the experts were quicker to locate the target than novice and have lower overall fixation times (Huemer et al., 2005; Nodine, Mello-Thoms, Kundel, & Weinstein, 2002; Van Gog, Paas, & Van Merrienboer, 2005). It has also been reported that during visual search, experts and novices show differences in where they focus attention (Charness et al., 2001; Kaakinen et al., 2003; Vonder Embse, 1987). Experts exhibit significantly longer fixations on salient features of images that are necessary for task completion, while novices showed little or no preference for salient versus non-salient features.

I hypothesize that experts exhibit shorter overall fixation times than novices. When comparing fixation durations on specific regions of the chemical equation, experts will have a greater number of fixations and spend significantly more time than novices on salient features (informative AOIs) related to the reactivity of compounds. Novices will show little or no preference for salient and nonsalient features of the chemical equation. Novices' fixations will have greater frequency and longer durations than experts for nonsalient features (distractor AOIs).

Measuring prior knowledge and eye movements. There is a special consideration that must be made when measuring prior knowledge in an eye-tracking study. It has been shown in the literature that repeated viewing of the same image will result in changes in eye movement behavior. According to Norton and Stark's scanpath theory (Noton & Stark, 1971), an individual scans a new image, fixating on various features of the image. The sequence of these fixations creates an internal representation of the image in the mind of the individual. When a subject is exposed to the same image again at a later time, the first few eye movements will tend to follow the same scan path as the previous one. Norton and Stark note that:

> The internal representation of a pattern in memory is a network of features and attention shifts, with a habitually preferred path through the network, corresponding to the scanpath. During recognition, this network is matched with the pattern, directing the eye or internal attention from feature to feature of the pattern. (Noton & Stark, 1971, p. 940)

This idea of forming habitual scanpaths can be related to chunk activation. Upon repeated viewing of the same image, the initial activation of that chuck will be increased due to frequency and recency effects. This, in turn, should decrease eye fixations and durations on the subsequent viewings. Pieters, Rosenbergen, and Wedel (1999) found that, by the third repeated viewing of the same stimuli (printed advertisement), the overall scan path remained stable but the fixation time was reduced by 50%. Hidalgo-Sotelo, Oliva & Torralba (2005) showed similar results when participants viewed the scenes with repeating elements. As

expected, repeated searches showed a large decrease in latency (time it takes to fixate on the target stimuli) and the duration of the fixations within the scene also decreased. However, the number of fixation remained unchanged. The average gaze time on the target decreased from 450 ms to 310 ms by the twentieth viewing.

Since these two works have very dissimilar numbers of exposures before effects were evident, it is unclear from the literature how many repeated viewings would result in a change in the viewing patterns for organic chemistry notation. What is clear is that repeated viewings do affect the viewing patterns. Any pre-test for prior knowledge of molecules and reactions would include viewing images of the reaction or parts of the reaction used in the study, therefore, including a pre-test in this study may introduce an unintended influence on eye movements. To prevent this, I have developed a post-test that participants take after viewing the chemical equations that assesses their self-reported familiarity with the chemical reaction and molecules given by the equation. This is discussed further in Chapter 3.

Expertise and organic chemistry. Research in the field of expertise itself shows that it is not sufficient for learners to have merely stored this type of knowledge in memory. Instead, knowledge must be organized to facilitate its easy retrieval. Most of the expertise research for the domain of organic chemistry focuses on the differences between how novices and experts use diagrammatic representations. For example, Bhattacharyya and Bodner (2005) studied how novices used the arrow notation in organic chemistry reaction mechanisms. They found that novice chemists do not fully understand chemical notation, more specifically, the arrow formalism that shows how electrons move during a chemical

transformation. The novices attached no conceptual understanding to the arrows, but used them as a means to move from the reactants to the products.

As students progress through an organic chemistry course, their level of expertise also increases and the concepts become more interconnected. However, at the end of their course work, their knowledge still lacks the organization of an expert with years of experience in the domain (Nash, Liotta, & Bravaco, 2000). This interconnectedness can be mapped using the ordered tree technique, which produces a hierarchical tree showing an individual's understanding of a specific domain. When novices' hierarchical trees from the beginning of the semester were compared to the ones created at the end of the semester, the trees changed significantly. Novices' initial trees were shallow, containing chunks of information based on surface features. At the end of the semester, the trees became more branched, showing the development of conceptual relationships between concepts. When these trees were compared to the professor's, it was found that, while some conceptual relationships were starting to develop, the professor's tree was much deeper and showed an overall structure to the knowledge based on conceptual understanding that "appears to arise from further expertise in the discipline" (Nash et al., 2000, p. 336).

This lack of overall structure in the knowledge of novices is evident in the way they answer questions that require multiple concepts. Coll and Treagust (2002) found that, as expertise increased, the ability of the individual to use a variety of concepts to explain chemical phenomena also increased. When asked to explain chemical phenomena, undergraduates and graduates were able incorporate ideas from other models of bonding,

while secondary school students tended to use a single model in their explanations. Graduate students also exhibited a greater "appreciation of the molecular nature of the covalent molecular substances used in the inquiry than their secondary school or the undergraduate counterparts" (Coll & Treagust, 2002, p. 260).

Spatial ability

Organic chemistry notation is a unique symbolic representation system that uses alphanumeric characters, Greek symbols, lines, and/or geometric shapes to convey the number and types of atoms present in a molecule of an organic compound (molecule). To understand a chemical equation, a viewer must construct and manipulate internal representations of the molecules presented in the equation. *Spatial ability* is defined as the ability to encode, store, process, and retrieve information about the spatial position of an object and its relationship to other objects in both two-dimensional and three-dimensional space (Cooper & Regan, 1982). Research has suggested that differences in spatial ability are related to differences in working memory resources for processing and storing of spatial information (Just & Carpenter, 1985; Just, Carpenter, Keller, Eddy, & Thulborn, 1996). According to this model, high spatial ability individuals have more resources for processing and storing spatial information than low spatial ability individuals. Research has shown that working memory span (a measure of verbal working memory) does not correlate with spatial ability (Hegarty, Shah, & Miyake, 2000; Shah & Miyake, 1996). This supports a model that separates working memory into separate subsystems, including Baddeley's model of working memory where separate subsystems are responsible for maintaining attention on

verbal, visuospatial, and episodic information. Although the Baddeley model suggests that spatial ability is a measurement of the visuospatial working memory, it is unclear from the literature whether this measurement is completely independent of the other subfactors for verbal memory and episodic memory. For this reason, measurements of both working memory capacity and visuospatial memory will be used in this study.

Since the process model for the comprehension of organic chemistry notation includes stages that search the two-dimensional problem for features of the structure (*intra-molecular search)* and processes relationships between groups in the molecules (*intra-molecular relationships* and *inter-molecular relationships*), I propose that spatial ability plays an important role in the processing of organic chemistry notation.

In a chemical equation, molecules are presented in specific orientations. In order to understand the reaction, a viewer may have to perform a series of mental manipulations to transform the reactants into the products. Many spatial ability factors have been identified in the literature that relate to the manipulation of mental representations (Carroll, 1993; McGee, 1979). Two such factors are *spatial visualization* and *spatial orientation* (Bodner & Guay, 1997). Spatial visualization includes the ability to carry out a series of mental manipulations on an object that is illustrated in a given perspective. Spatial orientation is the ability to imagine how an object or series of objects would look from a different perspective. Although McGee (1979) argues that these two factors are discrete, the meta-analysis performed by Carroll (1993) finds no evidence that these two factors are separate and classifies them both as spatial visualization. Measures for spatial orientation and spatial

visualizations are often highly correlated (Carroll, 1993; Price & Eliot, 1975). It has been suggested that tests designed to measure spatial orientation are often solved by mental rotation rather than reorienting one's perspective (Kozhevnikov & Hegarty, 2001). Since these two factors are indistinguishable with the measures available, a single measurement of spatial ability will be used in this study.

Spatial ability (SA) and eye movements. Although the effects of working memory capacity on eye movements were discussed earlier, there is limited research that suggests that this particular subscore of working memory may affects eye movement behavior. Research suggests that individuals with high SA are better at performing tasks that require the manipulation of a object than low spatial ability individuals. High SA individuals exhibit faster times to the target stimuli and shorter fixations than low SA individuals. When comparing eye fixation latencies, Stanfield and Zwaan (2001) found that individuals with high SA were better able match sentences with a picture that had the appropriate spatial orientation than low SA individuals. Just and Carpenter (1985) found that during a mental rotation task, low SA individuals had significantly longer gaze durations, especially for rotations that involved a longer trajectory than high SA individuals. Low SA individuals also exhibit a higher rate of regression (i.e., where an individual looks back at a previously viewed region) than their high SA counterparts. Just and Carpenter reason that the low spatial ability individuals exhibit these behaviors because they forget early results of mental rotation. As greater complexity is introduced by increasing the rotational trajectory, individuals with limited SA are not able to store and process the increasing amount of

complex information. These individuals must then look back over previously viewed regions to maintain the information in working memory. This, in turn, increases the frequency of fixation for individuals with low spatial ability.

In this study, it is hypothesized that participants with high spatial ability will have significantly shorter fixations than participants with low spatial ability on intramolecular and intermolecular regions of the equations. The frequency of these fixations will be significantly lower for participants with high spatial ability than participants with low spatial ability. Participants with low spatial ability will exhibit more regressions than participants with high spatial ability.

Spatial Ability and Chemistry. Research suggests that spatial ability, as measured by a test of spatial visualization ability, can affect student performance in chemistry. In general chemistry, it was found that those students who were classified as high spatial ability significantly outperformed their low spatial ability peers (Carter, Larussa, & Bodner, 1987). Spatial ability was also shown to significantly influence achievement on balancing equations (Staver & Jacks, 1988). Pribyl & Bodner (1987) found that, for problems where participants outline multi-step syntheses, complete a reaction scheme, or manipulate two-dimensional representations, students with high spatial ability are better at "understanding" a problem containing a reaction mechanism than students with low spatial ability.

Since reading chemical equations in organic chemistry requires mental manipulation of two-dimensional representations, it is hypothesized that spatial ability is a factor that influences the fixation times of viewers as they read chemical equations. According to the

eye-mind assumption underlying the process model for the comprehension of organic chemistry, the eye remains fixated on a portion of the chemical equation while the viewer is processing it. The length of time that the eye remains fixed on a given portion of the chemical equations is a direct measure of processing time. If high spatial ability viewers have a greater capacity to perform mental manipulations, it is hypothesized that they will have shorter fixation times than low spatial ability viewers.

Diagrammatic complexity

Larkin and Simon (1987) suggest that the reason why a diagram is "worth a thousand words" is because it makes relationships between objects explicit. For simple diagrams, extracting the relationships between objects is straightforward, however, when more elements are added to the diagram, locating relevant relationships can become more difficult for less knowledgeable viewers (Koedinger & Anderson, 1990; Larkin & Simon, 1987).

This difficulty in locating important relationships may be related to the demands that complex representations have on mental processing. This complexity "can be measured by the dimensionality of the relation, or the number of variables related" (Halford et al., 1998). As the relational complexity increases, the demands on available resources for processing information in working memory (cognitive load) also increase. As was discussed previously, working memory is limited. If the complexity of new information supplied to a learner is not managed and the processing demand exceeds the available working memory capacity, the learner will experience cognitive overload (Sweller, 1988). This overload impairs how information is stored in long-term memory and decreases his/her overall performance.

Sweller, Van Merrienboer, and Paas (1998) identified three types of cognitive load, namely, intrinsic, extraneous, and germane. Intrinsic cognitive load is the demand of the working memory that is inherent in the information being taught. Extraneous cognitive load is the demand that is placed on the working memory by the way the material was presented to the learner and is not inherent in the information being taught. The germane cognitive load is the process by which new information is stored in long-term memory. Intrinsic and extrinsic loads are cumulative, which means that when intrinsic load is high, as in the case of learning complex tasks like organic chemistry reactions, extraneous cognitive load can affect learning. The learner should have less trouble understanding if the intrinsic load is low or the extrinsic load is reduced (Chandler & Sweller, 1991, 1992).

If we consider the cognitive load on a student learning a new chemical reaction, we must take into account the complexity of the notation used. For example, consider the hydrohalogenation reaction, where a hydrohalic acid (e.g., HCl) is added to an alkene (compound that contains a carbon-carbon double bond). There is an almost infinite number of reactants, with a wide degree of complexity, can be developed that contain the carbon-carbon double bond (alkene group). Consider the complexity of the molecules in the following chemical reactions (Figure 23):

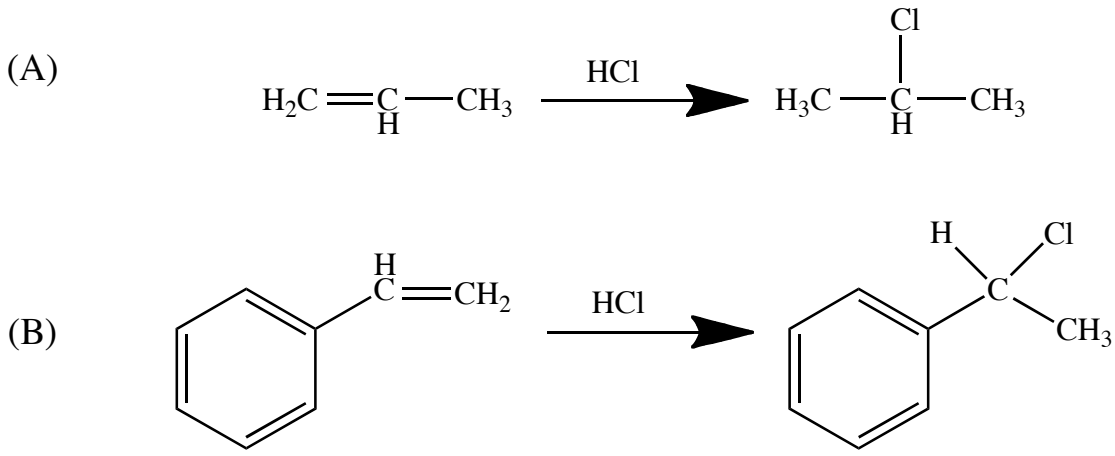


Figure 23. Examples of the hydrohalogenation reaction

The chemical equations in Figure 23 both describe the same chemical reaction, hydrohalogneation, in which hydrogen chloride is added to a double bond (alkene) yielding a chloroalkane. In equation (A), propene reacts with HCl to produce 2-chloropropane. In equation B, 1-phenylethene reacts with HCl to produce 1-cholo-1-phenylethane. Upon inspection, equation (A) contains less visual information than equation B. Most notably in equation (B), there is a six-membered ring with alternating double and single bonds (phenyl group) in both the reactant and the product that does not participate in the reaction. In order to understand equation (B), a portion of the limited working memory resources may be devoted to the encoding and processing of the phenyl group. For the organic chemistry expert, prior knowledge about the reactivity of phenyl groups and the hydrohalogenation reaction, would lead the expert to quickly dismiss the importance of the phenyl group in this reaction. However, the same would not necessarily be true for the novice. The additional complexity in equation (B) (e.g., alternating double and single bonds of the phenyl group)

may cause some confusion as to the site of hydrohalogenation and require the novice to engage in extraneous processing related to the structure and reactivity of this group. It is proposed that more complex chemical equations have a greater amount of visual information available to the reader. Depending on his/her level of expertise, this additional information may lead the reader to engage in extraneous processing, which would be demonstrated in the eye movement data as a larger number of fixations and longer fixation durations. It is expected that experts will show no significant difference in the number of fixations or the duration of fixations for equations of differing complexity level. In contrast, novices are expected to demonstrate an increase in both the number of fixations and durations for high complexity equations versus low complexity equations. This difference is due to the extraneous cognitive load caused by additional visual information in complex chemical equations.

Complexity and eye movement. Complexity has been shown to affect eye movements during both reading comprehension and diagrammatic comprehension. Text difficulty and characteristics of the writing system have been shown to influence eye movement. In Rayner's (1998) review of 20 years of research in eye movements during reading, he concluded that as the complexity of text increases, fixations are longer in duration, saccades are shorter, and the frequency of fixations increase. He notes that the complexity of vocabulary used in a sentence may be directly related to the frequency effect, where more common words are processed quicker and with more accuracy than words that appear less often. This may account for some of the variation in fixation times seen in the

literature. Low frequency words tend to be longer in character length, and sentences with "high complexity" tend to use these lower frequency words more often (Rayner, 1998). Since high frequency words are processed faster, individuals reading sentence with high frequency words exhibit shorter fixations durations.

A variety of typographical factors have also been shown to affect eye movements. Some of these include letter spacing, print quality, and line length (Morrison & Inhoff, 1981). Slattery and Rayner (2009) suggest that font choice can influence eye movement behavior. Fonts like Times New Roman, are easier to encode because of their simple shapes and lead to "faster reading times, fewer fixations, and shorter durations" (Slattery & Rayner, 2009).

Like sentential representations, complexity also affects the eye movements during the comprehension of diagrammatic representations. In general, fixation times for diagrams are longer than those for sentential representations (Rayner, 2009). According to Rayner, in sentential representations, there are well-defined tasks and an overall pattern for eye movements (left to right, top of the page to bottom). When viewing a diagram, the task becomes a visual search for key elements. As the number of elements in the diagram increases and the diagram becomes more complicated, the frequency of fixation and the duration of fixation increases (Vlaskamp & Hooge, 2006). Since there are more elements to in the scene, there are more spatial relationships. The search for key elements will take longer and require a more careful inspection of the relationships of each element.

I hypothesize that the complexity of the notation will affect eye movement. Participants reading visually complex equations will exhibit longer fixation durations and more frequent fixations. The largest effects will be observed for participants with low WMC, novices, and participants with low spatial ability.

Complexity and organic chemistry. It is unclear from the literature how the complexity of notation affects students' understanding of organic chemistry. There are no systematic studies reported in the literature on this topic. However, the identification of a critical attribute (salient feature) in an organic structure effects how an reader will classify the organic molecule (Domin, Al-Masum, & Mensah, 2008). When more than one salient feature exists, the reader will pick one to classify the molecule. Once the salient feature of a molecule is identified, the reader can use prior knowledge about that category of molecule to understand what he/she is reading. Domin, Al-Masum, and Mensah (2008) showed that additional training in organic chemistry may change the salient feature that the reader selects as a criteria for categorization. This implies that selection of the incorrect salient feature may lead to the access of inappropriate prior knowledge. It is reasonable to suggest that if the number of possible salient features increases the chances of misclassifying an organic molecule will also increase. More complex molecules, containing more salient features may lead the reader to focus on a feature of the molecule that is not helpful for comprehension (distractor). In turn, this would increase both the frequency and duration of eye fixations as the reader attempts to identify the correct salient feature.

This study will be the first to use a systematic way to classify organic chemistry notation according to perceptual elements (what Domin, Al-Masum and Mensah call salient features). The rubric used for this classification will be discussed in greater detail in Chapter 3.

Summary

By understanding how sentential and diagrammatic representations are processed, a new model has been proposed for the comprehension of organic chemistry notation that accounts for both the diagrammatic and sentential features of chemical equations.

This is a six-stage model that accounts for the eye movements of individuals as they read a chemical reaction for comprehension, accounting for eye movement and processing time from the point that they initially sees the reaction (*get next* and *search*) to processing *(encoding and access lexicon*, *intramolecular relationships, and intermolecular relationships*) to checking for errors in the final understanding of the reaction (*reaction wrap-up*). Several variables can affect how participants comprehend organic chemistry notation, including working memory capacity, expertise, spatial ability, and the complexity of the notation used in the equation. This research will use eye-tracking methodology to develop and validate the process model for the comprehension of organic chemistry notation. This study will also explore how variables discussed in this chapter affect the viewing patterns of participants as they read and comprehend organic chemistry equations. Chemical equations of both high and low complexity will be used to explore how expertise,

working memory capacity, and spatial ability affect eye fixations on various regions of a chemical equation.

The next chapter will detail the study designed to validate this new process model and explore how participant characteristics affect viewing behavior for various chemical reactions.

Chapter 3 - Methods

Two studies were conducted for this dissertation. Study 1 validated the *Complexity Rubric for Organic Chemistry Notation.* This dissertation required a common way to measure complexity of equations used to represent chemical reactions in organic chemistry. Since no such instrument existed in the literature, the *Complexity Rubric for Organic Chemistry Notation* was developed. It measures the complexity of a given symbolic representation. Before its use in this study, the validity of the rubric was investigated.

Study 2 used eye-tracking methodologies to develop and validate a process model for the comprehension of organic chemistry notation. Expertise, working memory capacity, spatial ability, and complexity of the notation were measured to determine their effects on how participants view and comprehend static representations of chemical reactions that employ organic chemistry notation.

Study 1: Validation of the Complexity Rubric for Organic Chemistry Notation

To solve any type of problem, an individual must create an internal mental representation of the problem from words and/or pictures supplied by an external representation (Mayer, 1991). To construct this internal representation, the individual encodes the external representation into working memory. Anderson, Matessa, and Douglass (2005) used a spotlight metaphor to describe how external information is encoded, or "chunked", in working memory. In this metaphor, visual attention is focused on an object, and features are recognized. These features become "chunks" that can be available for

higher-level processing. Figure 24 illustrates a possible "chunk encoding scheme" for a square. This scheme is similar to an example given by Anderson, Matessa, and Douglass (2005) for the letter "H". During processing of the object in Figure 24, the particular configuration of chunks (left vertical, right vertical, upper horizontal, and lower horizontal) is assigned a category ("square").

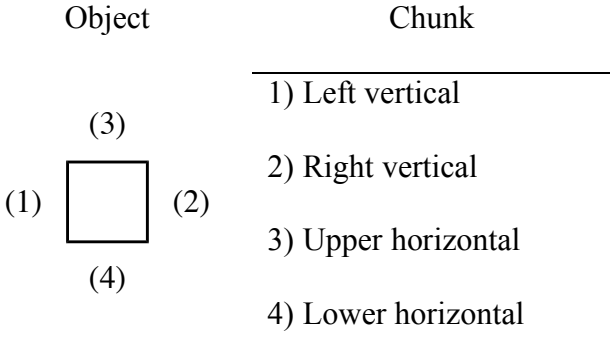


Figure 24. Chunk encoding scheme for a square, based on a similar example by Anderson, Matessa, and Douglass (2005).

This simple idea of looking at an external representation as chunks of information has been explored with different types of diagrams. When looking at a diagram for a geometry problem, Larkin and Simon were able to identify perceptual elements, such as "points, segments, angles, and triangles implied by the given problem statement, and evident in the diagram" (1987, p. 85). There are no set methods for defining these perceptual or diagrammatic elements of interest. Identified elements can be as specific as points or lines (Larkin & Simon, 1987), or as general as regions for a diagram (e.g. studies of meteorological charts of Australia (Lowe, 1994)). Since the complexity of organic molecules lies in the number of atoms and how they are interconnected, this research

hypothesized that perceptual elements must include both geometric features and symbolic elements.

The *Complexity Rubric for Organic Chemistry Notation* (Appendix A) was developed to identify the perceptual elements of organic chemistry notation in order to quantify the complexity of a structural drawing of an organic molecule. The *Complexity Rubric for Organic Chemistry Notation* identifies seventeen basic structural features (e.g. bonds, atoms, rings, chiral centers, etc.) used in representations of organic compounds and assigns a point value to each feature. The sum of these values is the *Organic Chemistry Notation Complexity score*.

Before this rubric could be used in Study 2, its validity needed to be investigated. Study 1 was a three-step validation process: 1) Content Validity, 2) Construct Validity, and 3) Predictive Validity (Groth-Marnat, 2009; Messick, 1995). In the discussion in Chapter 5, the results of the eye-tracking study will also be discussed as part of the score validation since it is hypothesized that the complexity of the notation will have a predictable effect on the eye movement behavior (Messick, 1995).

Research Questions

1. To what extent is the rubric consistent with expert opinion on visual information processing? (Content Validity)
2. To what extent does the rubric complexity score measure the visual complexity of the chemical notation? (Construct Validity)

3. To what extent does the rubric complexity score predict the visual complexity of a molecule? (Predictive Validity)

Part 1: Content Validity

Content validity is an external review process where experts assess each item on the rubric based on their knowledge of a given theoretical construct (Groth-Marnat, 2009). For this rubric, items were assessed for their agreement with what is known about how external representations are encoded into working memory. Since the rubric measures the complexity of the visual information to be encoded by the viewer, experts were chosen because of their familiarity visual information processing. It is important to note that the rubric does not measure the plausibility of a representation or the reactivity of the chemical species under examination. Therefore, little or no organic chemistry knowledge was required to evaluate the content validity of the rubric.

Participants. Three experts from the faculty at CUA and Northern Arizona State University were invited to participate. Two experts ultimately participated in this study. Both experts were PhDs in educational psychology, on the teaching faculty at their institutions, and had taught education psychology courses. Both experts had research experience, which included visual information processing, reading comprehension, and eye tracking methodologies. Dr. A was interviewed in person, and Dr. B was interviewed over the phone.

The total time commitment for the interview was 2 hours. Participants were asked to review the rubric materials on their own time and participate in a 1-hour semi-structured

interview. The purpose of the interview was to determine if the rubric adequately identified the perceptual chunks of information given in structural formulas that used organic chemistry notation.

Materials and Procedure. Experts were provided with an electronic copy of the rubric, the definition tables for each rubric element, and two worked examples illustrating how the rubric is used to score organic chemistry notation (Appendix A).

Visual sorting task. A visual sorting task was used as part of the interview process. Participants were given six structural formulas of organic compounds that ranged in preliminary *Chemical Notation Complexity Scores* from 19 to 79. A table of the structures, and complexity scores can be found in Appendix B.

Different formats were used in the presentation of the formulas. Five formulas used a bond-line format. Of these five formulas, two used notation with explicit terminal hydrogens. The sixth structure used condensed structural notation. The structures were presented to the participants in random order.

Procedure. A week before the interview, experts were given an electronic copy of the rubric and associated material. During the interview, I used a semi-structured interview protocol. Field notes were collected for analysis. Each participant was asked if he/she had any questions about the wording, terminologies, or definitions used in the rubric or accompanying material. Next, the participant was asked to comment on the ability of the rubric to adequately quantify the perceptual elements in the samples of chemical notation provided.

Each participant was asked to complete a visual sorting task where he/she had to arrange six structural formulas in order from least visually complex to most visually complex and comment on the criteria used for the final arrangement. I shared the ordering, as predicted by the rubric, and asked the expert to comment on differences, if any, between his/her initial ordering and the rubric's ordering. Finally, the expert was asked if there was anything that he/she would change about the rubric based on his/her knowledge of how humans encode information.

Analysis. Field notes were analyzed for emergent themes. Overlap between the experts and the theoretical construct were used to further develop the rubric. Modification to the rubric based on the emergent themes is discussed in Chapter 4.

Part 2: Construct Validity

This type of validity determines how well the rubric measures a theoretical construct. This is an ongoing measurement and "no single, quick, efficient method exists for determining construct validity" (Groth-Marnat, 2009, p. 20). For this study, rubric scores were correlated with those from related constructs (Groth-Marnat, 2009).

This rubric was designed to calculate a score for the visual complexity of an organic molecule based on the number of perceptual elements used in organic chemistry notation (*Organic Chemistry Notation Complexity Score*). It has been shown that as the number of elements in a diagram increases, the performance on a recall task decreases (Winn & Sutherland, 1989). Therefore, the ability of the students to reproduce the structure from memory should decrease as the *Organic Chemistry Notation Complexity Score* increases.

This was the first study that used the *Complexity Rubric for Organic Chemistry Notation.* In the future, new relationships between complexity predicted by the rubric and other variables will be investigated and validated. Additional data will increase the level of confidence that the rubric can be used to measure the visual complexity of organic chemistry notation.

Participants. Thirty-five undergraduate students enrolled in three separate sections of a general chemistry laboratory course participated in this study. This class was chosen because students in this course were able to identify elements on the periodic table (a skill taught in general chemistry) but had received little to no formal education in organic chemistry during the semester. Students were surveyed on their educational experience with organic chemistry. Of the thirty-five students, one student had one or more classes in organic chemistry in college and four had significant introductions to organic chemistry in high school. The rubric was designed to quantify the perceptual element of a structural formula as perceived by a novice early in organic chemistry instruction. As students progress in their study of organic chemistry, they develop strategies for "chunking" features of chemical notation. This ability to chunk certain configurations of bonds and/or atoms allows participants to recall more information than novices with little exposure to organic chemistry. Because of this advantage, the five students with significant experience in organic chemistry were omitted from the study.

Participation was voluntary. As compensation for participation in this portion of the study, all participants were entered in a drawing for two 25 dollar gift cards. Participation in

the study was voluntary. Sampling was not random because students self-selected into the course and the lab sections by enrolling in the course.

Materials and Procedure. A computer animation, developed in Microsoft PowerPoint, was used to present six molecules and six chemical equations. All molecules and equations were represented using structural formulas in either bond-line or condensed format. The animation consisted of a screen with a description of the experiment (self-paced), a screen of instructions (self-paced), the presentation of molecules, and the presentation of equations.

In the presentation of the molecules, the participant was shown each molecule for 30 seconds on the computer screen. Once the 30 seconds had elapsed, a blank screen appeared for 2 seconds. Then six choices were displayed on the screen – one correct choice and five distractors. Once the participant indicated that he/she was ready to proceed (keystroke), a blank screen appeared for 5 seconds, followed by a randomly selected molecule that appeared on the screen. This was repeated for all six molecules. The presented of equations was the same as that of molecule; however, the participant was shown the equation for 45 seconds instead of 30 seconds. Once the 45 seconds had elapsed, a blank screen appeared for 2 seconds, and then six choices were displayed on the screen. Once the participant indicated that he/she was ready to proceed, a blank screen appeared for 5 seconds and a new equation was presented. This was repeated for the remaining five equations.

Molecules used in this validation study were distributed across three levels of complexity based on *chemical notation complexity score* from the rubric: low (0-19),

medium (20-39), and high (40-59). I chose these cutoffs based on the range of complexity scores found during a previous informal analysis of two current commercially published organic chemistry textbooks. The typical range of complexity scores for the textbook molecules surveyed was 10 - 100, with a majority of the structures ranging from 10 - 60. Cutoffs were assigned by dividing this range into thirds. The molecules for each level are shown in Appendix C.

Equations used in this validation study all contained one reactant, a specified reaction condition, and one product. All the reactions selected were the addition of hydrochloric acid to an alkene producing an alkyl chloride. The reactants (alkenes) and products (alkyl chlorides) were selected so that the average complexity for the molecules in the equation (excluding the reaction conditions) were within the following ranges: 0-19, 20-39, and 40-59. Two equations were chosen for each range. The same criteria as that used for the molecules were used for the equations. The equations for each range are given in Appendix C.

Procedure. The Construct Validity Study was conducted during the end of the chemistry laboratory period. Using a paper-and-pencil survey, each participant was asked two multiple-choice questions relating to possible participation in other research related to this project and previous educational experience in organic chemistry. The first question was designed to ensure that there was no "cross-over participation" among the parts of the validation study. The second question was designed to identify those participants with significant educational experience in organic chemistry.

Participants were then instructed to read the directions carefully and not to make any drawings or notes during the experiment. The participants viewed a computer animation, which presented six molecules in random order, followed by six chemical equations in random order. After each molecule or equation was presented, the participant was given six choices and instructed to record the letter that best corresponded to the molecule he/she had viewed. All answers were recorded on the paper-and-pencil survey.

Analysis. Each response to the 12 multiple-choice selections was scored as follows: a correct answer received a score of 1 and an incorrect answer received a score of 0. Since the literature suggested that the ability of the participants to recall structures from memory would decrease as the complexity score increased, for each level of complexity, a reproduction score was calculated. The *low complexity reproduction score* was calculated by summing the scores for low complexity molecules and equations. The *medium complexity reproduction score* was calculated by summing the scores for the medium complexity molecules and equations. The *high complexity reproduction score* was calculated by summing the scores for the high complexity molecules and equations. These scores were compared to determine if there was a significant difference in the participants' ability to recall the structures based on complexity.

Since the responses to the survey were not normally distributed (Kolmogorov-Smirnov $D(108) = 0.221$, $p < 0.001$), the dataset was analyzed using the Friedman Test (Pallant, 2010), a non-parametric method of analysis analogous to the one-way ANOVA with repeated measures. A Friedman test was conducted to evaluate the differences in

reproduction scores for low, medium, and high visual complexity stimuli across all the participants.

When differences were identified, the Wilcoxon Signed-Rank Tests on the different combinations of related groups was used to compare the following combinations: low complexity figures to medium complexity figures; low complexity figures to high complexity figures; and medium complexity figures to high complexity figures. Since multiple comparisons were made on the results of the Wilcoxon test, I used the Bonferroni adjustment to reduce the likelihood of committing Type I error and concluding that a result was significant when it was not. To calculate the Bonferroni adjustment, the significance level initially used (0.05) was divided by the number of tests run (3), 0.05/3 = 0.017. This means that if the *p* value is larger than 0.017, the results are not statistically significant.

Part 3: Predictive validity

This step of the validation process determined if the rubric could predict the complexity of a molecule (Groth-Marnat, 2009). The rubric was used to identify and quantify the perceptual elements that a novice would identify during the encoding of such chemical notation. The central question for this validity study was as follows: Can the rubric predict how novices would score the complexity of series of structural formulas presented in organic chemistry notation?

Participants. Thirty-two undergraduate students enrolled in a general chemistry for non-science majors participated in this study. Students in this course were able to identify elements on the periodic table (a skill taught in general chemistry) but had received little to

no formal instruction in organic chemistry. A little over half (53%) of the participants reported that they had never taken a class that covered topics in organic chemistry. The remaining 47% reported that their only exposure to organic chemistry was a brief introduction to organic chemistry in high school.

Participation was completely voluntary. As compensation for participation in this part of the study, volunteers were entered into a drawing for a 25 dollar gift card. Sampling was not random because students self-selected into the course by enrolling in the class.

Materials and Procedure. A paper-and-pencil survey was used for this validation study. A copy of the survey is located in Appendix D. On the first page of the study, the participant was asked two multiple-choice questions relating to possible participation in other research related to this project and previous educational experience in organic chemistry. The first question was designed to ensure that there was no "cross-over participation" among the parts of the validation study. The second question was designed to identify those participants with significant educational experience in organic chemistry that may confound the results.

On the second page of the survey, the student was given structural formulas for six molecules of varying complexity labeled "A" through "F". The order of the molecules was random. The structural formulas used in this study were in the following ranges of complexity according to the *Complexity Rubric for Organic Chemistry Notation: 10-24, 25-39, 40-54, 55-69, 70-84, and 85-100.* These cutoffs were chosen by me and reflect the range of complexity scores found during an informal survey of two organic chemistry textbooks

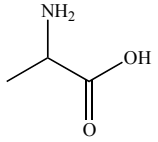
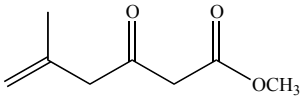
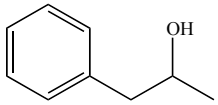
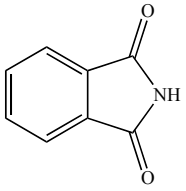
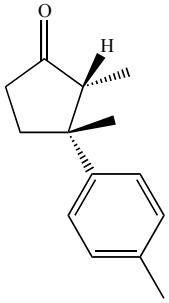
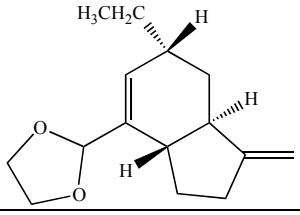
(Carey, 2006; McMurry, 2004). The typical range of complexity scores for the textbooks surveyed was from 10 to 100. Cutoffs were assigned by dividing this range into sixths.

Procedure. The Predictive Validity study was conducted in the last 10 minutes of a regular class period of general chemistry for non-science majors. Using a paper-and-pencil survey, participants were asked to judge the complexity of six structures and rank order the six structures from least complex to most complex. Participants were also asked to provide a brief written explanation of the criteria they used to order the molecules.

Analysis. To study the differences in the linear orderings of the participants, the linear order of structures A through F was determined based on the Complexity Rubric for Organic Chemistry Notation (Table 7). Based on the scores from the rubric, the predicted linear ordering of structures A - F was determined by me and validated by one other chemical education researcher.

Table 7

Molecules for Part 3: Predictive Validity and Their Molecular Complexities

Letter	Chemical Notation Complexity Score	Structural Formula
B	19	
A	38	
E	48	
F	58	
D	80	
C	98	

Each participant response was coded using the following scheme: the molecule that the participant ranked the least complex was given a position score of 1, the molecule that the participant ranked as the most complex was given a position score of 6. The remaining

molecules were assigned a score based on where they fell within this range. For example, a linear ordering B-A-C-D-F-E would have the following position scores assigned to each letter: A (2), B (1), C (3), D (4), E (6), and F(5).

A one-sample t-test for each item on the survey was conducted to determine if the mean position score for each molecule was equal to the position score assigned based on the *Complexity Rubric for Organic Chemistry Notation*. It was hypothesized that if the rubric worked correctly, there would be no significant difference between the mean score for at least five of the six (83% accuracy) structures and the assigned score predicted by the *Complexity Rubric for Organic Chemistry Notation*.

To compare the linear orderings assigned by the participants with the linear ordering predicted by the rubric, I used string edit distances (Levenshtein, 1966). In this technique, the amount of difference between two linear orderings, or strings, can be measured using the Levenshtein distance (LD). This metric is defined as the minimum number of deletions, additions, or replacements (edits) that must be made to one string so that it matches another string. For strings that are similar, this index value is small. However, as the strings become more dissimilar, the LD becomes increasingly larger. Each participant's linear ordering was compared to the linear ordering predicted by the rubric using custom java software designed for this project, LevD. Since the string length for all the data was the same, the average LD for all the linear orderings was calculated. If the average LD was greater than two, it indicated that more than two edits (deletion, addition, or replacement) was necessary to match the linear orderings from the participants to the one predicted by the rubric. A minimum of two

edits was chosen because this is the smallest Levenshtein distance for the transposition correction of two molecules in the linear ordering.

Since the LD was greater than two, the written responses of the participants were analyzed for common themes. To facilitate the analysis of themes, the mean position scores for the participant linear orderings were used to generate an mean linear ordering. This mean linear ordering was then compared to the predicted linear ordering and a LD was calculated. Written responses of participants whose linear ordering closely matched the mean linear ordering were analyzed.

Investigation of "Geometric Chunking"

The results of Part 2 and Part 3 of this study are presented in Chapter 4. They indicate that, while the rubric was able to adequately characterize the complexity of larger molecules, the rubric was not as successful with less visually complex molecules. The analysis suggested that familiarity with specific geometric features of the molecules might facilitate recall. The details of these analyses are discussed in Chapter 4.

As discussed in Chapter 2, familiar shapes have a higher base-level activation for the chunk and retrieval from memory is faster and more accurate. It was hypothesized that knowledge from domains outside of organic chemistry allowed participants to chunk visual information into familiar patterns. This in turn would facilitate recall. For example, consider the following structure of 1-bromo-2-methylcyclohexane in (Figure 25), whose *Organic Chemistry Notation Complexity Score* for this formula is 38.

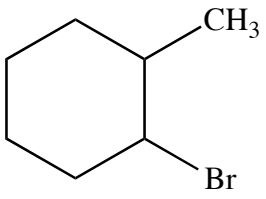


Figure 25. Bond-line structural formula of 1-bromo-2-methylcyclohexane.

It is hypothesized that instead of seeing the ring as six carbon atoms (five secondary carbons and one tertiary carbon) bonded together, the participant recognizes the ring as the hexagon, a geometric shape. During encoding, the participant might chunk the features as this familiar shape rather than as a collection of bonds with a specific arrangement of the carbon atoms. Unlike the participants, the rubric handles single rings as a collection of bonds rather than chunking them into a single geometric shape. As a result, it would overestimate the complexity score for structures containing a ring. To investigate this phenomenon the following small-scale study was carried out.

Participants. Ten volunteers were solicited from the undergraduate general chemistry laboratory course. Students in this course were able to identify elements on the periodic table (a skill taught in general chemistry) but had received little to no formal education in organic chemistry as part of the course. All ten participants reported that they either had never taken a class that covered topics in organic chemistry or had had only a brief exposure to organic chemistry in high school or college.

Participation was voluntary. As compensation for participation in this portion of the study, volunteers were entered into a drawing for a 25 dollar gift cards. Sampling was not random because students self-selected into the lab section and course by enrolling.

Materials and Procedure. Five molecules were selected for inclusion in this study (Appendix E). All the molecules selected contained at least 1 ring in the structural formula. Included in the study were a 5-membered ring, a 6-membered ring, a 7-membered ring, a benzene ring, and a bicyclic system that contained two rings fused along one edge. The 5- and 6-membered rings were selected because of their direct association with the geometric shapes, pentagon and hexagon. The benzene ring was chosen because it resembled a hexagon with alternating double bonds. The 7-membered ring was selected because a heptagon is not a commonly used shape, and I was interested in how participants would encode an unfamiliar geometric shape. Finally, the bicyclic system was selected because of its overall complexity due in part to the inclusion of two rings. All the structural formulas were presented in bond-line format with explicit terminal hydrogens. All structures were printed on index cards and shown to the participants in random order.

Procedure. This investigation was conducted at the completion of a general chemistry laboratory class. Sessions took approximately 10 minutes. The participant viewed a structural formula of an organic compound containing one or more rings for 15 seconds. The formula was hidden, and the participant was asked to verbally describe the molecule. The interviewer drew a structural formula from the participant's description. The drawing was shown to the participants, and he/she was given an opportunity to make corrections if necessary. This process was repeated for 5 structural formulas. The data collected included audio recordings, interviewer's notes, and written artifacts.

Analysis. The audio recordings were reviewed and directly coded using the qualitative

analysis software, "Observe" (version 0.9). Full transcripts were not made. Two chemical education researchers coded the interviews. From the codes, three themes for how participants remembered chemical structures were identified. Results from this investigation are reported in Chapter 4.

Study 2

Study 2 used eye-tracking methodologies to validate the proposed process model for the comprehension of organic chemistry notation proposed in this dissertation. It also addressed two questions that are directly linked to this validation process. These questions investigated how participant characteristics influence viewing patterns on specific regions of the reaction equation.

There were two levels of specificity used when categorizing specific regions of the reaction equation were area of interest (AOIs) and region of interest (ROI). AOIs were researcher-defined areas of the screen that contain one of three distinct features of the chemical equation, such as reactant(s), conditions, or products. In the case of bimolecular equations involving two reactants, each reactant had a separate AOI. Because they were the same in all the equations, other notational features (including arrows and plus signs) were ignored for this study and not included in AOIs. The second level of specificity looked at specific regions within the equation where participants focused attention. ROIs were mathematically defined areas of the screen based on the fixation patterns of the participants. ROIs were coded as informative or distractor ROIs. Informative ROI (iROI) contained

information necessary to understand the chemical reaction. Distractor ROI (dROI) contained information that was not necessary to understand the chemical reaction.

Research Questions

5. To what extent does the process model for the comprehension of organic chemistry notation account for eye fixations (frequency and duration) of participants reading organic chemistry equations?
6. For high versus low complexity chemical equations, what are the effects of different participant variables (expertise, spatial ability, and working memory capacity) on the frequency and duration of eye fixations as measured by the eye tracker for:
    c. Informative ROIs versus distractor ROIs?
    d. AOIs (reactant, condition, product)?
7. For high versus low complexity chemical equations, is there a difference in the sequence of fixations (both intramolecular and intermolecular) between AOIs as participants "read" organic chemistry equations for:
    d. Experts and novices?
    e. Participants of differing working memory capacity?
    f. Participants of differing spatial ability?

Participants

Recruitment for this study took place over one academic year. A total of 36 people volunteered to participate in this study, including 25 novice participants and 11 expert participants. The novice participants included undergraduates who were enrolled or had

completed the 2-semester sequence of organic chemistry (n = 17); graduate students with a bachelors degree in chemistry or biochemistry and were pursuing advanced studies in fields other than organic chemistry (n = 7), and a chemistry department staff member who completed a BS in chemistry (n = 1). The experts were instructors from three different institutions who had taught organic chemistry topics in courses for a minimum of 3 years. One expert had a Masters degree in organic synthesis, three experts were advanced graduate students in organic chemistry, and seven experts had doctorates in a variety of chemistry specializations (organic chemistry, n = 2; bioorganic chemistry, n = 2; analytical chemistry, n = 1; inorganic chemistry, n = 1; physical chemistry, n = 1). One expert participant withdrew from the study. These data were excluded from analysis. Participation in the study was voluntary, therefore, the sample for this study was self-selected.

The remaining participants (n = 35) were eye-tracked and useable reading time data was collected for all 35 participants. Technical problems with the eye-tracker that created data errors prevented access to useable eye movement data (fixation duration and scanpath) for one expert and six novices. For the remaining 28 participants, 19 novices and nine experts were successfully eye tracked. High error rates in the eye movement data for one expert lead to a sampling accuracy of 2%. The eye movement data for this expert was discarded. For this study, eye movement data (fixation duration, fixation frequency, and eye fixation pattern) were analyzed for 27 participants (novices, n = 19; experts, n = 8).

Compensation of participants. All participants were compensated a total of $30 for their participation in this study. Participation time was a maximum of two hours per participant.

Expertise and demographics. Expertise was assigned based on the participants' experience in organic chemistry. Novices were recruited from undergraduate students enrolled in the 1-year sequence in organic chemistry; advanced undergraduates in chemistry and biochemistry; and graduate students and staff whose highest level of education in chemistry was a bachelors of science in chemistry or biochemistry. The graduate students were pursuing advanced studies in fields outside of organic chemistry. Experts were recruited from instructors at three post-secondary institutions. The participants taught organic chemistry topics in lecture or lab for a minimum of three years. A demographic survey was used to validate this classification based on the participants' experience in chemistry. Separate surveys were developed for novices (Appendix F) and experts (Appendix G). Both surveys collected information on participants' educational background, research experience, and literature usage. The paper-and-pencil survey were delivered electronically a week before the eye tracking. The results of these surveys were used to inform the interpretation of eye movement data.

Materials and Procedure

Working memory span. The concept of working memory assumes that there exists a limited capacity system for a wide variety of cognitive tasks. For this study, the Digit Span Backwards (DSB) test was used to measure the working memory span of participants.

In the DSB, participants are read sets of numbers and asked to write them in reverse order. Both storage (number heard) and processing (mentally reverse the sequence of numbers) are involved in this task. The "digit span", an index of working memory capacity, was measured by measuring the largest set of numbers in which the participant consistently recalls the reversed sequence of numbers. Research suggested that achievement on organic synthesis problems decreases if both the amount of information that is held in working memory and the number of processes required to complete the task exceeds the working memory capacity as measured by the DSB (Tsaparlis, 1998; Tsaparlis & Angelopoulos, 2000).

Since it has been suggested in the literature that working memory capacity, as measured by the DSB test, can be used as a predictor for organic chemistry achievement, it was chosen as the measurement tool for working memory capacity in this study. For this study the DSB test was administered at the start of each eye-tracking session. The procedure used for this test is outlined in Appendix H. The complete test took approximately 10 minutes.

Spatial ability. The Purdue Visualization of Rotations test (ROT) was used to measure the spatial ability of participants (G. M. Bodner & Guay, 1997). The ROT is a subset of 20 multiple-choice questions from the Purdue Spatial Visualization Test Battery (Guay, 1977). The questions on the ROT are analogy-type questions using flat projections of three-dimensional objects. In the first analogy pair, participants are given two projections of the same object in different orientations and asked to study how the object was rotated.

Participants were then presented with a second object. They must mentally rotate the second object and select the figure from the five choices that were rotated the same way as the first analogy pair. The Kuder-Richardson 20 (KR-20) for this test is reported as 0.78 – 0.80, suggesting that the ROT is internally consistent (G. M. Bodner & Guay, 1997).

Research suggests that this test may be useful in studying performance in organic chemistry, especially for problems where participants outline multi-step syntheses, complete a reaction scheme, or manipulate two-dimensional representations (Pribyl & Bodner, 1987). The conclusion made by Pribyl and Bodner was that students with high spatial ability are better at "understanding" the problem containing a reaction mechanism than students with low spatial ability. As discussed in Chapter 2, success in problem solving relies on the ability of a student to read and comprehend a given problem statement and create accurate internal representations in working memory. Since spatial ability has been shown to influence achievement in organic chemistry, it may be a variable linked to the comprehension of organic chemistry notation.

For this study, the ROT was administered at the end of the eye-tracking session. Participants completed a paper-and-pencil version of the test. The total time commitment for the ROT was 10 minutes. A copy of the ROT, including directions, can be found in Appendix J.

Chemical Reactions. A total of 10 chemical equations were selected for Study 2. The *Complexity Rubric for Organic Chemistry Notation* was used to assign a complexity score to each of the equations used in this study.

Complexity of chemical notation. Complexity was measured using the *Complexity Rubric for Organic Chemistry Notation* developed and validated in Study 1. The average chemical notation complexity (ACNC) score was used to characterize reactions into low complexity and high complexity subsets. The *ACNC score* is the cumulative mean score for all the molecules in the chemical equation given by the equation $ACNC\ score = 1/n \sum X_i$,for i=1 to n. Where X is the *complexity* score as calculated using the *Complexity Rubric for Organic Chemistry Notation* for a molecule in the equation (i) and *n* is the total number of molecules in the equation. Since the reactions are in matched High/Low complexity pairs, scores are not be calculated for elements that remain the same between the pairs, namely the arrow, "+" sign, and reaction conditions. This average is used to classify chemical equations as high or low complexity.

Equations. Participants viewed a total of 10 equations. Five chemical reactions were selected from the material typically covered in the one-year organic chemistry course and were identified as reactions typically used in upper level chemistry courses, such as natural product synthesis. For each reaction type, a pair of equations was used - one with an average complexity score ranging from 50 to 90 (high) and the other with an average ranging from 1-25 (low). The average complexity score for reactants and products was used due to the difficult nature of finding chemical transformations that result in roughly equal complexity scores for the reactants and products. The ACNC score was calculated based on the complexity for all the molecules involved in the reaction (excluding the reaction conditions). The High/Low complexity pairs are given in Appendix I. Topics 1, 2, and 5 of

the high/low complexity pairs were unimolecular reactions, which involved the transformation of a single organic molecule into a new organic molecule under certain reaction conditions. The remaining two equations (Topics 3 and 4) were bimolecular reactions, which involve the combining of two molecules under specific conditions to form a single new molecule.

Post-test. A post-test was administered as part of this study (Appendix L). One set of questions was developed for each reaction high/low pair. Each set of questions consisted of two pages. On the first page, participants were given the picture of the reaction equation and asked about their familiarity with the overall equation, molecules, and functional groups. The second page of the post-test focused on specific questions about the reaction. These questions included an assessment of the viability of the reaction, types of conditions used in the reaction, specific characteristics of the chemical transformation, and information about how the reaction took place (reaction mechanism).

The purpose of the post-test was two-fold. The first purpose of the Post-test was to inform the analysis of the eye tracking data, but the main purpose was to help guide the participants in their reading. Participants completed the first set of questions on the Post-test after viewing the first equation. The questions on the second page were designed to reinforce the idea that comprehension meant reading the equation in an effort to understand the chemical transformation occurring, rather than just looking at surface changes to the structures (lines and letters). Because the main purpose of the Post-test was act as a prompt for readers, no formal analysis of the Post-test was planned as part of this study.

Equipment

Eye-tracking methodology was used to collect information on eye movements of participants as they read organic chemistry equations. Equations were displayed using a Tobii T120 Eye Tracker (Tobii Technologies, Inc., 2008). The T120 Eye Tracker hardware was integrated into a 17" thin-film transistor display (maximum resolution 1280X1024 pixels), appearing to the participants as a standard flat panel computer monitor. During tracking, the participant sat approximately 70 cm from the monitor. Near infrared diodes built into the display generated reflection patterns on the corneas of the participant's eyes. The image sensor hardware collected these reflection patterns and other visual information from the participant. The data rate for this eye tracker was 120 Hz, which translates to 120 points per second collected for each eye. The image processing software identified relevant features for each point, such as the position of each eye and the corneal reflection pattern. The three-dimensional positions of each eyeball in space and where the participant was looking (gaze point) were calculated. The Tobii T120 Eye Tracker reported the following data for each eye:

1. Time – a timestamp in microseconds when the gaze data was recorded.
2. Gaze point position – the normalized horizontal and vertical position of the gaze point.
3. Eye position – the horizontal and vertical position of the pupil from the camera image.
4. Eye Distance - the distance (millimeters) from the eye to the camera.

5. Pupil size– calculated size of the pupil in mm.
6. Validity Code – measurement of the system's certainty that the correct data was recorded.

Tobii-Studio analysis software was used to manage and analyze gaze point data.

Unlike head-mounted eye trackers, the Tobii T120 Eye Tracker did not impose physical restrictions on the participants. While looking at the monitor, data was collect simultaneously from both eyes during eye-tracking sessions. To compensate for head movements that are inevitable, the tracker uses a wide field of view (22x22x30 cm at a distance of 70 cm from the screen). This translates to the system tolerating head movements up to 30 x 22 x 30 cm with a maximum velocity of 35cm/s for a participant at a distance of 70 cm. The system recovers from "tracking failure" such as when a participant blinks or looks away from the screen, in 100 milliseconds (on average) after movements cease.

Procedure

This study was conducted during individual, one-hour sessions. Prior to each session, participants completed a paper-and-pencil demographic survey. During the session, participants completed the DSB test, the calibration of the eye tracker, eye tracking, and the ROT.

Prior to eye-tracking session. At least 48 hours before the scheduled eye tracking session, participants were emailed the demographic survey and asked to bring the completed survey to the eye tracking session. The survey was self-paced, with no time limit. Five

participants did not complete the survey prior to the eye tracking session. These participants were given time at the end of the one-hour session to complete the survey.

One-hour session. Each individual session lasted approximately one hour. The DSB was administered using the procedure outlined in Appendix G. Following the DSB, the Tobii eye tracker was calibrated for the participant. The participant was seated at the eye tracker, approximate 70 cm from the screen. The calibration process was automated by the system and took up to 60 seconds to complete. Next, the participant was eye tracked using the procedure outlined in Appendix K. During the eye-tracking session, participants viewed a series of static organic chemistry equations sequentially. Participants were given unlimited time to view the equations. All participants read the five high/low complexity pairs. The participants completed the Post-test. Finally, The paper-and-pencil ROT was administered to the participant with a 10-minute time limit.

Analysis

Data aggregation tools. Tobii Studio (version 2.0) analysis software used in conjunction with the Tobii eye-tracker hardware provided a means for aggregating the data set for analysis. Four semi-automated analysis tools were used to address the research questions including Area of Interest (AOI) definition tool, cluster tool, and hot spot visualization tool.

Area of Interest definition tool. This semi-automated analysis tool was used to define areas of interest (AOIs) in the stimuli. AOIs aggregate the data by defining regions of the screen that contain features of interest. Fixations within the AOI can be analyzed for

frequency and duration, giving the researcher an indication of how information in the AOI is processed. This technique has been used in a variety of content areas, including medicine (Augustyniak & Tadeusiewicz, 2006), mathematics (Cook & Reiser, 2005; Epelboim & Suppes, 2001), and physics (Kozhevnikov, Motes, & Hegarty, 2007).

For each equation, I defined an AOI for each of the features of a chemical equation, namely, the reactant(s), conditions, and product. Based on the Tobii recommendations, the AOIs were slightly larger than each of the features (30 additional pixels in each direction). Once defined, the system generated a report for each user that gave a time stamp, the exact XY coordinates (in pixels) for each eye at that time, a validity code for each eye measurement at that time, and a note as to whether the XY coordinates for each eye fell into a specific AOI. Validity codes were defined by the system on a scale of 0-4, with the following interpretation for each code (Table 8):

Table 8

Eye Tracker Validity Codes

Validity code	Meaning
0	All data for the eye has been recorded and there is no confusion between the left eye and the right eye. The user did not blink or look off-screen.
1	Data for only one eye was recorded. Estimations and assumptions are made by the system as to which eye was recorded. The eye that is not recorded receives a validity code of 3.
2	Data was collected for only one eye; however, there is no way to determine which eye (left or right) was recorded.
3	Data for this eye is incorrect or corrupt. The other eye will have a validity code set to 1.
4	The gaze data is missing or incorrect. This may be a sign of that the participant blinked or looked away.

Since this study deals with where the participant is looking rather than the position of each eye, the manufacturer recommended that validity codes for each eye be averaged. Following this guideline, the results are "generally more accurate, and more stable over long time and across changes in head position and light conditions" (Tobii Technologies, Inc., 2008, p. 63). All data points with an average validity code of 2 or higher were not included in this study (Tobii Technologies, Inc., 2008). This removed all data points that were missing, corrupt, incorrect, or based on estimation and assumptions.

The remaining gaze points were aggregated into fixations and the AOI tool calculated the following data for each participant including duration of each fixation within each AOI (ms); number of distinct fixations within each AOI; total duration of fixations in each AOI (ms); and the total number of fixations each AOI. The totals for each of these data

sets were also calculated for each equation across all participants.

Cluster tool. This automated tool is used for the aggregation of gaze data across multiple participants. It created regions of interest (ROI) that represented areas that had a high concentration of fixations. Unlike the area of interest tool, where the definition of AOIs was based on the features of the equation selected by the researcher, this tool used a clustering algorithm to find patterns of eye fixations. This algorithm, based on the robust clustering algorithm proposed by Santella and DeCarlo (2004), uses the iterative mean shift procedure to identify dense regions of fixations or "clusters". Two points are considered to be part of the same cluster if the maximum distance between them is below a pre-set threshold. The threshold for this analysis was set at 50 pixels because it provided good resolution of the clusters and was outside the range of error for the eye-tracker.

The resulting clusters were irregular shapes. Some contained features of the reaction equations. Others contained only white space. Each equation had a different number of ROIs. The ROIs were coded based on the features of the equation they highlighted. Informative ROIs (iROIs) were regions that highlighted features of the equation that were necessary for understanding the chemical reaction. Distractor ROIs (dROIs) were regions that contained features of the equation that were not necessary for understanding the chemical reaction. Off content ROIs (ocROIs) were regions of white space that had patterns of fixations. Off content ROIs were identified, but not analyzed in this dissertation. A second organic chemistry education researcher and an instructor of organic chemistry verified the coding of the ROIs.

The following data were calculated for each participant: duration of each fixation within each ROI (ms); number of distinct fixations within each ROI; total duration of fixations in each ROI (ms); and the total number of fixations within each ROI. The totals for each of these data sets were also calculated for each equation across all participants.

Hot Spot visualization tool. This tool aggregated the gaze data across multiple participants. A visualization of the frequency of fixations was superimposed over each equation creating a heat map. The resulting heat map shows how much participants looked at particular regions of the equation. This tool was used to visualize overall viewing patterns and to examine pattern differences.

Validation of the process model. To validate the process model developed for the reading comprehension of organic chemistry notation, specific eye movements were identified as participants read organic chemical equations. It was hypothesized that each stage of the model would exhibit characteristic eye movements.

Get input. According to the process model, the eyes will remain fixated on the specific region of the chemical equation until all the necessary processing has been completed. Once the processing is complete, the reader will end the fixation and move to a new fixation. The *get input* stage is responsible for the movement of the eye from one fixation to the next. It was hypothesized that the *get input* stage would be characterized by a series of fixations on different regions of the chemical equation. It was further hypothesized that the sequence of the fixations would be similar to that of reading English text, starting

with the leftmost reactant and ending with rightmost product. To validate this stage of the model, the fixations in the AOIs were analyzed. First, the frequencies of fixation within each AOI were examined for patterns of fixation. Heat maps were evaluated to determine if participants fixated on more than one discrete region of the screen.

To determine if there was an overall sequence of fixations for the AOIs across all participants, fixations on the AOIs were analyzed using string edit distances (Levenshtein, 1966) and Levenshtein distances were calculated for each equation. For sequences that are similar, this index value will be small. However, as the sequences become more dissimilar, the Levenshtein distance will become increasingly larger. This technique for analyzing sequence alignment has been used by other to analyze eye movement data (Josephson & Holmes, 2002; Lorigo et al., 2008; West, Haake, Rozanski, & Karn, 2006). For this study, the Levenshtein distances were calculated using a custom java program.

To determine if there is an overall sequence to reading a chemical equation similar to that for reading English text (left to right across a line of text), the pattern of first fixations for each of the AOIs were compared with the proposed string of fixation that starts with the leftmost reactants and ends with the rightmost product.

Regressive eye movements, where the participant looks back at a previously viewed AOI, were ignored for this analysis. There are two main causes of regression: 1) the initial saccade was too long and the participant must adjust the fixation for reading to continue efficiently, or 2) the participant did not understand the text from the previous fixation

(Rayner, 1998). In general these causes for regression are participant and case dependant. Since validation of this stage of the process model requires that I show that there exists several fixations across the chemical equation, only the sequence of initial fixations were analyzed. Fixations, caused by correction of a saccade or lack of comprehension, were ignored in this analysis. The patterns of first fixations were used to discuss the similarities and difference between the proposed sequence of fixations and the observed fixations. Number and percentages of specific first fixation patterns will be reported.

Search. This stage provides for the systematic intramolecular search of a given structure of an organic molecule. It was hypothesized that the *Search* stage would produce fixations that are specific to reading a structural drawing for one molecule in the chemical equations before moving to the structural drawing for another molecule. This stage would be characterized by a series of intramolecular fixations rather than one fixation per molecule. To validate this stage of the model, eye fixation frequencies for ROIs were reported.

Unlike the *get next* stage, the *Search* stage did not have a specific sequence but was highly dependant on the structure of the molecule being viewed. It was hypothesized that there would exist sequential searches within the same molecule, looking at various sub features of each molecule in turn. This was analyzed for all molecules in the equation. To analyze the sequence of eye fixations for each molecule for common or overlapping sequences of first fixations, custom software (NMerGen) was developed using Java. This software provides a frequency for each possible sequence, n units in length, in a given series

of eye fixations. For this study, a three-fixation sequence was used to investigate intramolecular search. Since the literature suggests that 3-fixations is the maximum sequence that can be interpreted (Underwood, et. al., 2003), 3-fixation patterns were used. The frequencies of intermolecular transitions for each molecule in the equations were reported.

Encoding and access lexicon. As the intramolecular features are encoded, an internal representation of the chemical equation is created. The meaning of features in the chemical notation (including arrangements of atoms, lines, alphanumeric characters, and geometric figure) is accessed from the lexicon. Linked by semantic networks, these meanings are connected to other concepts, which may include the name of a functional group, information about the three-dimensional shape of the feature, common reactions involving that functionalization, electronic effects, and reaction used to produce the functionalization. Just and Carpenter (1987) proposes that the reader has "an indexing scheme that allows him [or her] to evoke any lexical entry directly" (p. 69). As the reader is exposed to more chemical notation, he/she develops new links between the written form of the notation, entries in his/her mental lexicon, and associate concepts. These links influence the speed by which a reader can access the meaning of a word. Words that are used more frequently can be accessed faster and with more accuracy than lower frequency words. During the reading, once a word is encountered and working memory has accessed the meaning, the processing of subsequent instances of the word in the text will take less time. *Encoding and lexical access* can therefore be characterized by the duration of fixations on a

repeated viewing of portions of the molecules. It was hypothesized that the duration of the first fixation on a molecular feature is longer than the mean duration of all subsequent fixations on the same molecular feature. This is called the repetition effect.

ROIs were used for this analysis. The ROIs selected for this portion of the analysis contained the same molecular feature, for example a –CH3 group. Some chemical equations were not suited for this analysis because recurring molecular features could not be identified. A subset of the chemical equations was, therefore, used for this analysis, including Topic 1, low visual complexity (LVC); Topic 4, LVC; and Topic 5, high visual complexity (HVC). These equations were chosen because one set of ROIs could be closely matched based on molecular feature.

Figure 26 shows the equations and the ROIs selected for analysis. For example, three ROIs were chosen to study this effect in Topic 5, LVC. All three ROIs contained the same molecular feature, a (CH_2 =), in two separate molecules in the equation.

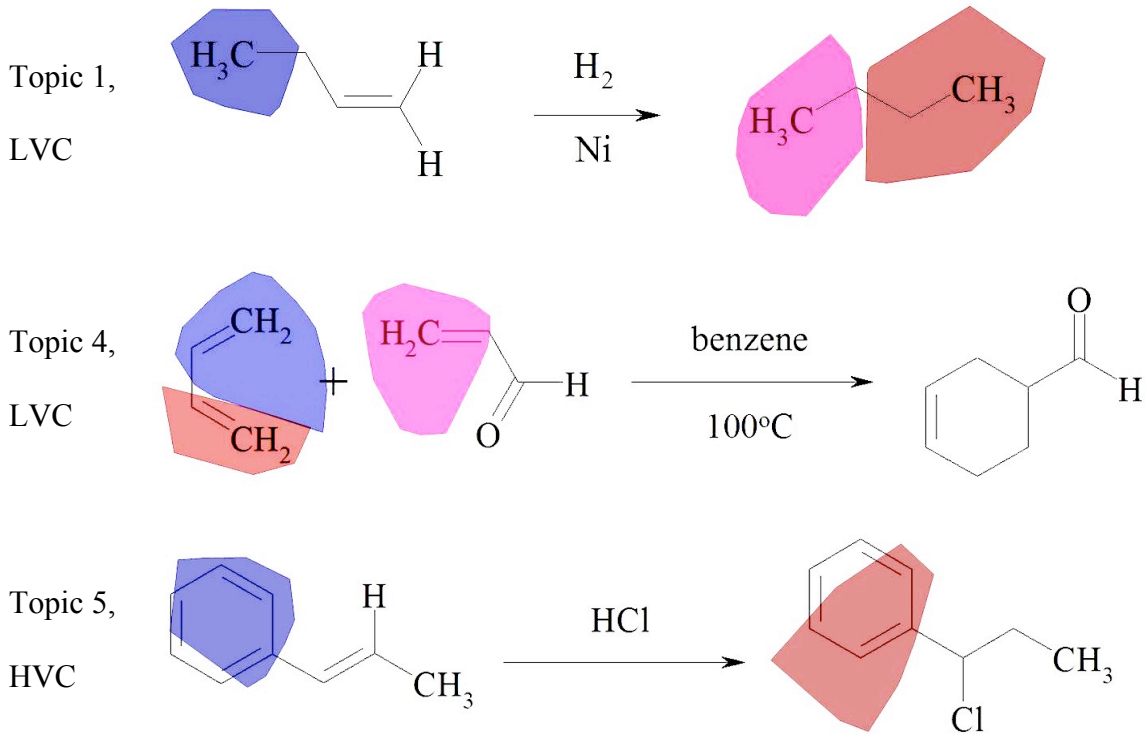


Figure 26. Equations and ROIs selected for analysis. The irregular shaped colored regions are ROIs, as defined by the cluster analysis.

The normality of the data was explored and appropriate data transformations were applied. The first fixation duration for that molecular feature was compared to the mean fixation duration for all subsequent fixations that contained the same molecular feature. Paired-sample t-tests were used to determine if there was a significant difference between the duration of the first fixation and mean of subsequent fixations. Geometric means and confidence intervals were reported as part of the analysis.

Intramolecular relationships. The Intramolecular relationship processes are responsible for determining the relationships (conceptual, spatial, etc) between features within a single molecule. This stage of the model is evidenced by a series of fixations within

the same molecule before the reader moves to a fixation in another part of the equation. The duration of these fixations is different depending on the role the molecular feature plays in the chemical reactivity of the molecule. Features that are directly involved in or influence the chemical reaction (iROI) require more processing than features that do not (dROI). Therefore, I hypothesized that iROIs would have longer fixation durations than dROIs in each molecule.

The normality of the fixation durations was explored. If the data were normally distributed, repeated measures ANOVA would be used to determine if there was a difference in fixation durations for iROI and dROI. However, results from the normality assessment (presented in Chapter 4) indicated that the dataset was not normally distributed. The nonparametric Wilcoxon signed rank test was used to compare the percent fixation duration on iROI to dROI for each molecule ($n = 21$).

To better understand the types of relationships that participants identify within the molecule, 4-fixation patterns were analyzed to look for trends in the reading patterns. A sequence of four fixations was chosen for analysis because it is the maximum number of ROI in a given molecule for this dataset. Since the patterns were only analyzed for frequency and not interpreted for intention of the participant, the larger fixation pattern was examined. The top five fixation patterns for each equation (according to frequency) were coded for the following patterns: fixations within the same iROI; a combination of fixations between one iROI and one dROI; fixations among different iROI; fixations within the same

dROI; and the combination of 2 iROI and 1 dROI. The frequency of each type of fixation is presented.

Intermolecular relationships. The Intramolecular relationship processes are very similar to those of *Intramolecular Relationship*. *Intermolecular Relationships* are responsible for determining the relationships (conceptual, spatial, etc) between molecules in the entire equation. This stage of the model is evidenced by a series of fixations across all the regions of interest in the entire equation. Like the intramolecular relationship stage of the process model, the duration of these fixations is different depending on the role of the molecular feature plays in the entire chemical reaction. Features that are directly involved in the chemical reaction (iROI) require more processing than features that do not participate in the reaction (dROI). Therefore, iROI have longer fixation durations than dROI across the entire equation.

The normality of the fixation durations was explored. If the data had been normally distributed, repeated measures ANOVA would have been used to compare the fixation durations of iROI and dROI across the entire equation. However, results from the normality assessment (presented in Chapter 4) indicated that the dataset was not normally distributed. The nonparametric Wilcoxon signed rank test was used to compare the percent fixation duration on iROI to dROI for each molecule ($n = 21$).

To better understand the types of relationships that participants created during the reading process, three-fixation patterns among the AOI were analyzed to look for trends in

reading patterns. Three-fixation patterns were chosen for this analysis because I was interested in how participants interacted with all three elements of the equation, namely, reactant(s), conditions, and products. All three-fixation scan paths were coded for one of four types of patterns including: 1) fixations on the same AOI (RRR, CCC, PPP), 2) regressions (RCR, RPR, etc), 3) fixation patterns containing 2 different AOIs with no regression, and 4) fixations patterns containing 3 different AOIs. The frequency and percentage of fixations were reported.

Reaction wrap-up. During this stage of the process model, participants check their internal representation for inconsistencies, such as reproduction errors where functionalization is either added or subtracted. In reading studies, the reader tends to pause longer on the last word of a sentence or on the final punctuation (Just & Carpenter, 1980; Mitchell & Green, 1978). This pause is attributed to the process of integrating all the relationships assigned into an overall meaning for the sentence and to check for inconsistencies in these relationships. It was proposed that reading chemical equations would exhibit the same integration stage. This stage would be characterized by a long fixation, just before the participant indicates that he/she comprehends the chemical reaction. The fixation may be on white space, the reaction center, or another feature of the chemical equation.

The normality of the fixation durations was explored. If the data were normally distributed, repeated measures ANOVA would have been used to compare the final fixation

durations to the mean fixation duration of all previous fixations. However, results from the normality assessment (presented in Chapter 4) indicated that the dataset was not normally distributed. The nonparametric Wilcoxon signed rank test was used to compare percent final fixation duration to the average percent fixation duration for all other fixations to determine if there was a difference in the fixation durations. In an effort to understand final fixation patterns further, separate Wilcoxon tests were run on experts and novices to determine if there was a difference in final fixation patterns.

The final fixations were coded for all participants to determine what they looked at before indicating that they understood the reaction. The following codes were used in this analysis: conditions; white space; reactant iROI; product iROI; reactant dROI; and product dROI. Frequencies and percentage of final fixations were reported.

Questions 5. A variety of analyses were used to investigate the following questions: For high versus low complexity chemical equations, what are the effects of different participant characteristics (working memory capacity, expertise, and spatial ability) on the frequency and duration of eye fixations as measured by the eye tracker for:

a. Informative ROIs versus distractor ROIs?

b. AOIs (reactant, condition, product)?

The normality of the dependent variable for each group was explored using SPSS (version19.0) Explore. For each dataset, *z* scores were calculated for the skew and kurtosis using the following formula: z_{skew} = skew / SE_{skew} and $z_{kurtosis}$ = kurtosis / $SE_{kurtosis}$. Because the sample size was less than 30, skew and kurtosis were rejected as non-normal if the

absolute value of the *z-score* was greater than 1.96 (Cramer & Howitt, 2004). The Kolmogorov-Smirnov statistic was also calculated for each dataset. The data was transformed to improve the normality of the distribution using the natural logarithm transformation.

I hypothesized that there would be a significant difference in the viewing patterns of participants while reading equations of high verses low visual complexity.

Participants with low WMC, whose working memory capacity might be overtaxed by the high cognitive demands of reading the chemical equation, would be expected to exhibit longer fixation times and a greater number of fixations than the high WMC participants. This was explored for ROIs, as well as AOIs. Low WMC participants compensated for the high cognitive demand by using diagrammatic offloading. This, in turn, increased the duration and frequency of fixation. As the complexity of the equation increases, the cognitive demands also increase. Therefore, these differences will be greater for HVC equations versus LVC equations. In addition, participants with high WMC will be expected to spend significant more time viewing iROI than dROI. However, there should be no difference in viewing pattern between HVC and LVC equations because the high WMC compensate for the cognitive demands of the equation.

I also hypothesized that there would be a significant difference in viewing patterns based on the expertise of the participant. Experts, who have prior knowledge of the equations and the concepts necessary to understand the reaction, should have overall shorter fixation times and exhibit fewer fixations than novices. This would be exhibited at both

levels of specificity. Considering the ROIs, the prior knowledge of experts allows them to filter out competing information. Therefore, the experts will focus more of their attention on iROIs, successfully filtering out the dROIs. Novices will be unable to quickly filter out the distractor information and will focus more attention on dROIs than the experts. Because HVC equations contain more distractor information, it is hypothesized that differences will be greater for HVC equations than LVC equations.

Finally, I hypothesize that there will be a significant difference in the viewing patterns of participants based on spatial ability (SA). These patterns are similar to those of working memory capacity. Since high SA participants are not overtaxed by the cognitive demands of the notation, they are better at identifying information necessary to understand the reaction. Therefore, participants with high SA will be expected to exhibit fewer and shorter fixations than participants with low SA on both ROIs and AOIs. The high spatial ability participants will spend a greater percentage of their fixations on iROIs than low SA participants, because they are better able to filter out the distractor information. Low SA participants will have a significantly higher number of fixations for dROI and iROI than the participants with high SA because they may be use diagrammatic offloading or other strategies (e.g. comparison) to compensate for the cognitive demands of the equation. These effects are expected to be greater for HVC than for LVC equations.

Separate split-plot repeated measure ANOVAs were conducted to assess the effects of each participant variable on viewing patterns for chemical equations of differing complexity. Two-molecule and 3-molecule equations were analyzed separately using similar

procedures. The within-subject variable was the participant *characteristic* (working memory capacity, expertise, or spatial ability), each with two levels (WMC- high WMC, low WMC; expertise - expert, novice; and SA - high SA, low SA). The within-subject variables were *complexity* of the equation (HVC and LVC) and *content*. For investigation of the ROI, *content* had two levels (dROI and iROI). The within-subject variable *content* had different levels depending on the type of equation - 3 levels (reactant, condition, product) for the 2-molecule equations and 4 levels (reactant 1, reactant 2, condition, product) for the 3-molecule equations. The dependent variables were the mean fixation duration and frequency for the overall comparisons. The mean percent fixation duration and frequency were used to compare ROI viewing patterns.

For ANOVAs that violated the assumption of homogeneity of intercorrelations, a separate analysis was planned. This proposed analysis used separate split-plot ANOVA to characterized differences in viewing behaviors for the HVC and LVC equations. The within-subject variable was the participant *characteristic* (working memory capacity, expertise, or spatial ability), each with two levels (WMC- high WMC, low WMC; expertise - expert, novice; and SA - high SA, low SA). The between-subject variable for the AOI analysis was *content* with 3 levels (reactant, condition, product) for the 2-molecule equations and 4 levels (reactant 1, reactant 2, condition, product) for the 3-molecule equations. While this analysis does not provide a direct comparison of HVC to LVC equations, it does offer insights into the viewing behaviors of participants while reading these types of equations.

Question 2. For high versus low complexity chemical equations, is there a difference in the sequence of fixations (both intramolecular and intermolecular) between areas of interest as participants "read" organic chemistry equations for:

a. Participants of differing working memory capacity?

b. Experts and novices?

c. Participants of differing spatial ability?

I hypothesize that there will be a significant difference in the viewing patterns of participants based on participant characteristics. These differences will be more pronounced in HVC equations than in LVC equations. According to the literature, longer eye fixation sequences indicate a less efficient search (Goldberg, Stimson, Lewenstein, Scott, & Wichansky, 2002). I hypothesize that participants with low WMC or low SA will exhibit significantly longer eye fixation sequences than their counterparts. For low WMC and low SA participants, the high demands of the chemical notation will overtax cognitive resources and hinder these participants from identifying the areas of interest necessary for understanding the reaction. This will lead to more inefficient searching and longer eye fixation sequences. This effect will be more pronounced in the HVC equations.

Prior knowledge is also hypothesized to play a role in the length of the eye fixation sequence. For novices, lack of prior knowledge about the reaction will lead to longer eye fixation sequences. Unable to quickly prioritize areas of interest based on their contribution to the chemical reaction, novice participants cannot easily filter out distractor information. This leads to less efficient searching and, therefore, longer eye fixation sequences than

experts. Experts use their prior knowledge to prioritize informative regions of the equation and create efficient search patterns, leading to shorter eye fixation sequences.

A mixed between-within repeated measure ANOVA was used to compare the length of the eye fixation sequence. The within-subject variable is the participant characteristic (WMC - high WMC, low WMC; expertise - expert, novice; SA - high SA, low SA). The between-subject variables are *complexity* (HVC and LVC) and *equation* (2-molecule equations - Topic 1, Topic 2, and Topic 5; 3-molecule equations - Topic 3 and Topic 4). The dependent variable is the length of the eye fixation sequence.

To further investigate the sequence of fixations during reading, the 3-fixation patterns within the eye fixation sequence were analyzed for common patterns of fixations. Two fixation patterns were chosen for investigation, based on the literature. It has been suggested that regression patterns, fixations that are back and fourth between AOIs/ROIs, indicate inefficient searching (Goldberg & Kotval, 1999). The cognitive resources of participants with low WMC or low SA may become overtaxed with the demands of reading chemical notation and thus hinder their ability to identify features of the equation that are important for understanding the reaction. Similarly, novices' lack of prior knowledge may hinder their ability to prioritize informative features of the equation and they would be less successful at filtering out distractor information than the experts. Both cases would lead to inefficient searching of the equation. I hypothesize that regression patterns will be more common for novices than expert. Similarly, regression patterns will be more common for

participants with low SA and participants with low WMC than their high ability counterparts.

For the intramolecular ROIs, the presence of patterns with successive fixations within the same ROI may be linked to the conceptual importance of that ROI. The literature also suggests that successive fixations within the same AOI can be collapsed into a gaze or dwell (West, Haake, Rozanski, & Karn, 2006; Parasuraman & Rizzo, 2007). Dwells are sequential fixations within the same AOI. Dwell frequency has been linked to the importance of an ROI (Kasarskis, Stehwien, Hickox, Aretz, & Wickens, 2001). ROIs that provide important information have higher dwell frequencies less informative ROIs.

Because of their prior knowledge, experts are able to better filter out distractor information and focus on informative ROIs. It is predicted that the frequency of dwell fixation patterns for iROI will be significantly higher for experts than novices, and the frequency of dwell patterns on dROIs will be significantly lower for experts than novices. Similarly, it is predicted that participants with high SA or high WMC will exhibit the same pattern of dwell fixations as the experts. The high SA or high WMC participants are better able to differential iROI from dROI and filter out the distractor information. Their counterparts, whose cognitive resources may be overtaxed by the high demands of the chemical notation, will be less successful at identifying the iROI, splitting their attention between iROI and dROI.

Eye fixation sequence analysis. People develop perceptual strategies for interpreting visual stimuli that is evidenced by eye fixation sequences (e.g. Augustyniak &

Tadeusiewicz, 2006). To analyze the eye fixation sequences for common or overlapping sequences of fixations, or scan patterns, custom software (NMerGen) was developed using Java. This software was used in conjunction with eyePatterns (West et al., 2006) to identify fixation patterns. NMerGen provided a frequency for each possible transition, n units in length, for a given eye fixation sequence. For this analysis, all possible 3-fixation patterns were isolated. Consider the three AOIs in a 2-molecule equation: reactant (R), condition (C), and product (P). The total possible number of 3-fixation patterns, allowing for multiple fixations within the same AOI, is 27. The frequency of these fixation patterns in participants' eye fixation sequences were analyzed.

Each participant generated up to ten eye fixation sequences (one for each equation). Eye fixation sequences were aggregated across participants for each type of stimuli. Analysis of the eye fixation sequences for the 2-molecule and 3-molecule equations using the Java application eyePatterns (version 0.91) (West et al., 2006) provided the total number of 3-fixation patterns observed. NMerGen, generated the frequency for the observed patterns in the eye fixation sequences of each participant. Descriptive statistics will be used to provide information on the types of eye fixation sequences for 3-fixation patterns.

Three-fixation patterns were coded based on content. For the AOIs, the patterns were coded using the following scheme: successive fixations on the same AOI (e.g., RRR or PPR); regression fixation between two AOI (e.g., RPR); and search fixations of three different AOIs (e.g., RCP). For ROIs, patterns of fixations among iROI and dROI were coded using the following scheme: successive fixations on the same iROI (e.g., iROI-iROI-

iROI and iROI-iROI-dROI); successive fixations on the same dROI (e.g., dROI-dROI-dROI and dROI-dROI-iROI); immediate regression fixations between two ROI (e.g., iROI-dROI-iROI and dROI-iROI-dROI); and search fixations of three different ROI (e.g., $dROI_1$-$iROI_1$-$iROI_2$). Successive fixations were not collapsed into gazes but were retained to preserve the temporal qualities of the eye fixation sequences. Descriptive statistics will be used to provide information on the types of eye fixation sequences for each 3-fixation pattern.

Regression patterns and successive fixations patterns were chosen for further study. Separate split-plot repeated measure ANOVAs were conducted to determine if there was a significant difference in these patterns based on participant characteristics.

For the regression pattern analysis, a split-plot ANOVA was conducted to compare the impact of two different types of equations (HVC and LVC) on the frequency of regression fixations exhibited in the eye fixation sequences of participants. The within-subjects variable was the *participant characteristic* (WMC, Expertise, or SA). The between-subjects variable was *complexity* (HVC and LVC). The dependent variable was the frequency of the regression pattern expressed as a percentage of the total number of 3-fixation patterns.

For the successive fixation pattern analysis, a 2x2x2 complex mixed design was used to assess the frequency of successive fixations patterns. The within-subjects variable was the *participant characteristic* (WMC, Expertise, or SA). The between-subjects variables were *complexity* (HVC and LVC) and *content* (dROI and iROI).

Chapter 4 will present the data from these studies, followed by a discussion of the results.

Chapter 4 - Results

This chapter will present the data and results of the studies presented in Chapter 3. In this dissertation, two studies were conducted. The results of this study will be discussed first, starting with the content validity, followed by construct validity, and, finally, predictive validity. A follow-up study will also be discussed.

Study 2 used the rubric developed for this dissertation to develop and validate a process model for the comprehension of organic chemistry notation using eye tracking methodologies. Since the literature suggests that expertise, working memory capacity, spatial ability, and complexity of the notation may play a role in how an equation is read, the effect of these variables on the eye movement data was also studied. The data and results of Study 2 will be presented, beginning with the validation study of the process model for the comprehension of organic chemistry notation, followed by the analysis of eye tracking data to address research questions 5 and 6.

Study 1

As previously discussed, this study, Study 1 was a validation study of the *Complexity Rubric for Organic Chemistry Notation*, a tool used in Study 2. This validation study involved three steps, namely, 1) Content Validity, 2) Construct Validity, and 3) Predictive Validity. A follow-up study was carried out to further examine the validity of the rubric.

Part 1: Content Validity

Two experts in educational psychology (Dr. A and Dr. B) agreed to participate in separate interviews to address the following question: To what extent is the rubric consistent with expert opinion on visual information processing? (Research question 1)

Wording and content. The experts were asked to review the rubric and accompanying definitions and comment on the wording and content of the rubric. Three issues were identified through the rubric including clarification of chemical terms, the encoding of two character elemental names, and the treatment of implicit carbons and hydrogens in the total score.

The rubric contained a large among of organic chemistry concepts related to implicit carbons, bonding, and symbols. Dr. A suggested that there should be greater clarification of these terms. It was agreed that additional descriptions were needed in the accompanying material. Chemical symbols, definitions, and examples were added to address this issue. These changes are reflected in the rubric in Appendix A.

Both experts raised the question about the encoding of elements that contained two alphanumeric characters in the symbol, for example chlorine has the symbol Cl. In the rubric given to the experts, chlorine would add a +1 under "non-carbon atoms". Dr. A pointed out that, although these symbols represent one atom, the novice may not be familiar enough with the periodic table to know this and will most likely read these letters initially as two separate characters. Dr. A and Dr. B separately argued that these two characters symbols should have a value of +2, rather than "chunking them together" and giving them

the value of +1. The rubric was amended to have all two letter symbols count as +2 under non-carbon atoms.

The final issue that was raised related to the perceived double counting of carbon atoms in the rubric. Dr. B was concerned that the rubric "double counted" carbon atoms when both implicit and explicit carbons were considered. Dr. B pointed out that the rubric was about "visual information and has nothing to do with elaboration". Since this was true, Dr. B argued, the rubric should not give weight and counts to carbons that are only implied by the vertices of geometric shapes. If it does count the implicit carbons, then the rubric should also count the implicit hydrogens attached to those carbons. In our discussion, I pointed out that both implicit and explicit carbons participate in bonding that effect the local and overall structure of the molecule. In turn, their presence increases the visual complexity. The implicit hydrogens in the molecules, while conceptually important, do not affect the 2D representations presented in structural formulas. It was concluded that the "assignment of counts for implicit carbons is necessary to account for the geography of the molecule (Dr. B)".

Visual sort task. The second part of the interview was the card sort task. Dr. A and Dr. B were given a set of structural formulas for six organic molecules in no particular order. They were asked, using what they know about visual information processing, to arrange the molecules in order from least complex to most complex. Both experts produced the same linear ordering. The experts were then shown the linear ordering produced by the

rubric, which was in agreement with their ordering. It was concluded by both experts that the rubric worked as expected.

Changes were made to the rubric and the definition table to reflect discussions with the experts. This included the scoring of elements with two character symbols that were later supported with subsequent research. A copy of the finalized rubric is included in Appendix A.

Part 2: Construct Validity

Research question 2: To what extent does the rubric complexity score measure the visual complexity of the chemical notation? Participants completed a multiple-choice test to measure their ability to recall 12 organic chemistry diagrams of varying complexity.

The Friedman test was conducted to evaluate the difference in the medians for recall scores across three levels of complexity. Thirty participants were scored on the recall of diagrams with low, medium, and high visual complexity. The results from this non-parametric test indicated that there was a statistically significant difference in the ability of the participants to recall a figure depending on the level of complexity (low complexity, medium complexity, and high complexity χ^2 (2, n = 30) = 13.747, $p < 0.01$).

Post hoc analysis used the Wilcoxon Signed-Rank Tests with Bonferroni adjusted alpha levels of 0.017 per test (0.05/3) for the following three comparisons: medium complexity to low complexity figures; high complexity to low complexity figures; and high complexity to medium complexity figures. Results are given in Table 9.

Table 9

A Wilcoxon Signed Rank Comparison of Ability of Participant to Recall Based on Figure Complexity

Comparison (Complexity)	*z*	*r*
Medium – Low	-1.468	0.19[a]
High – Low	-2.828*	0.37[b]
High – Medium	-3.303*	0.43[b]

Note. [a] indicates a small effect size using Cohen (1988). [b] indicates a medium effect size using Cohen (1988). * $p < .05$.

As predicted, participants had a harder time recalling figures with high visual complexity when compared to those with medium or low visual complexity. In the high to low comparison, the mean for the ranks in recall ability for high visual complexity figures was 8.50, while the mean rank for the low visual complexity figures was 12.74. In the high to medium comparison, the mean for the ranks in recall ability for high visual complexity figures was 7.00, while the mean rank for the medium visual complexity figures was 8.15. These results indicate that complexity rubric differentiated figures that contained molecules of high visual complexity from those of either low or medium visual complexity. However, the rubric could not differentiate between molecules of medium and low visual complexities.

Part 3: Predictive Validity

Question 3: To what extent does the rubric complexity score predict the visual complexity of a molecule? For this step of Study 1, participants assigned a linear ordering to six organic structures, from least complex to most complex, and briefly described the criteria used to order the structures. The linear orderings were coded using the scheme described in Chapter 3 and compared to the linear ordering predicted by the rubric. For each molecule,

separate one-sample t-tests were performed to compare the mean position of the molecule in the participants' linear ordering with its position as predicted by the *Complexity Rubric for Organic Chemistry Notation*. Results from the t-tests are given in Table 10.

Table 10

Comparison of the Observed and Predicted Linear Orderings using One-Sample t-Tests

	Mean	*SD*	*df*	*t*
B (least complex)	2.39	1.086	30	7.114*
A	2.97	1.402	31	3.98*
E	1.61	0.830	31	1.61*
F	3.23	0.884	30	-4.879*
D	4.84	0.574	31	-1.539
C (most complex)	5.91	0.390	31	1.61

Note. The t-test compared the observed position of each molecule in the linear orderings of participants with its position in the linear ordering predicted by the rubric. * $p < .05$

These results suggest that the *Complexity Rubric for Organic Chemistry Notation* accurately predicted the complexity of visually complex molecules. However, the rubric did not accurately predict the complexity of molecules with low to medium complexity.

String edit distances were used to compare the differences between the linear ordering assigned by the participants and the predicted linear ordering. The Levenshtein distances were calculated for all the participants in this study, comparing their linear ordering to the string predicted by the rubric: B-A-E-F-D-C. The mean Levenshtein distance was $M = 2.98$, $SD = 1.27$. On average, there would need to be almost 3 edits (deletions, additions, or replacements) to match the participants' linear orderings of linear sequence predicted by the rubric.

To investigate the source of the differences, the mean scores for each molecule were used to generate the average participant linear ordering (Table 11).

Table 11

Descriptive Statistics for Participant Linear Orderings

Structure	n	Mean (*SD*)	
E (least complex)	31	1.61	(0.80)
B	31	2.39	(1.09)
A	32	2.97	(1.40)
F	31	3.23	(0.88)
D	32	4.84	(0.57)
C (most complex)	32	5.91	(0.39)

This average participant linear ordering (E – B – A – F – D – C) was then compared with the one predicted by the rubric (B - A - E - F - D – C). The Levenshtein distance was $LD = 2$. Two edits are necessary to transform the mean participant linear ordering into the predicted linear ordering. This transformation requires the following steps: 1) the deletion of E in the average participant linear ordering and 2) the insertion of E between A and F in the resulting string. The structures of the three molecules affected by the edits were compared. Structures A ($C_8H_{13}O_3$) and B ($C_3H_7NO_2$) were linear molecular formulas, containing at least one double bond. Structure E ($C_9H_{12}O$) had a six-membered ring (hexagon) with alternating double bonds in addition to a chain of carbons. Just over half (53%) ranked this molecule as the least complex. An additional 25% ranked it as second least complex molecule.

Participants' brief written responses were analyzed to determine factors that would account for why a structural formula for a compound that contains more carbons and a ring

would be ranked less visually complex than smaller, linear molecules. The analysis focused on participants who listed molecule E as either the least complex (n = 17) or the second least complex (n = 8). Two major themes emerged from the written responses - 1) traditional chemical terms and 2) geometric or spatial terms. Traditional chemical terms deal with references " chemical", "elements", "letters", "bonds", and "symbols". In the written responses, 16 of the 25 students used chemical terms or concepts to describe the criteria for linear ordering the molecules. These references to chemical terms and concepts include, for example "I figured those with more bonds, lines, molecules, or elements were the more complex structures" (participant 103921); "The least have very few bonds [and] molecules whereas the others are bigger and have more" (participant 103354); and "I ordered the molecules based on … how many chemicals or elements were given" (participant 103753).

The second theme to emerge was geometric and spatial terms, which included geometric terms (e.g., line or angle) and spatial characteristics (e.g., size, shape, or quality of the drawing). Eighty percent of the participants (n = 20) used these terms to describe the criteria for ordering the molecules. For example, "The number of bonds and hexagonal structures" (participant 103111); "By: Simitry or pattern. Shape. Different lines. Letters" (participant 103500); and "The first ones I chose have the least amount of different aspects, with similar not a lot of crazy rings. Last ones have many different shapes and lines that are scary" (participant 103353). The written descriptions were brief, so determining the exact meanings of "shape" and "size" was not possible. Since it was possible that participants

were referring to the recognizable hexagon shape in structure E, a follow-up experiment was conducted to determine how novices in organic chemistry interpret structural formulas that contain rings.

Investigation of "Geometric Chunking"

The purpose of this small-scale study was to investigate how novice participants encode structural formulas that contain at least one ring. Participants were asked to describe five structural formulas of molecules they viewed briefly. Verbal responses from the participants were analyzed for emergent themes. Three ways that participants described molecules that they viewed were: chemical, geometric, and numeric categories. Seven of the ten participants (70%) used more than one way to describe the shape of molecules.

Chemical descriptions of the molecules used chemistry vocabulary and concepts of bonding to describe the structure of molecules. This included terms like "bond", "covalent", and "prime". Eight of the participants (80%) used these terms in their descriptions. Three participants used the names of specific sub-structures (e.g., benzene or oxygen), and one participant referred to all the ring structures as "benzene".

Geometric descriptions included terms from geometry to describe the structures. These included the names of geometric shapes (e.g., triangle, pentagon, hexagon, and octagon) and "line" to describe a bond. Eighty percent (n = 8) of the participants used specific shape names to describe the ring portion of the molecule. Seven of the ten participants (70%) mentioned the word "line" to describe bonds in the molecule. Two participants (20%) used exclusively geometric terms to describe the molecular formulas,

never mentioning chemical names or chemical concepts. Five participants used terms like "vertices", "point", "triangle" or "angle" to describe the arrangement of carbon atoms in the ring.

Numeric descriptions, such as "six member ring" and "seven-sided shape" were also used to describe the rings in the molecules. Eighty percent of participants chose this type of description for at least one of the molecules they viewed. Seven of the 10 participants used this type of description for the molecule that contained a 7-membered ring. One identified the 7-membered structure as an octagon, and only one participant was able to correctly identify the geometric shape as a heptagon. One participant commented that identifying the shape was hard since "I haven't had geometry since the seventh grade" (participant 103272).

All the participants in this study carried out some variation of chunking when remembering the structures presented to them. One participant used chemical names to chunk structures, referring to all the rings as benzene. Almost all the participants (90%) displayed evidence of "geometric" chunking, using words and concepts from geometry to describe the shape of organic molecules. The extent of this geometric chunking is unknown, and how this relates to the rubric score is an area for future research.

Summary

Research questions 1, 2, and 3 investigated the validity of the *Complexity Rubric for Organic Chemistry Notation*. Results from Study 1 seem to indicate that the rubric was able to differentiate the visual complexity of molecules with a high degree of visual complexity (Chemical Notation Complexity Score > 40) from molecules with low visual complexity (0

– 19) and medium visual complexity (20 – 39). However, the rubric has difficulties differentiating the visual complexity of molecules that it would classify as either low or medium complexity. This difficulty in differentiation may be due to the effects of participants' prior knowledge in domains that are visually related, such as geometry.

Conclusion

The equations used in Study 2 have Chemical Notation Complexity Score in the low to medium-low range (< 25) and high range (50 – 90). Because the rubric works adequately well differentiating high visual complexity equations from those in the medium - low range, it was used to classify the molecules used as stimuli in Study 2.

Study 2

The purpose of this study was to validate the process model for the comprehension of organic chemistry notation. As part of this study, the effects of participant characteristics (expertise, working memory capacity, and spatial ability) and the complexity of the organic chemistry equations on the reading process were investigated.

Eye-tracking data. The eye movements of 27 participants were analyzed for this study. The stimuli used in the study were self-paced, meaning that participants controlled viewing time for each equation. All participants viewed ten equations. Both novice and expert participants were included in this study. Differences in the viewing time, fixation frequency, and fixation durations were analyzed between these two groups to determine if there were significant differences in reading behaviors that would affect the validation. It was expected that the viewing times and fixation durations of the novices would be

significantly longer than those of the experts, and that novices would exhibit a higher frequency of fixations than experts. However, both experts and novices should exhibit similar viewing patterns when reading 2-molecule versus 3-molecule equations. It was expected that the additional visual information in 3-molecule equations would cause an increase the viewing times, fixation durations, and fixation frequencies exhibited by both groups of participants.

Two types of equations were used for this validation. The 2-molecule stimuli (Topics 1, 2, and 5) contained one reactant, conditions, and one product . The 3-molecule stimuli (Topics 3 and 4) contained two reactants, conditions, and one product. Conceptually and structurally, these types were considerably different. The addition of a second reactant increased the number of AOIs and ROIs in the analysis. These additional AOIs and ROIs could artificially increase the percent fixation durations and fixation frequencies for the 3-molecule stimuli. Therefore, the two types of stimuli were analyzed separately.

Viewing time. Viewing time was the total amount of time the participants viewed each stimulus from the time it appeared on the screen until the time the participant indicated that they understood the equation. The mean viewing time across all participants for the 2-molecule stimuli was 16.39 s (SD = 10.35, Mdn = 14.63 s) and for 3-molecule stimuli, was 27.13 s (SD = 15.34, Mdn = 25.61).

For the expertise subgroups, the mean and median viewing times for each equation type are given in Table 12.

Table 12

Viewing Times for Novices and Experts

Stimuli	Expertise	Viewing time	
		M (s)	*Mdn (s)*
2-molecule	Expert	10.03 (6.1)	8.19
	Novice	19.07 (10.61)	17.26
3-molecule	Expert	16.15 (14.16)	12.98
	Novice	31.75 (13.41)	29.02

Note. Standard deviation is in parentheses.

To determine if there was a significant difference between expert and novice viewing times, a 2-way mixed model ANOVA was used. Exploratory data analysis investigated the normality of the reading times distribution. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated the datasets were not symmetrical. The Kolmogorov-Smirnov test was significant ($p < 0.05$), suggesting that it did not follow a normal distribution. These datasets were transformed using the natural logarithm to improve normality.

To determine if there was a significant difference in the viewing times of experts and novices, the natural log of the total viewing time was analyzed using a 2 way mixed model ANOVA with one within-subject factor (equations) and one between subjects factor (Expertise - expert and novice). The dependent variable was the natural log of the viewing time.

There was a significant main effect comparing the viewing times of reaction equations for 2-molecule equations ($F(5,115) = 14.37$, $p < 0.001$, partial eta squared = 0.38)

and 3-molecule equations ($F(3,72) = 9.01$, $p < 0.001$, partial eta squared = 0.27). This indicated that at least two of the equations differ significantly in viewing times. There was also a significant main effect comparing the viewing times based on expertise for 2-molecule equations ($F(1, 23) = 13.664$, $p < 0.001$, partial eta squared = 0.37) and for 3-molecule equations ($F(1, 24) = 24.00$, $p = 0.00$, partial eta squared = 0.50). There was no significant interaction between expertise and equation for either the 2-molecule stimuli ($F(5, 115) = 0.59$, $p > 0.05$, partial eta square = 0.05) or the 3-molecule stimuli ($F(3, 72) = 0.05$, $p > 0.05$, partial eta square = 0.02). Novices had significantly longer viewing times than experts (moderate to large effect size).

Table 13

Viewing Times for Experts and Novices Across Equation Type

			Geometric Mean	95% Confidence Interval	
Stimuli	Expertise	*n*	(*s*)	Lower Bound	Upper Bound
2-molecule	Expert	7	8.85	6.49	12.06
	Novice	18	17.00	14.00	20.61
3-molecule	Expert	8	12.01	8.28	16.61
	Novice	18	30.36	24.43	37.68

Note. The dependent variable in the ANOVA was the natural log of the fixation durations. The mean and confidence interval were back-transformed and presented as the geometric mean and associated confidence interval.

The novices spent significantly more time viewing the equations than the experts. For 2-molecule equations, novices viewed the equation approximately twice as long as experts. The novices viewed the 3-molecule stimuli 2.5 times longer than the experts. This difference remained constant regardless of the equation that was read.

Frequency of fixations. The mean frequency of fixations for 2-molecule equations was $M = 44.03$ ($Mdn = 39.00$, $SD = 28.16$) and for 3-molecule equations was $M = 66.16$ ($Mdn = 62.00$, $SD = 35.30$). The mean and median fixation frequencies of each equation type for novices and experts are given in Table 14.

Table 14

Fixation Frequency Based on the Expertise

		Frequency of Fixation	
Stimuli	Expertise	*M (s)*	*Mdn (s)*
2-molecule	Expert	28.17 (15.59)	25.00
	Novice	51.16 (29.36)	44.00
3-molecule	Expert	37.5 (20.87)	33.5
	Novice	78.22 (33.17)	72.5

Note. Standard deviation is in parentheses.

Exploratory data analysis was used to assess the normality of the frequencies of fixations. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated the datasets were not symmetrical. The Kolmogorov-Smirnov test was significant ($p < 0.05$), suggesting that the data did not follow a normal distribution. The datasets were transformed using the natural logarithm to improve normality.

To determine if there was a significant difference in the frequencies of fixation of experts and novices, the natural log of fixation frequencies was analyzed using a 2-way mixed model ANOVA with one within-subject factor (equations) and one between subjects

factor (Expertise - expert and novice). The dependent variable was the natural log of the fixation frequency. For the 2-molecule equations, there was a significant main effect comparing the fixation frequency based on expertise ($F(1, 23) = 11.02$, $p < 0.001$, partial eta squared = 0.42). For the 3-molecule equations, there was also a significant main effect for expertise ($F(1, 24) = 22.45$, $p < 0.001$, partial eta squared = 0.48). Novices had significantly more fixations during reading than the experts (Table 15).

Table 15

Geometric Mean of Fixation Frequency for Experts and Novices

				95% Confidence Interval	
Equation	Expertise	*n*	Geometric Mean (s)	Lower Bound	Upper Bound
2-molecule	Expert	8	24.19	18.99	30.81
	Novice	17	43.3	36.63	51.06
3-molecule	Expert	32.17	32.17	24.36	42.44
	Novice	69.20	69.20	57.51	83.26

Note. The dependent variable in the ANOVA was the natural log of the fixation durations. The mean and confidence interval were back-transformed and presented as the geometric mean and associated confidence interval.

For 2-molecule stimuli, novices made 1.75 more fixations than the expert. For the 3-molecule equations, novice made more than double the number of fixations as the experts. This includes fixations on the content within the equation as well as fixations on white space.

There was also a significant main effect for the type of equation. This indicated that the equations had fixation frequencies that differed significantly - 2-molecule equations ($F(5,115) = 23.22$, $p < 0.001$, partial eta squared = 0.502) and 3-molecule equations ($F(3,72)$

= 7.56, $p < 0.001$, partial eta squared = 0.24. There was no significant interaction between expertise and equation for the 2-molecule equations ($F(5, 115) = 1.40$, $p > 0.05$, partial eta square = 0.06) or the 3-molecule equations ($F(3, 72) = 0.55$, $p > 0.05$, partial eta square = 0.02). While novices had more fixations than experts, this difference remained constant regardless of the equation that was read (Table 15).

Duration of fixations. The mean duration of fixations for 2-molecule equations was $M = 26.67$ ($SD = 69.33$, $Mdn = 11.94$) and for 3-molecule equations was $M = 42.77$ ($SD = 107.32$, $Mdn = 20.77$). The mean and median fixation duration for novices and experts viewing each equation type are given in Table 16.

Table 16

Fixation Duration Based on the Expertise

		Duration of Fixation	
Equation	Expertise	*M (s)*	*Mdn (s)*
2-molecule	Expert	7.22 (5.15)	4.96
	Novice	16.17 (9.95)	13.92
3-molecule	Expert	10.15 (6.04)	8.67
	Novice	26.65 (12.43)	24.19

Note. Standard deviation is in parentheses.

Exploratory data analysis was used to assess the normality of the distribution of fixation durations. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated the datasets were not symmetrical. The Kolmogorov-Smirnov test was significant ($p < 0.05$), suggesting that the data did not follow

a normal distribution. These datasets were transformed using the natural logarithm to improve normality.

To determine if there was a significant difference in the fixation durations of experts and novices, the natural log of the fixation duration was analyzed using a 2-way mixed model ANOVA with one within-subject factor (equations) and one between subjects factor (Expertise - expert and novice). The dependent variable was the natural log of the fixation durations. For the 2-molecule stimuli, there was a significant main effect comparing the fixation frequency based on expertise ($F(1, 18) = 27.57$, $p < 0.001$, partial eta squared = 0.61). For the 3-molecule equations, there was also a significant main effect for expertise ($F(1, 23) = 34.31$, $p < 0.001$, partial eta squared = 0.60). Back-transformed means and 95% confidence intervals are given in Table 17.

Table 17

Geometric Mean of Fixation Duration for Experts and Novices

				95% Confidence Interval	
Equation	Expertise	*n*	Geometric Mean (s)	Lower Bound	Upper Bound
2-molecule	Expert	6	5.52	10.08	14.14
	Novice	14	11.94	4.27	7.15
3-molecule	Expert	6	7.43	5.20	10.62
	Novice	19	23.71	19.39	28.96

Note. The dependent variable in the ANOVA was the natural log of the fixation durations. The mean and confidence interval were back-transformed and presented as the geometric mean and associated confidence interval.

The novices made significantly longer fixations during reading than the experts. For 2-molecule stimuli, novice fixations were 2.2 times longer than those of the experts. For 3-molecule stimuli, they were 3.2 times longer than those of experts.

The analysis also had a significant main effect for equations. For 2-molecule equations ($F(5,90) = 13.07$, $p < 0.001$, partial eta squared = 0.42) and 3-molecule equations ($F(3,69) = 7.22$, $p < 0.001$, partial eta squared = 0.24), at least two of the equations had significantly different fixation durations. There was no significant interaction between expertise and equation for the 2-molecule equations ($F(5, 90) = 1.31$, $p > 0.05$, partial eta square = 0.07) or the 3-molecule equations ($F(3, 69) = 0.15$, $p > 0.05$, partial eta square = 0.01). Overall, novices made significantly longer fixations than experts. However, this difference remained constant regardless of the equation that was read.

Summary. From the analysis of viewing time, fixation frequency, and fixation duration, it was determined that there were significant differences between the expert and novice subpopulations participating in this study. Novices spent significantly more time viewing the chemical equations than the experts. When compared with the experts, they also had a higher number and longer fixations on the equation. However, the analysis also showed that there was no interaction between the expertise and the equation type, meaning that although these differences existed, they did not differ significantly from equation to equation type. Therefore, both populations were included in the validation study. Fixation frequency and duration were converted to percentages for the total fixation frequency and total fixation duration so that the two subpopulations could be analyzed together.

Validation of Process Model for the Comprehension of Organic Chemistry Notation

Eye tracking methodology was used to address Question 4 - To what extent does the process model for the comprehension of organic chemistry notation account for eye fixations (frequency and duration) of participants reading organic chemistry equations? Observations and analysis of eye tracking data was used to support each stage of the model.

Stage: *Get Input*. This stage of the process model is responsible for moving the eyes. The *Get Input* stage controls the movement of the eyes from one fixation to another. Over the course of reading a chemical equation, this stage would be responsible for multiple eyes movements across the content of the equation, each time ending in a fixation. Eye tracking data were analyzed for the frequency of fixation in AOIs for each equation. Multiple fixations in the equations were confirmed using the heat map visualization tool.

Two-molecule equations. In each of the equations, participants viewed at least two of the three AOIs (Table 18).

Table 18

Number of Participants Fixating in AOIs and Percentage of Total Fixations for 2-Molecule Equations

	Reactant		Condition		Product	
Topic	*n*	Percent (%)	*n*	Percent (%)	*n*	Percent (%)
Topic 1 HVC	27	44.48	27	12.26	27	43.26
LVC	25[a]	46.98	25[a]	22.64	25[a]	30.38
Topic 2 HVC	27	49.61	27	23.98	27	26.41
LVC	27	41.78	27	27.62	27	30.60
Topic 5 HVC	27	56.21	23	10.92	27	32.87
LVC	27	49.98	25	13.17	27	37.85

Notes. [a] For this equation, the eye tracker failed to successfully track 2 participants.

On average the lowest percentage of fixation was on the conditions. This is not surprising since the conditions contained very little visual and conceptual information when compared to the other AOIs. The reactants had the highest percentage of fixations. Since the chemical equation is concerned with the transformation of reactant to product, it is not surprising that the largest percentage of the fixation was here.

Heat maps are used to visualize the frequency of fixations across stimuli. Using a color gradient, heat maps help visualize the cumulative fixations across all the participants, with the most intense color indicating the highest number of frequencies for that stimuli. For example, consider the heat map for Topic 1, HVC (Figure 27).

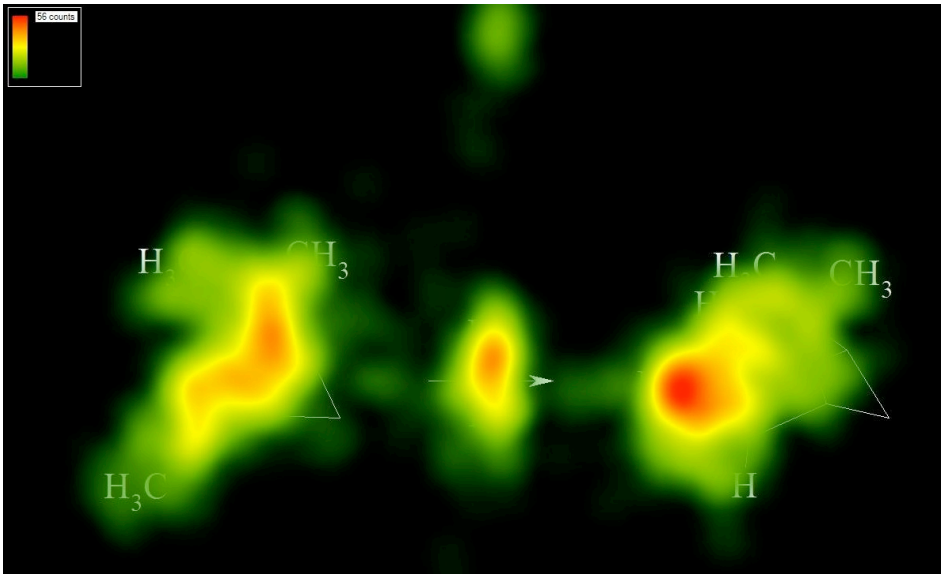


Figure 27. Heat map for Topic 1 HVC. The fixations are localized on three regions of the equation: reactants (left), conditions (middle), and product (right).

Here we see the localization of fixations on the conditions and the site of the chemical reaction in the reactant and product of the chemical equation.

Three-molecule equations. Similar trends in fixation patterns are observed in the 3-molecule stimuli (Table 19). Participants viewed at least three of the four AOIs in each equation. When compared to the 2-molecule equations, the lowest percentage of fixation was on the conditions for 3-molecule equations. With the addition of a second reagent, the percentage of fixations for each of the reactants and the product are partitioned across all three regions.

Table 19

Number of Participants Fixating in AOIs and Percentage of Total Fixations for 3-Molecule Equations

	Reactant 1		Reactant 2		Condition		Product	
Equation	*n*	Percent (%)	*n*	Percent (%)	*n*	Percent (%)	*n*	Percent (%)
Topic 3 HVC	27	28.5	27	30.69	25	12.42	27	28.39
LVC	27	27.55	27	25.43	26	18.53	27	28.50
Topic 4 HVC	27	26.55	27	33.64	26	6.99	27	32.82
LVC	27	24.68	27	40.39	27	13.28	27	21.65

The heat map for Topic 4 LVC (Figure 28) illustrates the localization of fixations on the four regions of the equation: reactant 1 (far left), reactant 2 (left of center), condition (right of center), and product (far right).

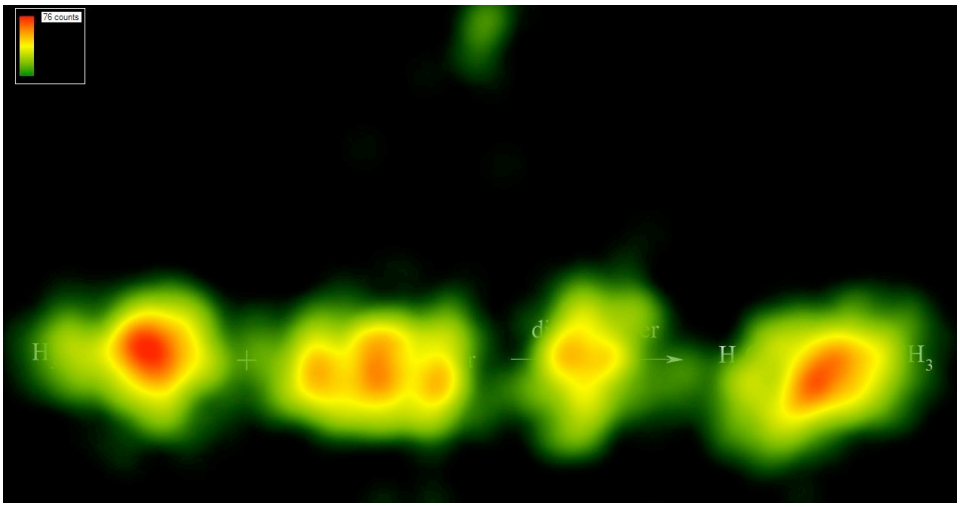


Figure 28. Heat map of Topic 4 LVC.

The color gradient indicates that the fixations are partitioned fairly evenly across the four regions of the equation. Using fixation frequencies and heat maps, I was able to show

that participants fixate across the chemical equation and participants' eyes move while reading chemical equations. The pattern of this movement will be discussed next.

Sequence of fixations. It was hypothesized that participants would read the chemical equations from left to right, similar to the pattern for reading English text. The sequence of fixations would start at the reactant (R,S), move to condition (C), and end at product (P) (see Figure 29). For this study, this reading pattern would yield two predicted strings, RCP (2-molecule stimuli) and RSPC (3-molecule stimuli).

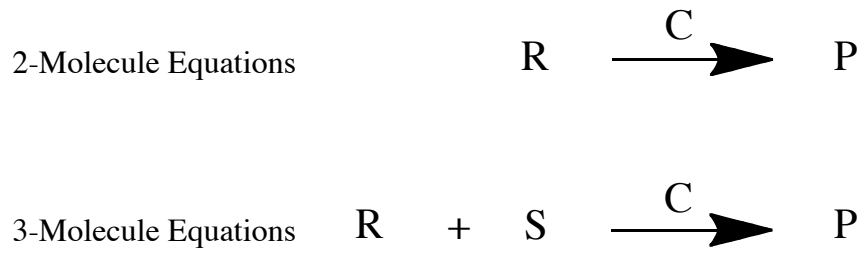


Figure 29. Schematic of equations for sequence of fixations

To determine the sequence of fixations for each participant, regressions between AOIs were ignored. Only the patterns of first fixations in AOIs were analyzed. This pattern indicated the order that the participants processed the individual features of the chemical equation. A string edit metric was used to compare the viewing patterns of the participants to that of the predicted string. The Levenshtein distance (LD) is a measure of how different two strings are. The magnitude of LD indicates the minimum number of edits needed to transform the participant's pattern of first fixation into the predicted string. An LD = 0 would mean that the predicted string and the participant's pattern of first fixations matched.

The first fixation patterns for each participant were compared to the predicted strings for the 2-molecule and 3-molecule equations. Levenshtein distances were calculated for all first fixation patterns. The mean Levenshtein distance (*mLD*) was calculated for all the equations in each type of equation. For the 2-molecule equations, the *mLD* = 0.96 (*SD* = 0.983), indicating that the participants do not always follow the predicted eye movement pattern. There are six possible permutations of first fixation patterns given three AOIs. Of the six possible, the participants exhibited only four. I examined the patterns of first fixations to determine in what order participants read a chemical equations. The distribution of fixation patterns is given in Table 20.

Table 20

Observed Instances of Each First Fixation Pattern in AOI for 2-Molecule Equations

First Fixation Pattern	*n*	Observed (%)
RCP	81	52.9
RPC	19	12.4
CRP	48	31.4
CPR	5	3.3

While almost two-thirds of the participants (65%) read from left to right, the other third (35%) start at the condition rather than the reactants. One possible reason may be that participants have developed strategies for reading chemical equations that allow them to organize and better recall information about the chemical reaction. Through lab work and learning experiences, participants may have learned to look at the conditions as a way to

categorize the chemical reaction. This categorization then helps the participant focus subsequent fixations on regions of the equation important to the chemical reaction.

The same trends were observed for the 3-molecule equations. The *mLD* = 1.80 (*SD* = 0.918), indicating that participants are even less likely to read from left to right when there are two reactants in the equation. There are twenty-four possible permutations of first fixation patterns given four AOIs, but participants exhibited only twelve. I examined the patterns of first fixations to determine the order participants were reading the chemical equations. The distribution of fixation patterns is given in Table 21, for all fixation patterns with a frequency 2 or more.

Table 21

Observed Instances of Each First Fixation Pattern in AOI for 3-Molecule Equations

First Fixation Pattern	*n*	Observed (%)
SRCP	45	43.3
RSCP	19	18.3
SRPC	13	12.5
SCRP	8	7.7
RSPC	7	6.7
SCPR	4	3.8
CSRP	2	1.9
CRPS	2	1.9

Under these conditions, the participants tended to start reading by focusing on the reactant closest to the tail of the arrow (43%). One reason for this may be that the arrow provided the participant with a visual cue to focus their first fixation. Overall, participants

focused their first fixation on the reactants side of the equation (94%) - either R or S. Only 5% of the participants started reading by viewing the conditions first.

Summary. This data suggest that while reading chemical equations, participants move their eyes from one fixation to another across the chemical equation. According to the model, the Get Next process governs this movement. Unlike reading English text, once a fixation is complete and the eyes move to the next fixation, the location of that fixation is not set. The data in Table 20 and Table 21 illustrate a variety of patterns that are used as the participants' eyes move across the equation.

Stage: *Search*. In this stage of the process model, a search is conducted for molecular features that are key to understanding the chemical reaction. Before moving to the next molecule, the reader makes a series of intramolecular fixations within the same AOI.

To determine if participants make a series of intramolecular fixations, scanpaths were analyzed to determine the frequency of fixations within the same AOI, and a pattern of three fixations was chosen to study. Sequences of 4-fixations within the same AOI were isolated using custom software NMerGen. Frequencies were calculated for each participant. Table 22 provides is the average number of 4-fixation patterns for each molecule in the reaction equations.

Table 22

Average Frequency of Intramolecular Four-Fixation Transitions for Each Equation

Equation	Reactant 1	Reactant 2	Product
Topic 1, HVC	9.1	-	9.5
Topic 1, LVC	4.3	-	8.7
Topic 2, HVC	5.2	-	16.2
Topic 2, LVC	6.1	-	9.5
Topic 3, HVC	6.3	7.4	5.6
Topic 3, LVC	5.8	5.9	5.3
Topic 4, HVC	11.5	9.1	9.6
Topic 4, LVC	3.0	3.9	6.8
Topic 5, HVC	2.9	-	8.5
Topic 5, LVC	4.2	-	6.6

Notes. For each molecule in the equation, patterns of 4-fixation within the molecule were identified. The average frequency of these patterns is given for each molecule in the equation.

The intramolecular transitions in Table 22 accounts for 33% of all the four-fixation sequences that the participants exhibited. While participants are making these intramolecular fixations, they are processing information about various features of the molecule.

Summary. The presences of intramolecular search were confirmed by AOI scanpath analysis. The data suggests that participants engaged in a searching process for a portion of their viewing time. Thirty-three percent of all the four-fixation sequences follow the pattern of intramolecular search, either within the reactants or the products.

***Stage: Encode and Access Lexicon*.** This stage of the process model is responsible for encoding the features of the molecule and retrieving information from long-term memory (LTM) to create an internal representation of the equation. The meanings of molecular features and notation are activated in LTM during the building of this

representation. The model proposed in this study predicts that the participant will exhibit a significant decrease in the fixation durations when he/she encounters a molecular feature that was already viewed. Since the meaning of this feature was already activated in LTM, when the participant encounters a second instance of this same feature somewhere else in the equation, he/she should need less time to process it.

To study this phenomenon, ROIs resulting from the cluster analysis were used to aggregate the data. Three equations were chosen for this analysis that had at least two ROIs that contained nearly identical molecular features.

Two variables were calculated for each subject, namely, Fixation Duration (FD) and the Average Fixation Duration (AFD) for subsequent fixations. The FD is the total time of fixation on a given molecular feature. The duration of the first fixation on the molecular feature was given the designation of First Fixation Duration, or FFD. The AFD is the average fixation time for all subsequent fixations on the same molecular feature (either the same ROI or other ROI containing the same feature). Since the viewing times for each equation was controlled by the participant, the total viewing time varied. In order to compare the participants, the fixation times were given as a percentage of the total viewing time. The following variables were computed as percentages of the total fixation time for each participant:

- Fixation Duration (FD) = duration of a given fixation (ms) / total equation viewing time (ms)

- First Fixation Duration (FFD) is the duration of the first fixation on the molecular feature
- Mean Fixation Duration (AFD) = $\sum X_i$ / number of subsequent fixations, where X_i is the fixation durations for all subsequent fixations.

To determine if there was significant difference in fixation durations, exploratory data analysis was conducted to assess the normality of the data. For the analysis, each equation was tested separately. The skew and kurtosis indicated that the distribution of the durations were not symmetrical, exhibiting a left-handed skew. Kolmogorov-Smirnov test results were significant ($p < 0.05$), indicating that the dataset was not normally distributed. A natural logarithmic transformation was applied to the data, improving the normality of the distribution.

To determine if there was a significant difference in duration times between the first fixation and the average of subsequent fixations, paired samples t-tests were used to compare the natural log transformed FD with the natural log transformed AFD. Results are given in Table 23. The results from the t-test were back-transformed and reported as the geometric mean.

Table 23.

Comparison of First Fixation and Subsequent Fixations Durations in ROIs for Similar Molecular Features

	Geometric Mean				
Equation	First Fixation	Subsequent Fixations	t [a]	df	η^{2} [a]
Topic 1, LVC	2.18	1.67	2.27*	23	0.10
Topic 4, LVC	1.56	2.29	-4.11*	23	0.27
Topic 5, LVC	1.87	1.44	3.33*	17	0.25

Note. The dependent variable for the t test was the natural log of the fixation duration. The mean was back-transformed and presented as the geometric mean. [a] t statistic and eta squared for the difference in the natural logs of the FD and AFD. These values were not back-transformed. * $p < .05$.

For Topic 1 and 5, the participants spent a greater proportion of their viewing time looking at the molecular feature the first time they encountered it compared to the mean viewing time for all other fixations. For Topic 4, the inverse was true. After viewing the molecular feature, participants spent significantly more time viewing a molecular feature when they encountered it on subsequent viewings. A comparison of the type of ROIs used in this study was conducted. For Topic 1 and 5, the ROIs contained information that was not necessary for understanding the chemical reaction (dROIs). The ROIs selected in topic 4 contained groups that were taking part in the chemical reaction (iROIs). While the identified ROIs contained the same molecular features in each molecule, the role these regions played in the overall chemical reaction was different, which could account for the longer fixation times on the iROIs in Topic 4.

Summary. The results from Topic 1 and 5 indicate a significant difference between the first fixation time and subsequence fixations for all participants. This supports the existence of the Encoding and Access Lexicon stage of the process model. While the results

from Topic 4 show a negative difference, I believe that the iROIs selected for study had additional processing requirements. These ROIs were directly involved in the chemical reaction and needed additional processing to define the important relationships among the ROIs. I believe the addition processing may have confounded the results, thus making them suspect. This additional processing will be discussed in the next two sections.

Stage: *Intramolecular Relationships.* The Intramolecular relationship processes are responsible for determining the relationships (conceptual, spatial, etc) between features within a single molecule. As a result, I hypothesize that iROIs have longer fixation durations than dROIs in each molecule.

To determine if there was a significant difference in fixation durations, exploratory data analysis was conducted to assess the normality of the data. For the AOI analysis, 2-molecule and 3-molecule equations were tested separately. Skewness and kurtosis indicated that the distribution was not symmetrical, but had a left-hand skew. The Kolmogorov-Smirnov test results were significant ($p < 0.05$). Using standard methods, attempts to transform the data yielded no significant improvement in the normality of the distribution. Therefore, non-parametric Wilcoxon signed rank test was used to analyze the data.

Wilcoxon signed rank test. For each molecule in the equations, a separate Wilcoxon signed rank test was used. This test compared the percent fixation duration in iROIs to dROIs for each molecule to determine if there was a difference in the amount of time participants spent viewing information necessary to understanding the reaction vs. information that is superfluous. In 18 of the 21 molecules (90%), the percentage of total

fixation duration was significantly different between fixations in iROIs and dROIs. The results for these tests are reported in Table 24.

Table 24

Summary of the Wilcoxon Signed Rank Test Comparing Fixation Durations in iROIs and dROIs for Molecules

Equation			Median	*Z*	*r*
Topic 1 HVC	Reactant	iROI	6.26	-3.75*	.72
		dROI	25.06		
	Product	iROI	26.88	-4.20*	.80
		dROI	6.75		
Topic 1 LVC	Reactant	iROI	23.57	-4.09*	.82
		dROI	11.74		
	Product	iROI	11.03	-.09	.02
		dROI	10.94		
Topic 2 HVC	Reactant	iROI	40.31	-3.62*	.88
		dROI	3.72		
	Product	iROI	18.47	-3.72*	.90
		dROI	2.38		
Topic 2 LVC	Reactant	iROI	33.20	-4.37*	.93
		dROI	4.24		
	Product	iROI	20.15	-4.11*	.79
		dROI	3.00		

(continued)

Equation			Median	*Z*	*r*
Topic 3 HVC	Reactant 1	iROI	18.44	-3.72*	.79
		dROI	2.42		
	Reactant 2	iROI	13.07	-.43	.08
		dROI	12.50		
	Product	iROI	16.16	-4.27*	.85
		dROI	7.15		
Topic 3 LVC	Reactant	iROI	17.48	-4.20*	.88
		dROI	3.52		
	Product	iROI	20.26	-2.53*	.63
		dROI	4.29		
Topic 4 HVC	Reactant 1	iROI	193	-3.92*	.88
		dROI	2.63		
	Reactant 2	iROI	10.72	-1.85	.35
		dROI	12.55		
	Product	iROI	23.50	-4.07*	.87
		dROI	3.18		
Topic 4 LVC	Reactant 2	iROI	16.70	-2.52*	.48
		dROI	12.50		
Topic 5 HVC	Reactant	iROI	28.20	-3.49*	.68
		dROI	13.27		
	Product	iROI	19.65	-4.11*	.88
		dROI	5.61		
Topic 5 LVC	Reactant	iROI	34.14	-2.52*	.89
		dROI	2.52		
	Product	iROI	19.06	-3.43*	.71
		dROI	8.54		

Note. * $p < .05$.

Of those equations that were significant, with one exception (Topic 1 HVC product), the Wilcoxon signed rank test indicated that the percentage of total fixation was higher when participants viewed iROIs than when they viewed dROIs within the same molecule. Participants spent more time viewing iROIs than dROIs. To explain the discrepancy observed in Topic 1 HVC, consider the structure of the reactant and product (See Appendix J). Both molecules contained a bridging carbon. For novice participants, the bridging carbon

may have been an unfamiliar feature because it is not commonly used in the 1-year chemistry sequence of organic chemistry. For those novices, the bridging structures would have lower chunk activation, requiring additional time to processes the feature of the equation. Responses on the follow-up task indicated that three novices were unfamiliar with this feature of the molecule. More analysis is needed to explore this fully.

Scanpath analysis. To better understand the types of relationships that participants identify within the molecule, 4-fixation patterns were analyzed to look for trends in the reading patterns. A sequence of 4 fixations was chosen because it is the maximum number of ROIs in a molecule. As the fixation pattern gets larger, the intent of an eye fixation and its relationship to the initial fixation becomes progressively harder to interpret. Using ROIs, each series of fixation were turned into a string that could be analyzed linearly. Each molecule in the equations presented had two to four ROIs. Therefore, the number of possible combinations of ROIs in each molecule ranged from to 4 to 256 combinations, which allowed for repeats. To narrow the analysis, the five most frequent transitions were coded for each molecule. These represented approximately 60 percent of all 4-fixation patterns (n = 1,541).

Table 25 gives a summary of the types of intramolecular transitions observed. Examples assume a molecule with 4 ROIs: two iROIs (A and B) and two dROIs (C and D).

Table 25

Frequency of the Top Five Fixations Patterns for Each Molecule

Fixation pattern	Example	*n*	Percent
Same iROI	AAAA or BBBB	851	55.22%
Combination of iROI and dROI	CAAA or BBDD	483	31.43%
Different iROI	AABB or ABAB	115	7.46%
Same dROI	CCCC or DDDD	58	3.76%
Combination of two iROI and one dROI	ABDA or BBCA	34	2.21%

The most common sequence of fixations occurred within the same iROI. Participants fixated multiple times within the same iROI before moving to the next fixation. During these fixations, the participants are thought to be processing different features of the same iROI. Approximately 41% of the fixation patterns were the processing of two or more ROIs. During these fixation sequences, participants processed various features of the same molecule to create relationships within working memory. Not accounted for in this table are regression patterns, where participants look at a ROI, look at a different ROI, and then return to the original ROI. For 4-fixation patterns that contain two or more ROIs, approximately 17% ($n = 255$) of the fixation patterns contained an immediate regression pattern (i.e. ABAA, ADAC). It is believed that these regression patterns are 1) characteristic of comparative strategies used by the participant, where he/she is looking for similarities or difference between the features of the two ROIs or 2) a result of forgetting, when the participant, after moving to a new fixation forgets a feature of the previous fixation. In both

cases, the participant, building an internal representation of the molecule, needs to determine the relationship of one molecular feature to another within the same molecule.

Summary. For 81% of the molecules (17 our of 21 molecules), participants spent a larger percentage of their viewing time looking at informative molecular features than distracting features. During viewing, the participants spent more time processing informative data about the molecule and less time processing distracting information. In order to give preference to informative regions, participants assigned priority by creating relationships among features within the same molecule. This analysis supports the proposed stage of the process model responsible for identifying *Intramolecular Relationship*.

The analysis of 4-fixation patterns indicated that participants made a series of fixations within the same molecule. During these fixations, participants processed molecular features. The preferential fixation on informative regions of the molecule (63% of 4-fixation scanpaths) indicates that the participants created relationships between the features of the molecule they viewed and assigned priority to regions that contained information necessary to understand the reaction. Fixation patterns uniquely within a dROI account for only 4% of the of the fixation patterns analyzed.

Stage: *Intermolecular Relationships.* The *Intermolecular Relationship* processes are very similar to those of *Intramolecular Relationships*. *Intermolecular Relationships* are responsible for determining the relationships (conceptual, spatial, etc) between molecules in the entire equation. This stage of the model is evidenced by a series of fixations across all the ROIs in the entire equation. Like the intramolecular relationship stage of the process

model, the duration of these fixations is different depending on the role the molecular feature plays in the chemical reaction. Features that are directly involved in the chemical reaction (iROIs) require more processing than features that do not participate in the reaction (dROIs). Therefore, iROIs should have longer fixation durations than dROIs.

Normality assumption. To determine if there was a significant difference in fixation durations, exploratory data analysis was conducted to assess the normality of the data. The results of the Kolmogorov-Smirnov indicated that the percent fixation duration was not normally distributed. Analysis of skewness and kurtosis indicated that the distribution was not symmetrical. Attempts to transform the data yielded no significant improvement in the normality of the distribution. Therefore, non-parametric means were used to analyze the data.

Wilcoxon signed rank test. For each equation, a separate Wilcoxon signed rank test was used to compare the percent total fixation duration in iROIs to dROIs across the entire equation. This determines if there is a difference in the amount of time participants spent viewing information necessary to understanding the chemical reaction vs. information that was unnecessary. I hypothesized that participants would spend more time viewing iROIs than dROIs. The results of this analysis are given in Table 26.

Table 26

Summary of the of Wilcoxon Signed Ranks Tests Comparing Fixation Durations in iROIs and dROIs for Equations

Equation		Median	*Z*	*r*
Topic 1 HVC	iROI	36.95	-2.23*	.43
	dROI	31.14		
LVC	iROI	36.02	-3.65*	.72
	dROI	22.03		
Topic 2 HVC	iROI	62.07	-4.29*	.87
	dROI	3.63		
LVC	iROI	52.79	-4.46*	.87
	dROI	8.54		
Topic 3 HVC	iROI	50.46	-3.77*	.73
	dROI	22.08		
LVC	iROI	64.67	-4.54*	.87
	dROI	6.48		
Topic 4 HVC	iROI	58.72	-4.54*	.87
	dROI	18.58		
LVC	iROI	58.19	-4.54*	.87
	dROI	12.67		
Topic 5 HVC	iROI	47.74	-4.31*	.84
	dROI	17.90		
LVC	iROI	58.98	-4.20*	.88
	dROI	8.54		

Note. * $p < .03$.

There was a significant difference in the percent of time participants spent viewing informative and distracting regions of the equation across all topics. For all equations, they spent more time viewing iROIs than dROIs. Because participants preferentially fixated in iROIs over the dROIs, they had to develop relationships and assign priorities to the regions containing informative features of the equations. If no relationships were established, there would be no difference in the fixation durations of iROIs and dROIs.

Scanpath analysis. To better understand the types of relationships that participants created during the reading process, three-fixation scanpaths among the AOIs were analyzed to look for trends in the reading patterns. Three-fixation patterns were chosen for this analysis because I was interested in how participants interacted with all three elements of the equation, namely, reactant(s), conditions, and products.

On average, participants made a total of approximately 41 3-fixation transitions for equations with a single reactant and almost 62 transitions for equations with two reactants. This difference in the number of transitions can be accounted for by the increase in the number of relationships that need to be established in the equation with an additional reagent.

All 3-fixation patterns were coded for one of four categories, such as: 1) fixations on the same AOI (RRR, CCC, PPP); 2) regressions (RCR, RPR, etc); 3) fixation patterns containing two different AOIs with no regression; and 4) fixations patterns containing three different AOIs. The frequency and percentage of fixations are given in Table 27.

Table 27

Frequency of Three-Fixation Patterns in AOI Across All Equations

Fixation pattern	Examples	*n*	Percent (%)
Two different AOIs	RRC, CRR, PPR	6784	50
Same AOI	RRR, CCC, PPP	5143	37
Three different AOIs	RCP, PRC, CRP	969	7
Regression	RCR, PRP, CPC	808	6

Fixation patterns within the same AOI (37%) are characteristic transitions for *Intramolecular Relationships.* Here participants fixate on different regions of the same molecule. The most common type of transition indicating the formation of *Intermolecular Relationships* was between two different ROIs (not regressive). In these types of transitions, participants studied the molecular features of one portion of the equation (reactant, condition, or product) before moving to a different feature of the equation. Approximately 63% of all the 3-fixation transitions were between different features of the chemical equation (reagents, conditions, and products). These transitions between features of the chemical equation support the idea that participants establish relationships between molecules and conditions in the reaction.

Summary. The preferential fixation in iROIs over dROIs across the equation indicates that participants created relationships among features of equations. These relationships help participants identify important features key to helping them understand the reaction. ROIs that contained these important features experienced higher percent fixation duration than ROIs that contained distractor information.

The analysis of 3-fixation patterns indicated that participants made a series of fixations across all features of the equation. During these fixations, participants processed each feature of the equation. Approximately two thirds of the 3-fixation patterns were transitions between two or more AOI in the equation. While fixation patterns uniquely within the same AOI indicated that participants were examining relationships within the

molecules, the fixation patterns between different AOIs supported the proposed processes for identifying relationships between molecules in the equation (*Intermolecular Relationships*).

Reaction Wrap-up. The final stage of the process model occurs just before the participant indicates that they understand the equation. During this final stage, the participant integrates all the relationships, check for inconsistencies in his/her internal representation, and assigns meaning to the chemical equation. In the reading of English text, this integration stage is characterized by a long pause on the final punctuation of the sentence. Similar to the reading of English, I hypothesized that this stage would also be characterized by a long fixation just before the participant indicates that he/she comprehends the chemical reaction. For each chemical equation, the final fixation duration would be significantly longer than the mean fixation duration of all the other fixations. For this analysis, these fixations were computed as percentages of the total fixation time for each participant.

Normality assumption. I examined the variables for assumption violations using SPSS (version 19) Explore. For the percent final fixation duration and percent average fixation duration, the Kolmogorov-Smirnov test statistics were statistically significant ($p < .05$), indicating the normality assumption was violated. Examination of the skewness and kurtosis indicated that the distributions were not symmetrical. Skew was to the right with heavy tailing. Attempts to transform the data using common transformations were

unsuccessful at significantly improving the normality of the distribution. Therefore, non-parametric means were used to analyze the data.

Wilcoxon signed rank test. The percent final fixation duration was compared to the average percent fixation duration for all other fixations to determine if there was a difference in the fixation durations. I hypothesized that the final fixation would be significantly longer than the average of the other fixation durations because of the amount of processing that occurs during this final stage. A Wilcoxon signed ranks test indicated that the final fixation duration (Mdn = 1.86) was longer than the average duration for all other fixations (Mdn = 1.70, Z = -4.36, $p < 0.00$, d = 0.26). The effect size was determined to be small indicating that the difference in fixation durations was small.

According to the process model, the final fixation is used to look for inconsistencies and apply meaning to the chemical equation. Since experts are more likely to recognize meaningful patterns and have a highly structured long-term memory, these processes should take less time for the expert to complete than the novice. This would be reflected in the final fixation times for experts and novices. To determine if there was an expertise effect on the final fixation, two separate Wilcoxon signed ranks tests were run. For the experts, the test indicated that the final fixation duration (Mdn = 3.74) was not significantly longer than the average duration for all other fixations (Mdn = 2.84, Z = -1.49, p = 0.135, d = 0.16). However, the second Wilcoxon signed rank test indicated that the novices had significantly longer final fixation duration (Mdn = 1.64) than compared to the average duration for all

other fixations (*Mdn* = 1.44, *Z* = -4.66, *p* = 0.00, *d* = 0.34). There was a moderate effect size.

To better understand the final fixation patterns, the ROI of the final fixations were coded to determine what participants looked at just before indicating that they understood the reaction. Table 28 gives the frequency and percent for the content of the final fixations.

Table 28

Content of the Final Fixation Across All Equations

Content Type	Frequency	Percent (%)
Conditions	97	36.3
White space	52	19.5
Reactant iROI	51	19.1
Product iROI	32	12.0
Reactant dROI	30	11.2
Product dROI	5	1.9

Just over a third (36%) of all final fixations for participants were on the conditions. Another 30% of the final fixations were on the reactants, and about 13% were on the product. A final fixation on content like the conditions makes sense. Participants check the internal representation against some information from the equation. Organic chemistry is often taught with an emphasis on conditions or the reactants as means of organizing the chemical reactions, so it is not surprising that these were the most common final fixations. However, almost 20% of the final fixations were on areas of the screen that contained no

content. The equations were examined to see if off content viewing occurred preferentially in LVC or HVC equations. It was determined that off content viewing was more common in HVC equations (n = 32) than for LVC equations (n = 20). The reason for this may be related to the cognitive demands of processing the additional information in a HVC equation.

Summary. This analysis indicates that there is a final stage in the process model, just before the participants indicate that they understand the reaction. This stage is marked by a longer fixation. It is believed that during this longer fixation, additional processing takes place that allows participants to process the entire equation and give meaning to their internal representation.

Conclusion. Eye-tracking methodology provided means to explore the processes that support the six stage process model described in Chapter 1 of this dissertation. As the eyes of the participant moved across the chemical equation (*Get Next)*, fixation patterns were evident. The participants searched the molecule for features that were key to understanding the reaction (*Search)* before moving to another molecule. Patterns of fixations on molecular features were observed. As the participants read, other processes took place. Participants encoded information and activated LTM to give meaning to the molecular features (*Encoding and Access Lexicon*). This encoding required time to activate memory. Features that were important to understanding the chemical reaction had significantly longer fixation times than features that were not important in the reaction. Participants defined relationships between the informative and distracting features of the molecules in the chemical equation

(*Intramolecular Relationships* and *Intermolecular Relationships*), as evidenced by the patterns of fixations and fixation durations. Once this processing was complete, the participants paused briefly to possibly integrate the internal representation and give meaning to the chemical equation (*Reaction Wrap-up*).

Research Question 5

This analysis addressed research question 5:

> For high versus low complexity chemical equations, what are the effects of different participant variables (expertise, spatial ability, and working memory capacity) on the frequency and duration of eye fixations as measured by the eye tracker for
>
> a. Informative ROIs versus distractor ROIs?
> b. AOIs (reactant, condition, product)?

Since I was interested in the difference between high versus low visual complexity equations, fixation durations and fixation frequencies were collapsed across observations and reported as mean fixation durations and mean fixation frequencies for HVC equations and LVC equations. A mixed between-within subject ANOVA was uses to address this research question.

Informative ROIs verses distractor ROIs. To investigate the effects of different participant characteristics (expertise, spatial ability, and working memory capacity) on the frequency and duration of eye fixations as measured by the eye tracker for Informative ROIs versus distractor ROIs, a complex mixed design was proposed. Separate mixed between-within repeated measure ANOVAs were used to compare the frequency and duration of eye

fixations in ROIs. The between-subject factor was the participant characteristic (expertise, spatial ability, or working memory capacity) and two within-subjects factors (visual complexity of the chemical equation and the type of ROI). Two-molecule and 3-molecule equations were analyzed separately. In cases where datasets were transformed for analysis, results from the ANOVA were back-transformed. For these datasets, geometric means and 95% confidence intervals were reported.

Expertise. Based on status in the educational system, participants were split into two groups based on expertise. Experts ($n = 8$) were instructors and novices ($n = 19$) were undergraduate and graduate students. One trial was incomplete for the 3-molecule analysis and was removed from the dataset.

Exploratory data analysis was conducted on each dataset to assess the normality of the distribution. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated frequency data were symmetrical. However, duration data were not. The Kolmogorov-Smirnov test was significant ($p < 0.05$) for the duration datasets, suggesting that it did not follow a normal distribution across all participant types. These datasets were transformed using the natural logarithm to improve normality. The datasets for the frequency of fixations followed a normal distribution and were not transformed.

The natural log of the mean duration was entered into a 2x2x2 mixed factorial ANOVA with expertise as the between-subject variable and complexity of the equation

(HVC and LVC) and ROI content type (iROI and dROI) as the between-subject variables. A summary of the result from the ANOVA is given in Table 29.

Table 29

Summary of ANOVAs on Eye Fixation Duration in ROIs - Expertise

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	18.04*	1, 25	0.00	0.42
	Content	298.05*	1, 25	0.00	0.92
	Complexity*Content	1.05	1, 25	0.32	0.04
	Complexity*Expertise	0.22	1, 25	0.23	0.06
	Content*Expertise	0.20	1, 25	0.25	0.05
	Complexity*Content*Expertise	0.07	1, 25	0.37	0.03
	Expertise	16.69*	1, 25	0.00	0.40
3-Molecule	Complexity	36.58*	1, 23	0.00	0.61
	Content	179.33*	1, 23	0.00	0.89
	Complexity*Content	30.13*	1, 23	0.00	0.57
	Complexity*Expertise	1.19	1, 23	0.29	0.05
	Content*Expertise	1.25	1, 23	0.27	0.05
	Complexity*Content*Expertise	4.49*	1, 23	0.05	0.16
	Expertise	26.84*	1, 23	0.00	0.54

Note. * significant at $p < 0.05$.

From the results in Table 29, there is a significant main effect for complexity, content, and expertise for equations containing 2-molecules. Novices (M = 4.56 s, 95% CI [3.68, 5.66]) made significantly longer fixations than experts (M = 1.17 s, 95% CI [1.50, 2.90]) in the ROIs in the equations, regardless of the content of the ROIs. Fixations in ROIs of HVC equations (M = 3.66 s, 95% CI [2.98, 4.51]) were significantly longer than those of LVC equations (M = 2.60 s, 95% CI [2.09, 3.24]) for all participants. Finally, fixations in iROIs (M = 6.07 s, 95% CI [5.01, 7.34]) were significantly longer than the mean fixations in dROIs (M =1.57 s, 95% CI [1.24, 1.98]). There were no significant interactions. This

indicates that although participants exhibited longer fixation durations in iROI versus dROI, the expertise level of the participants influenced this difference.

In 3-molecule equations, there was a significant interaction among complexity, content, and expertise. The graph of the interaction is given in Figure 30. The simple effect analysis indicated the following results: both novices and experts made significantly longer fixations on iROIs than dROIs. However, experts spent significantly more time on the iROIs than the novices. Experts also spent significantly less time viewing the dROIs than novices. But, for both the experts and novices, there is a significant decrease in the duration of the fixations on dROIs from HVC to LVC equations.

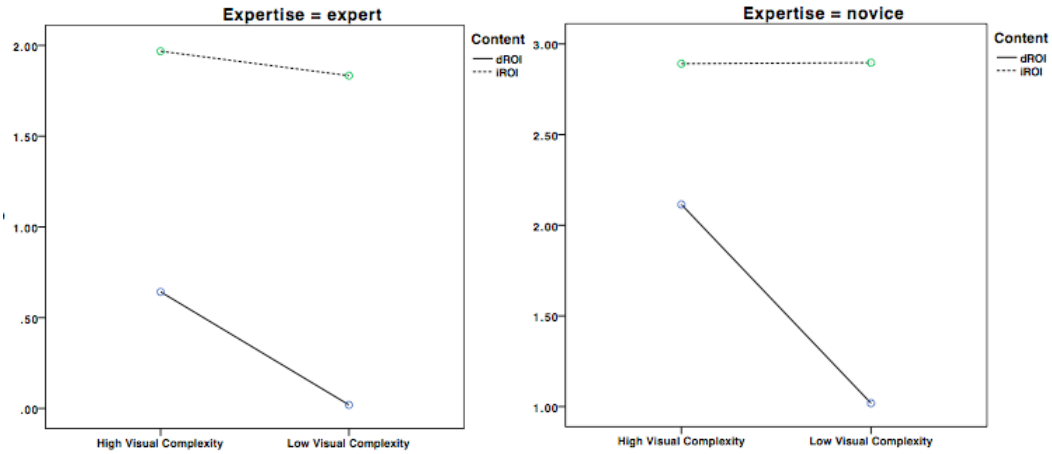


Figure 30. Three-way interaction of complexity, content, and expertise for duration of fixation in ROIs

Next, the mean frequency of the eye fixations were entered into the 2x2x2 mixed factorial ANOVA. The results of the analysis are given in Table 30.

Table 30

Summary of ANOVAs on Eye Fixation Frequency in ROIs - Expertise

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	24.77*	1,25	0.00	0.50
	Content	499.75*	1,25	0.00	0.95
	Complexity*Content	0.71	1,25	0.41	0.03
	Complexity*Expertise	1.03	1,25	0.32	0.04
	Content*Expertise	0.84	1,25	0.37	0.03
	Complexity*Content*Expertise	1.16	1,25	0.29	0.04
	Expertise	1.42	1,25	0.25	0.05
3-Molecule	Complexity	8.86*	1,24	0.01	0.27
	Content	343.25*	1,24	0.00	0.94
	Complexity*Content	86.53*	1,24	0.00	0.78
	Complexity*Expertise	0.17	1,24	0.68	0.01
	Content*Expertise	1.60	1,24	1.60	0.06
	Complexity*Content*Expertise	21.46*	1,24	0.00	0.47
	Expertise	1.20	1,24	0.29	0.05

Note. * significant at $p < 0.05$.

In 2-molecule equations, there was a significant main effect for complexity, indicating that HVC equations ($M = 39.87$, $SE = 0.51$) had significantly more fixations than the LVC equations ($M = 35.54$, $SE = 0.72$). There was also a significant main effect for content. Informative AOIs ($M = 57.27$, $SE = 0.85$) had a significantly larger number of fixations than dROIs ($M = 18.14$, $SE = 0.85$). There were no significant interactions indicating that these effects were not dependant on the expertise of the participant.

In 3-molecule equations, there was a significant interaction among complexity, content, and expertise. The graph of the interaction is given in Figure 31.

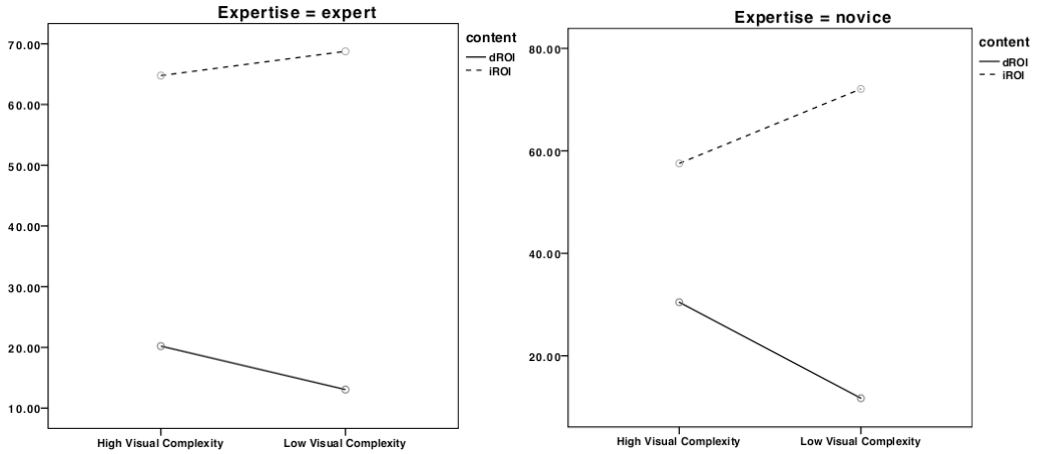


Figure 31. Three-way interaction of complexity, content, and expertise for frequency of fixations in ROIs.

The results of the simple effect analysis indicate that there is a significant difference in the frequency of fixations for experts and novices in the HVC equations. As predicted, experts made significantly more fixations in iROIs and fewer fixations in dROIs than the novices. In the LVC equations, experts made more frequent fixations in iROIs than the novices. However, there was no significant difference in the number of fixation in dROIs for experts and novices for LVC equations. The novices made significantly fewer fixations in the iROIs in HVC equations than in LVC equations and made significantly more fixations in the dROIs in the HVC equations than in the LVC equations. As predicted, there was no significant difference in the number of fixations experts made in iROIs for HVC and LVC equations. However, experts made significantly fewer fixations in dROIs in the LVC equations versus the HVC equations.

Spatial ability (SA). As part of this study, participants completed the Purdue Visualization of Rotations test (ROT), a measure of spatial ability. The mean score for the

participants on the ROT was $M = 13.56$ ($SD = 4.16$). The distribution of the scores ($n = 27$) was divided into thirds - low SA ($n = 8$), medium SA ($n = 9$), and high ($n = 10$). One incomplete trail for high spatial ability was removed from the 3-molecule analysis.

Exploratory data analysis was used to determine if frequency and duration of eye fixations followed a normal distribution for participants of differing spatial ability. Each dataset was assessed for normality of distribution. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated frequency data was symmetrical. However, duration data was not. The Kolmogorov-Smirnov test was significant ($p < 0.05$) for the duration datasets, suggesting that it did not follow a normal distribution across all participant types. These datasets were transformed using the natural logarithm to improve normality. The datasets for the frequency of fixations followed a normal distribution.

For this analysis, two separate mixed between-within subjects ANOVA were conducted to assess the role of visual complexity (HVC and LVC) and content of the ROI (iROIs and dROIs) on the fixation duration of participants with different spatial ability (High SA and Low SA). The results of the ANOVA with mean fixation duration as the dependent variable are given in Table 31.

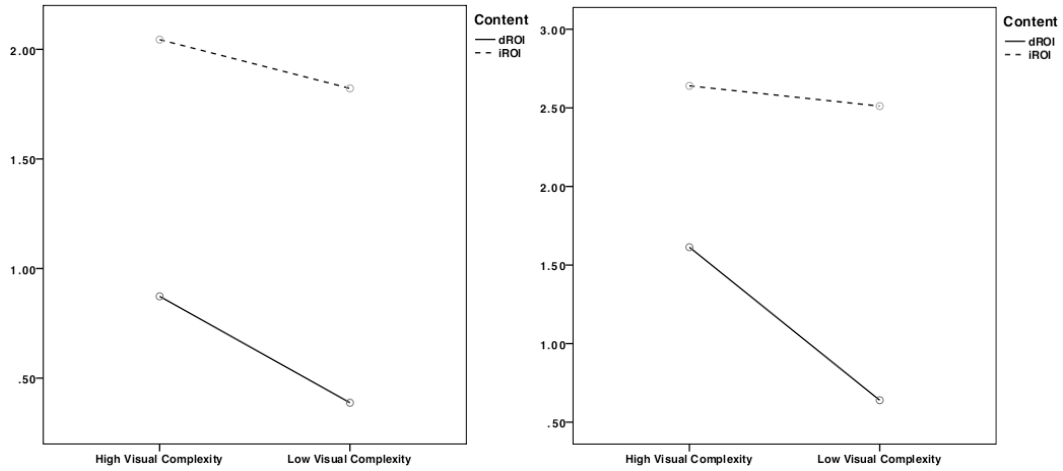
Table 31

Summary of ANOVAs on Eye Fixation Duration in ROIs – Spatial Ability

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	12.91*	1,16	0.00	0.45
	Content	165.46*	1,16	0.00	0.91
	Complexity*Content	5.78*	1,16	0.03	0.27
	Complexity*SA	1.74	1,16	0.21	0.10
	Content*SA	0.58	1,16	0.46	0.04
	Complexity*Content*SA	0.73	1,16	0.41	0.04
	SA	1.73	1,16	0.21	0.10
3-Molecule	Complexity	50.88*	1,14	0.00	0.78
	Content	172.29*	1,14	0.00	0.93
	Complexity*Content	24.43*	1,14	0.00	0.64
	Complexity*SA	1.14	1,14	0.31	0.08
	Content*SA	2.71	1,14	0.12	0.16
	Complexity*Content*SA	2.19	1,14	0.16	0.14
	SA	1.43	1,14	0.47	0.04

Note. * significant at $p < 0.05$.

In both the 2-molecule and 3-molecule equations there was a significant interaction between complexity and content. The graphs for the interactions are given in Figure 32.



A **B**

Figure 32. Interaction of complexity and content in eye fixation durations for 2-molecule equations (A) and 3-molecule equations (B).

For both 2 and 3-molecule equations there is a significant difference in the duration of eye fixations in iROIs and dROIs of LVC and HVC equations. In the 2-molecule LVC equations, the duration of fixations in dROIs is M = 1.47 s, 95% CI [0.98, 2.21] and the duration in iROI is M = 6.18 s, 95% CI [4.57, 8.36]. For the HVC equations, the duration in both types of ROIs increased. The dROIs have a mean fixation of M = 2.39 s, 95% CI [1.71, 3.36] and the iROIs have a mean fixation of M = 7.72 s, 95% CI [6.01, 9.92]. For the 3-molecule equations, there is a similar trend. For the LVC equations, duration of fixations in dROIs is M = 1.90 s, 95% CI [1.14, 3.15] and the duration in iROIs is M = 12.32 s, 95% CI [8.04, 18.88]. For the HVC equations, the duration of fixation in the ROIs increases. The dROIs have a mean fixation of M = 5.02 s, 95% CI [2.88, 8.75] and the iROIs had a mean fixation of M = 14.01 s, 95% CI [10.00, 19.63]. In both instances, participants spent more time fixated on dROIs in the HVC equations than in the LVC equations.

Next the frequency of fixation was investigated. The results from the 2x2x2 mixed factorial ANOVA are given in Table 32.

Table 32

Summary of ANOVAs on Eye Fixation Frequency in ROIs – Spatial Ability

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	24.94*	1,16	0.00	0.61
	Content	432.91*	1,16	0.00	0.96
	Complexity*Content	1.16	1,16	0.30	0.07
	Complexity*SA	3.08	1,16	0.10	0.16
	Content*SA	1.21	1,16	0.29	0.07
	Complexity*Content*SA	0.48	1,16	0.50	0.03
	SA	0.20	1,16	0.66	0.01
3-Molecule	Complexity	4.70*	1,15	0.05	0.24
	Content	436.08*	1,15	0.00	0.97
	Complexity*Content	68.84*	1,15	0.00	0.82
	Complexity*SA	0.63	1,15	0.44	0.04
	Content*SA	1.48	1,15	0.24	0.09
	Complexity*Content*SA	4.77*	1,15	0.05	0.24
	SA	4.77*	1,15	0.05	0.24

Note. * significant at $p < 0.05$.

For 2-molecule equations, there is significant main effect for complexity and content. The ROIs in HVA equations ($M = 40.26$, $SE = 0.56$) had significantly more fixations than the ROIs in LVC equations ($M = 35.32$, $SE = 0.90$), which was not unexpected considering HVC equations have more visual information and a greater number of ROIs. As expected, iROIs ($M = 56.50$ fixations, $SE = 1.07$) received more fixations than dROIs ($M = 19.08$ fixations, $SE = 1.05$). However, there was no significant main effect for SA and the interactions were also not significant. This suggests that SA does not affect the fixations on dROIs and iROIs.

For the 3-molecule equations, there was a significant interaction between complexity and content. The graph of the interaction is given in Figure 33.

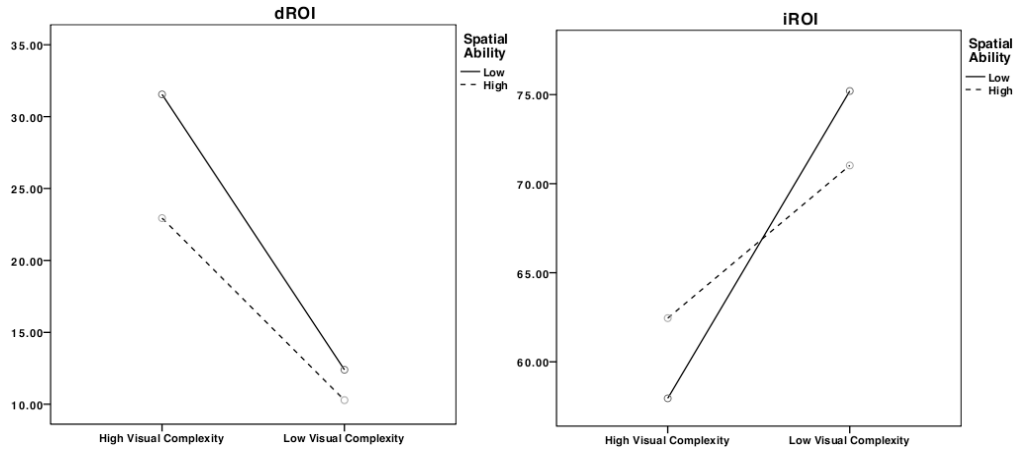


Figure 33. Three-way interaction of content and visual complexity for the frequency of fixation in ROIs of 3-molecule equations.

The results of simple effects analysis are as follows. There is a significant difference in the fixation patterns for high and low spatial ability participants for iROIs and dROIs in both HVC and LVC equations. For the dROIs, low SA participants made significantly more fixations than the high SA participants in the HVC equations. However, in the LVC equations, the frequency of fixation in dROIs was not significantly different for high SA and low SA participants. For the iROIs, low SA participants made significantly fewer fixations on iROIs in the HVC equations than in the LVC equations. The same was true for the high SA participants. However, the difference was not as great as the low SA participants.

Working memory capacity (WMC). As part of this study, participants completed the Digit Span Backwards test (DSB), a measure of WMC. The mean scores for the participants on the DSB are $M = 4.19$ ($SD = 0.96$). The distribution of the scores ($n = 27$) was divided

into thirds - low WMC (n = 6), medium WMC (n = 11), and high WMC (n = 10). Failure successfully eye-track two participants for one equation in 2-molecule stimuli caused 2 incomplete datasets, which were removed from that analysis

To determine if frequency and duration of eye fixations followed a normal distribution for participants of differing working memory capacity, exploratory data analysis was conducted on each dataset to assess the normality of the distribution. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated frequency data was symmetrical; however, duration data was not. The Kolmogorov-Smirnov test was significant ($p < 0.05$) for the duration datasets, suggesting that they did not follow a normal distribution across all participant types. These datasets were transformed using the natural logarithm to improve normality. The datasets for the frequency of fixations followed a normal distribution.

The mean duration of eye fixations in ROIs was entered into a 2x2x2 mixed factorial ANOVA with WMC as the between-subjects factor. Complexity of the equation and the content of the ROIs were the within-subject factors. The results of this ANOVA are given in Table 33.

Table 33

Summary of ANOVAs on Eye Fixation Duration in ROIs – Working Memory Capacity

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	16.90*	1,14	0.00	0.55
	Content	211.30*	1,14	0.00	0.94
	Complexity*Content	0.57	1,14	0.46	0.04
	Complexity*WMC	1.41	1,14	0.26	0.09
	Content*WMC	0.77	1,14	0.40	0.05
	Complexity*Content*WMC	0.17	1,14	0.69	0.01
	WMC	0.21	1,14	0.65	0.02
3-Molecule	Complexity	14.82*	1,12	0.00	0.55
	Content	86.13*	1,12	0.00	0.88
	Complexity*Content	20.37*	1,12	0.00	0.63
	Complexity*WMC	0.83	1,12	0.38	0.07
	Content*WMC	3.37	1,12	0.09	0.22
	Complexity*Content*WMC	0.33	1,12	0.57	0.03
	WMC	0.92	1,12	0.36	0.07

Note. * significant at $p < 0.05$.

As in previous analyses in this section, there was a significant main effect for complexity and content in the 2-molecule equations. Fixations were significantly longer in ROIs of HVC equations ($M = 3.99$ s, 95% CI [3.11, 510]) than in LVC equations ($M = 2.70$ s, 95% CI [2.04, 3.56]). This is not surprising since HVC equations have more ROIs and more visual information than LVC equations. Fixations in iROIs ($M = 6.70$s, 95% CI [5.35, 8.41]) were over four times longer the fixations in dROIs ($M = 1.69$ s, 95% CI [1.19, 2.16]). There were no significant interactions and WMC was also not significant. This suggests that these differences were not influenced by the WMC of the participants.

For 3-molecule equations, there was a significant interaction between complexity and content. The graph of the interactions is given in Figure 34.

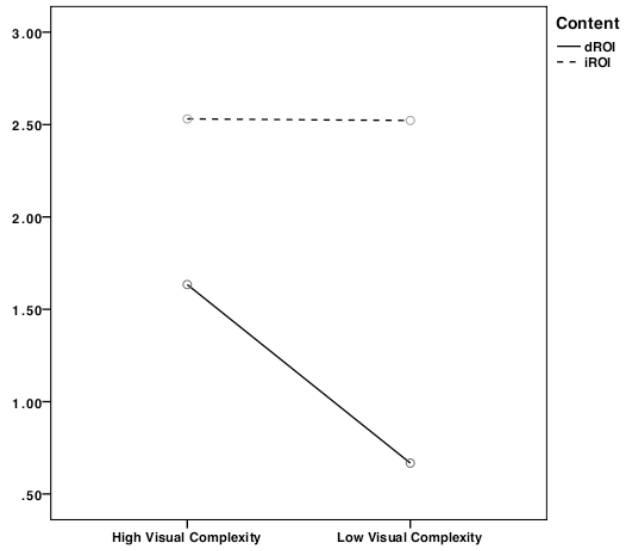


Figure 34. Interaction of complexity and content for fixation duration in ROIs of 3-molecule equations

In this interaction, the duration of fixations on iROIs is not significantly different for HVC equations (*M* = 12.57 s, 95% CI [8.75, 18.03]) or LVC equations (*M* = 12.45 s, 95% CI [8.48, 18.28]). However, there is a significant difference in the fixations durations for dROIs. These fixation durations were over 2.5 times longer in HVC equations (*M* = 5.12s , 95% CI [3.33, 7.88]) than in LVC equations (*M* = 1.95 s, 95% CI [1.03, 3.40]). The fixation durations on iROIs are significantly different from dROIs regardless of the equation complexity.

Next, the frequencies of fixations in ROIs of the fixations were entered into the 2x2x2 mixed ANOVA with SA as the between-subject factor. The results are given in Table 34.

Table 34

Summary of ANOVAs on Eye Fixation Frequency in ROIs – Working Memory Capacity

Equation	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Complexity	10.78*	1,14	0.01	0.44
	Content	561.26*	1,14	0.00	0.98
	Complexity*Content	0.28	1,14	0.61	0.02
	Complexity*WMC	0.16	1,14	0.70	0.01
	Content*WMC	3.47	1,14	0.08	0.20
	Complexity*Content*WMC	0.02	1,14	0.89	0.00
	WMC	2.29	1,14	0.15	0.14
3-Molecule	Complexity	15.55*	1,12	0.00	0.55
	Content	167.13*	1,12	0.00	0.93
	Complexity*Content	48.06*	1,12	0.00	0.79
	Complexity*WMC	3.90	1,12	0.07	0.23
	Content*WMC	2.58	1,12	0.13	0.17
	Complexity*Content*WMC	1.03	1,12	0.33	0.07
	WMC	1.82	1,12	0.20	0.12

Note. * significant at $p < 0.05$.

There are significant main effects for complexity and content for the 2-molecule equations. There are significantly fewer fixations in ROIs in the LVC equations ($M = 35.46$ fixations, $SE = 1.04$) than in the HVC equations ($M = 35.46$ fixations, $SE = 0.62$). This is not surprising since LVC equations have fewer ROIs than LVC equations. As expected, iROIs ($M = 58.12$, $SE = 1.11$) have a significantly higher number of fixations than dROIs ($M = 17.22$, $SE = 0.91$). There are no significant interactions and the main effect for WMC is also not significant. Therefore these differences were not influenced by the WMC of the participants.

For 3-molecule equations, there is a significant interaction between complexity and content for the frequency of fixation in ROIs. The graph of the interaction is given in Figure 35.

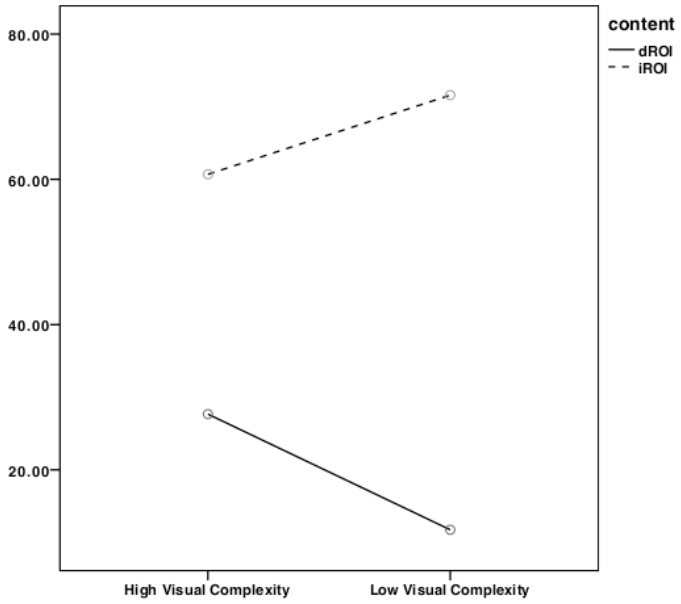


Figure 35. Interaction of complexity and content for fixation frequency in ROIs of 3-molecule equations.

In this interaction, the frequency of fixations in iROIs is significantly different for the two types of equations. The number of fixations in dROIs for HVC equations (M = 27.67, SE = 1.56) is significantly higher than the number of fixations for LVC equations (M = 11.75, SE = 1.51). For iROIs, the number of fixation in iROIs for HVC equations (M = 60.69, 2.35) is lower than for LVC equations (M = 71.59, SE = 2.90). The fixation durations on iROIs are significantly different from dROIs regardless of the equation complexity.

Summary. Overall, there appears to be no effect of participant variables on the viewing patterns of ROIs in 2-molecule equations. However, effects due to expertise and

spatial ability were observed in 3-molecule equations. As predicted, experts exhibited fewer but longer fixations in iROIs than the novices. Experts also made fewer, shorter fixations in dROIs than the novices in these equations. However this was only true in HVC equations. This effect was not seen in the LVC equations.

It was predicted that high SA participants would have fewer fixations in iROIs and dROIs than the low SA participants. However, the data presented here suggest that the relationship of SA to fixation frequency is not that simple and needs to take into account the complexity of the equation that is being read. While these general trends hold true for content that is not informative, high SA participants spend significantly more of their fixation time in iROIs then the low SA participants. This data suggest that participants with high SA are able to find key visual information about the chemical reaction and focus a greater proportion of their fixations in iROIs versus dROIs. This would translate into a larger number of fixations and greater total fixation duration in iROIs than dROIs.

Working memory capacity showed no significant effect on reading patterns. There was no significant main effect or interaction, suggesting that WMC may not play a role in reading chemical equations as first thought.

While not part of the overall question, it is important to note that there was a significant main effect for complexity and a significant interaction between complexity and content in all three participant variables. This suggests that the amount of visual information in the equations affects viewing patterns, regardless of the level of expertise or SA of the

participant. Participants reading equations with high visual complexity experienced longer reading times and made more fixations than they did when they read LVC equations.

Areas of interest (AOIs). The purpose of the investigation was to examine the effects of different participant characteristics (expertise, spatial ability, and working memory capacity) on the frequency and duration of eye fixations in AOIs of 2-molecule and 3-molecule equations. A complex mixed design was proposed. However, the small sample size and the unbalanced design of the experiment violated the assumption of homogeneity of intercorrelations for the mixed between-within subject ANOVA, preventing the proposed analyses. No value was calculated for the Box's M statistic because there were fewer than two nonsingular cell covariance matrices.

To compare fixation patterns of participants with different characteristics, I used separate 2x2 mixed ANOVA for each AOI in the equation. The within-subject variable was the participant characteristic. The between-subject variable was the complexity of the equations (HVC and LVC) that contained the AOIs. The mean fixation duration and mean fixation frequency for each AOI was entered into the ANOVA.

Exploratory data analysis was used to determine if frequency and duration of eye fixations followed a normal distribution for each participant characteristic. Two-molecule and 3-molecule equations were tested separately. Analysis of the skew and kurtosis data indicated frequency and duration datasets for 2-molecule equations and the duration dataset for the 3-molecule equations were not symmetrical. The dataset for the frequency of fixation for 3-molecule equations showed little skew. The Kolmogorov-Smirnov test was

significant ($p < 0.05$) for both the duration and the frequency datasets for 2-molecule equations, suggesting that they did not follow a normal distribution across all participant types. These datasets were transformed using the natural logarithm to improve normality. The datasets for the frequency of fixations for 3-molecule equations followed a normal distribution.

Expertise. The mean duration and frequency of fixations in AOIs were entered into two separate mixed ANOVAs with expertise as the within-subject factor and the complexity of the AOIs as the between-subject factor. The results of the ANOVA for the duration of fixation are given in Table 35.

Table 35

Summary of ANOVAs on Eye Fixation Duration in AOIs - Expertise

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	19.27*	1,25	0.00	0.44
		Complexity*Expertise	3.70	1,25	0.07	0.13
		Expertise	16.36*	1,25	0.00	0.40
	Condition	Complexity	3.30	1,25	0.08	0.12
		Complexity*Expertise	0.52	1,25	0.48	0.02
		Expertise	15.12*	1,25	0.00	0.38
	Product	Complexity	17.31*	1,25	0.00	0.41
		Complexity*Expertise	2.03	1,25	0.17	0.08
		Expertise	16.07*	1,25	0.00	0.39
3-Molecule	Reactant 1	Complexity	16.97*	1,25	0.00	0.40
		Complexity*Expertise	1.63	1,25	0.21	0.06
		Expertise	16.55*	1,25	0.00	0.40
	Reactant 2	Complexity	10.16*	1,25	0.00	0.29
		Complexity*Expertise	0.23	1,25	0.64	0.00
		Expertise	20.08*	1,25	0.00	0.45
	Condition	Complexity	2.83	1,25	0.11	0.10
		Complexity*Expertise	0.00	1,25	0.93	0.00
		Expertise	12.45*	1,25	0.00	0.33
	Product	Complexity	52.09*	1,25	0.00	0.68
		Complexity*Expertise	0.19	1,25	0.67	0.01
		Expertise	14.46*	1,25	0.00	0.60

Note. * significant at $p < 0.05$.

For each type of AOI, expertise had a significant main effect. In all cases the experts had significantly shorter fixation durations than novices (Table 36).

Table 36

Geometric Mean of Fixation Durations for Experts and Novices in AOIs

				95% Confidence Interval	
	Feature	Expertise	Geometric Mean	Lower bound	Upper Bound
2-Molecule	Reactant	Novice	6.78	5.67	8.56
		Expert	3.32	2.42	4.56
	Condition	Novice	2.89	2.32	3.60
		Expert	1.34	0.63	1.89
	Product	Novice	4.58	3.67	5.72
		Expert	2.08	1.47	2.92
3-Molecule	Reactant 1	Novice	21.78	18.03	26.34
		Expert	12.29	9.18	16.48
	Reactant 2	Novice	9.12	7.52	11.03
		Expert	5.07	3.77	6.81
	Condition	Novice	15.39	12.68	18.69
		Expert	7.34	5.45	9.90
	Product	Novice	6.55	5.05	8.51
		Expert	2.54	1.70	3.80

However, there are no significant interactions, which indicate that the expertise of the participants does not influence the duration of the fixation for HVC and LVC equations. There is a main effect for complexity in five of the seven types of AOIs. Just as in previous analyses, experts exhibit significantly shorter fixation durations than novices. The two AOIs that did not show a significant main effect were both on conditions.

Mean frequency of fixation was also entered into the same ANOVA. The results are given in Table 37.

Table 37

Summary of ANOVAs on Eye Fixation Frequency in AOIs - Expertise

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	26.60*	1,25	0.00	0.52
		Complexity*Expertise	5.29*	1,25	0.03	0.17
		Expertise	11.42	1,25	0.00	0.31
	Condition	Complexity	0.53	1,25	0.48	0.02
		Complexity*Expertise	0.98	1,25	0.33	0.04
		Expertise	11.75*	1,25	0.00	0.32
	Product	Complexity	16.61*	1,25	0.00	0.40
		Complexity*Expertise	2.81	1,25	0.11	0.10
		Expertise	18.34*	1,25	0.00	0.42
3-Molecule	Reactant 1	Complexity	15.62*	1,25	0.00	0.39
		Complexity*Expertise	1.42	1,25	0.25	0.05
		Expertise	13.09*	1,25	0.00	0.34
	Reactant 2	Complexity	8.20*	1,25	0.01	0.25
		Complexity*Expertise	2.95	1,25	0.10	0.11
		Expertise	10.15*	1,25	0.00	0.29
	Condition	Complexity	6.19*	1,25	0.02	0.20
		Complexity*Expertise	0.01	1,25	0.92	0.00
		Expertise	6.94*	1,25	0.01	0.22
	Product	Complexity	18.69*	1,25	0.00	0.43
		Complexity*Expertise	2.56	1,25	0.12	0.09
		Expertise	26.50*	1,25	0.00	0.52

Notes. * significant at $p < 0.05$.

There was a significant main effect for expertise. Experts exhibited significantly fewer fixations than novice participants. Table 38 gives a summary of the back-transformed means for the frequency of fixations in 2-molecule equations. Table 39 provides the summary of the means for the 3-molecule equations.

Table 38

Geometric Mean of Fixation Frequencies for Experts and Novices in AOIs of 2-Molecule Equations

			95% Confidence Interval	
Feature	Expertise	Geometric Mean	Lower bound	Upper Bound
Reactant	Novice	7.48	5.92	9.44
	Expert	2.94	2.05	4.22
Condition	Novice	2.59	1.94	3.46
	Expert	1.04	0.66	1.63
Product	Novice	7.02	5.71	8.64
	Expert	2.26	1.64	3.11

Table 39

Mean Fixation Frequencies for Experts and Novices in AOIs of 3-Molecule Equations

Feature	Expertise	Mean	(*SE*)
Reactant 1	Novice	20.79	(1.53)
	Expert	10.66	(2.35)
Reactant 2	Novice	25.03	(2.09)
	Expert	12.81	(3.22)
Condition	Novice	9.50	(0.91)
	Expert	5.09	(1.40)
Product	Novice	22.91	(1.48)
	Expert	8.94	(2.28)

Spatial ability. The mean duration and frequency of fixations in AOIs were entered into two separate mixed ANOVAs with SA as the within-subject factor and the complexity of the AOIs as the between-subject factor. The results of the ANOVA for the duration of fixations are given in Table 40. There is no main effect for SA and no interactions, indicating that the SA of the participant did not play a significant role in influencing the fixation durations in AOIs.

Table 40

Summary of ANOVAs on Eye Fixation Duration in AOIs – Spatial Ability

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	9.55*	1,16	0.01	0.37
		Complexity*SA	0.44	1,16	0.52	0.03
		SA	1.38	1,16	0.26	0.08
	Condition	Complexity	2.74	1,16	0.12	0.15
		Complexity*SA	0.00	1,16	0.96	0.00
		SA	0.22	1,16	0.64	0.01
	Product	Complexity	8.30*	1,16	0.01	0.34
		Complexity*SA	1.77	1,16	0.20	0.10
		SA	1.48	1,16	0.24	0.08
3-Molecule	Reactant 1	Complexity	16.83*	1,16	0.00	0.51
		Complexity*SA	0.01	1,16	0.94	0.00
		SA	0.46	1,16	0.51	0.03
	Reactant 2	Complexity	19.15*	1,16	0.00	0.55
		Complexity*SA	0.24	1,16	0.63	0.02
		SA	0.47	1,16	0.51	0.03
	Condition	Complexity	1.00	1,16	0.33	0.06
		Complexity*SA	1.02	1,16	0.60	0.01
		SA	0.23	1,16	0.64	0.01
	Product	Complexity	48.62*	1,16	0.00	0.75
		Complexity*SA	0.89	1,16	0.36	0.05
		SA	0.02	1,16	0.91	0.00

Note. * significant at $p < 0.05$.

For 5 out of the 7 AOIs, there is a significant main effect for complexity. As seen in other analyses, HVC equations have longer fixation durations in AOIs than LVC equations. With more visual information in the AOIs of HVC equations, these results are expected.

Table 41 gives the results of the ANOVA for the eye fixation frequencies. Like fixation duration, there were no significant interactions and no main effect for SA. This indicates that SA does not play a significant role in the frequency of eye fixations in AOIs.

Table 41

Summary of ANOVAs on Eye Fixation Frequency in AOIs – Spatial Ability

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	11.47*	1,16	0.00	0.42
		Complexity*SA	0.09	1,16	0.77	0.01
		SA	1.46	1,16	0.25	0.08
	Condition	Complexity	1.11	1,16	0.31	0.07
		Complexity*SA	0.00	1,16	0.98	0.00
		SA	0.53	1,16	0.48	0.03
	Product	Complexity	7.04*	1,16	0.02	0.31
		Complexity*SA	1.25	1,16	0.28	0.07
		SA	1.62	1,16	0.22	0.09
3-Molecule	Reactant 1	Complexity	17.41*	1,16	0.00	0.52
		Complexity*SA	0.00	1,16	0.99	0.00
		SA	0.87	1,16	0.37	0.05
	Reactant 2	Complexity	18.20*	1,16	0.00	0.53
		Complexity*SA	0.30	1,16	0.59	0.02
		SA	0.42	1,16	0.53	0.03
	Condition	Complexity	2.81	1,16	0.11	0.15
		Complexity*SA	1.99	1,16	1.18	0.11
		SA	0.11	1,16	0.74	0.01
	Product	Complexity	12.84*	1,16	0.00	0.45
		Complexity*SA	0.20	1,16	0.66	0.01
		SA	0.14	1,16	0.71	0.01

Note. * significant at $p < 0.05$.

Working memory capacity. The mean duration and mean frequency of fixations in AOIs were entered into two separate mixed ANOVAs. Working memory capacity (high WMC and Low WMC) was the within-subject factor, and the complexity of the AOIs (HVC and LVC) was the between-subject factor. The results of the ANOVA for the duration of fixation are given in Table 42. The results showed no main effect for WMC and no

interactions. This indicates that WMC also did not play a significant role in influencing the fixation durations in AOIs.

Table 42

Summary of ANOVAs on Eye Fixation Duration in AOIs – Working Memory Capacity

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	18.15*	1,14	0.00	0.57
		Complexity*WMC	0.87	1,14	0.37	0.06
		WMC	0.40	1,14	0.54	0.03
	Condition	Complexity	2.07	1,14	0.17	0.13
		Complexity*WMC	0.63	1,14	0.81	0.01
		WMC	0.31	1,14	0.59	0.02
	Product	Complexity	17.28*	1,14	0.00	0.55
		Complexity*WMC	1.94	1,14	0.19	0.12
		WMC	0.01	1,14	0.98	0.00
3-Molecule	Reactant 1	Complexity	18.00*	1,14	0.00	0.56
		Complexity*WMC	2.26	1,14	0.34	0.20
		WMC	0.18	1,14	0.68	0.01
	Reactant 2	Complexity	10.16*	1,14	0.01	0.42
		Complexity*WMC	0.56	1,14	0.47	0.04
		WMC	0.13	1,14	0.72	0.01
	Condition	Complexity	2.62	1,14	0.13	0.16
		Complexity*WMC	0.62	1,14	0.45	0.04
		WMC	1.18	1,14	0.30	0.08
	Product	Complexity	40.90*	1,14	0.00	0.75
		Complexity*WMC	6.47*	1,14	0.02	0.32
		WMC	0.00	1,14	0.95	0.00

Note. * significant at $p < 0.05$.

Next, the mean frequency of fixations for AOIs was entered into a 2x2 ANOVA. Table 43 provides a summary of the results. The main effect for the participant variable is not significant. The interaction is also not significant. Both results indicate that WMC does not have a significant effect on the frequency of eye fixations in AOIs.

Table 43

Summary of ANOVAs on Eye Fixation Frequency in AOIs – Working Memory Capacity

	Feature	Effect	*F*	*df*	*p*	Partial Eta Squared
2-Molecule	Reactant	Complexity	21.39*	1,14	0.00	0.60
		Complexity*WMC	0.01	1,14	0.92	0.00
		WMC	0.20	1,14	0.66	0.01
	Condition	Complexity	0.10	1,14	0.75	0.01
		Complexity*WMC	0.01	1,14	0.94	0.00
		WMC	0.15	1,14	0.71	0.01
	Product	Complexity	12.18*	1,14	0.00	0.47
		Complexity*WMC	0.45	1,14	0.51	0.03
		WMC	0.02	1,14	0.88	0.00
3-Molecule	Reactant 1	Complexity	16.15*	1,14	0.00	0.54
		Complexity*WMC	5.99	1,14	0.03	0.30
		WMC	0.03	1,14	0.88	0.00
	Reactant 2	Complexity	11.73*	1,14	0.00	0.46
		Complexity*WMC	1.70	1,14	0.21	0.11
		WMC	0.00	1,14	0.97	0.00
	Condition	Complexity	6.58*	1,14	0.02	0.32
		Complexity*WMC	0.93	1,14	0.35	0.06
		WMC	0.41	1,14	0.54	0.03
	Product	Complexity	16.26*	1,14	0.00	0.54
		Complexity*WMC	3.07	1,14	0.10	0.18
		WMC	0.16	1,14	0.70	0.01

Note. * significant at $p < 0.05$.

Summary. Overall, both SA and WMC of participants do not affect the viewing patterns across AOIs. The main effect for expertise indicates that experts and novices have different viewing patterns across all AOIs. Experts have significantly shorter fixation durations and made fewer fixations than novices, regardless of the complexity of the equation.

Research Question 6

For high versus low complexity chemical equations, is there a difference in the sequence of fixations (both intramolecular and intermolecular) between areas of interest as participants "read" organic chemistry equations for:

d. Participants of differing working memory capacity?

e. Experts and novices?

f. Participants of differing spatial ability?

Exploratory data analysis was conducted to assess normality and homogeneity of variance. Two-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test was not significant ($p > 0.05$) for all equations under both equation types, indicating a normal distribution of eye fixation sequence lengths for high WMC and low WMC participants. Levene's test for equality of variances was not significant ($p > 0.05$) for all equations.

To investigate the overall sequence of fixations, separate mixed between-within repeated measure ANOVAs was used to compare the length of the eye fixation sequence. The within-subject variable was the participant characteristic (WMC - high WMC and low WMC; Expertise – expert and novice; SA - high SA and low SA). The between-subject variables were *complexity* (HVC and LVC) and *equation* (2-molecule equations - Topic 1, Topic 2, and Topic 5; 3-molecule equations - Topic 3 and Topic 4). The dependent variable is the length of the eye fixation sequence.

Working memory capacity. To determine if there were significant differences in eye fixation sequence length between participants of differing working memory capacity, exploratory data analysis was conducted for normality and homogeneity of variance. Two-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test was not significant ($p > 0.05$) for all equations under both stimuli types, indicating a normal distribution of eye fixation sequence lengths for high WMC and low WMC participants. Levene's test for equality of variances was not significant ($p > 0.05$) for all equations.

Two-molecule equations. For the 2-molecule equations, there were unequal sample sizes for the participants when considering AOIs (high working memory capacity, $n = 10$; low working memory capacity, $n = 3$) and ROIs (high working memory capacity, $n = 10$; low working memory capacity, $n = 4$). Incomplete data sets were seen as responsible for the reduced number of low WMC participants. A 2x2x3 mixed factor ANOVA (WMC (high WMC and low WMC) x complexity of equation (HVC and LVC) x equation topic (Topic 1, Topic 2, and Topic 5)) was proposed for the analysis of 2-molecule AOIs and ROIs. However, limitations in the data (small, unbalanced sample size) prevented the computation of Box's test of equality of covariance matrices because there were fewer than 2 nonsingular cell covariance matrices. Therefore, the mixed factor ANOVA was not used for this analysis.

A two-way mixed ANOVA was used to compare the eye fixation sequence lengths of high WMC and low WMC participants reading each pair of equations. The mean eye

fixation sequence length for each equation, broken down by specificity, topic, complexity and working memory capacity is given in Table 44.

Table 44

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and WMC for 2-Molecule Equations

			High		Low	
Specificity	Topic	Complexity	Mean (*SD*)	*n*	Mean (*SD*)	*n*
AOI	1	HVC	41.60 (17.63)	10	47.33 (8.39)	3
		LVC	31.50 (20.15)		49.67 (18.58)	
	2	HVC	61.70 (24.19)	10	68.83 (32.68)	6
		LVC	40.40 (15.21)		50.83 (16.93)	
	5	HVC	32.40 (12.10)	10	29.17 (6.55)	6
		LVC	26.80 (9.62)		34.50 (7.74)	
ROI	1	HVC	43.40 (17.83)	10	54.24 (12.58)	4
		LVC	34.80 (20.54)		48.50 (19.55)	
	2	HVC	64.30 (24.72)	10	70.67 (32.14)	6
		LVC	42.70 (15.27)		53.50 (17.65)	
	5	HVC	35.20 (13.00)	10	33.50 (8.74)	6
		LVC	26.80 (9.62)		34.50 (7.74)	

Results from the ANOVA for AOI fixations are presented in Table 45.

Table 45

Summary of ANOVAs on Eye Fixation Frequency Lengths in AOIs of 2-Molecule Equations – Working Memory Capacity

Topic	Effect	*F*	*df*	*p*	Partial Eta Squared
1	Complexity	0.80	1, 11	0.39	0.07
	Complexity*WMC	2.06	1, 11	0.18	0.16
	WMC	1.15	1, 11	0.31	0.31
2	Complexity	13.90*	1, 14	0.00	0.50
	Complexity*WMC	0.10	1, 14	0.76	0.01
	WMC	0.72	1, 14	0.41	0.05
5	Complexity	0.00	1, 14	0.96	0.00
	Complexity*WMC	5.27*	1, 14	0.04	0.27
	WMC	0.25	1, 14	0.62	0.02

Note. . * significant at $p < 0.05$.

Of interest was the significant interaction only for topic 5 ($F(1,14) = 5.27$, $p = 0.04$, partial eta squared = 0.27). Participants with high WMC exhibited longer eye fixation sequences for the HVC equation ($M = 32.40$, $SD = 12.10$) than the LVC equation ($M = 26.80$, $SD = 9.62$). However, when viewing the same topic, low WMC participants exhibited longer eye fixation sequences for the LVC equation ($M = 34.50$, $SD = 7.74$) than the HVC equation ($M = 29.17$, $SD = 6.55$). This indicates that for some types of equations, working memory does play a role in the eye fixation sequence length. The graph of the interaction is given in Figure 36.

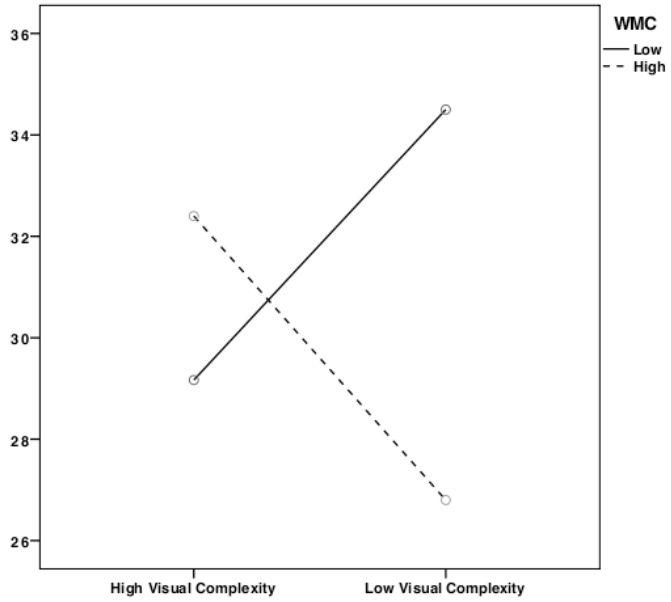


Figure 36. Interaction of WMC and complexity on the eye fixation sequence lengths in Topic 5.

The significant main effect for complexity in topic 2 (Table 45) suggests that for some topics, the overall participants' eye fixation sequences are significantly longer for HVC equations (M = 64.38, SD = 26.83) than for LVC equations (M = 44.31, SD = 16.17).

Results of the ANOVA for the ROIs revealed that there is a significant main effect for complexity only for Topic 2, where HVC equations (M = 66.69, SD = 26.85) had significantly longer eye fixation sequences than LVC equations (M = 46.75, SD = 16.52). For the other 2-molecule equations, there is no main effect for complexity. There are also no significant interactions ($p > 0.05$) between complexity and WMC across all the topics. This suggests that for 2-molecule equations, the scan lengths may be topic dependent. The

test of between-subjects variables showed no significant effect for WMC across all the topics. Results of the ANOVAs for the fixations in ROIs are given in Table 46.

Table 46

Summary of ANOVAs on Eye fixation Sequence Lengths in ROIs of 2-Molecule Equations – Working Memory Capacity

Topic	Effect	*F*	*df*	*p*	Partial Eta Squared
1	Complexity	2.23	1, 12	0.16	0.16
	Complexity*WMC	0.08	1, 12	0.78	0.01
	WMC	1.55	1, 12	0.24	0.11
2	Complexity	12.25*	1, 14	0.00	0.47
	Complexity*WMC	0.16	1, 14	0.695	0.01
	WMC	0.70	1, 14	0.42	0.05
5	Complexity	1.84	1, 14	0.20	0.12
	Complexity*WMC	2.97	1, 14	0.11	0.18
	WMC	0.42	1, 14	0.03	0.03

Note. * significant at $p < 0.05$.

Three-molecule equations. For the 3-molecule equations, there were also unequal ns for the participants when considering AOIs (high WMC, $n = 10$; low WMC, $n = 6$) and ROIs (high WMC, $n = 10$; low WMC, $n = 6$). The 2x2x3 mixed ANOVA, (WMC (high WMC and low WMC) x complexity of equation (HVC and LVC) x equation topic (Topic 3 and Topic 4)) was used to compare the eye fixation sequence lengths. Separate ANOVA were carried out for AOI and ROI fixations. The mean eye fixation sequence length for each equation, broken down by specificity, topic, complexity and working memory capacity is given in Table 47.

Table 47

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and WMC for 3-Molecule Equations

Specificity	Topic	Complexity	High Mean (*SD*)		*n*	Low Mean (*SD*)		*n*
AOI	3	HVC	58.20	(28.95)	10	68.17	(25.04)	6
		LVC	52.90	(29.54)		57.00	(20.64)	
	4	HVC	66.50	(28.12)	10	77.33	(26.58)	6
		LVC	47.20	(23.48)		61.00	(25.61)	
ROI	3	HVC	62.10	(29.23)	10	69.50	(25.02)	6
		LVC	61.40	(33.09)		65.50	(23.42)	
	4	HVC	68.90	(28.20)	10	80.33	(27.57)	6
		LVC	49.80	(24.51)		64.17	(26.13)	

The results from the ANOVA for AOI fixations, given in Table 48, did not indicate a significant effect of WMC on the scan lengths for participants. Although there appears to be a difference in the eye fixation sequence lengths of participants with high WMC versus low WMC, this difference did not reach the level of significance at $p < 0.05$. The interactions of WMC x complexity and WMC x equation were not significant.

Table 48

Summary of ANOVA on Eye fixation Sequence Lengths in AOIs of 3-Molecule Equations – Working Memory Capacity

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	12.59*	1, 16	0.00	0.47
Equation	0.71	1, 16	0.41	0.05
Complexity*Equation	2.07	1, 16	0.17	0.13
Complexity*WMC	0.04	1, 16	0.85	0.00
Equation*WMC	0.32	1, 16	0.58	0.02
Complexity*Equation*WMC	0.44	1, 16	0.52	0.03
WMC	0.66	1, 16	0.43	0.05

Note. * significant at $p < 0.05$.

The main effect for complexity was significant at $p < 0.05$, indicating that HVC equations have significantly longer eye fixation sequences ($M = 67.55$, $SE = 6.81$) than those for LVC equations ($M = 54.53$, $SE = 5.61$).

Next, the eye fixation sequence lengths for the ROI fixations were compared. The results from the ANOVA are given in Table 49.

Table 49

Summary of ANOVA on Eye Fixation Sequence Lengths in ROIs of 3-Molecule Equations – Working Memory Capacity

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	6.07*	1, 14	0.03	0.30
Equation	0.06	1, 14	0.82	0.00
Complexity*Equation	5.00*	1, 14	0.04	0.26
Complexity*WMC	0.00	1, 14	0.98	0.00
Equation*WMC	0.51	1, 14	0.49	0.04
Complexity*Equation*WMC	0.21	1, 14	0.66	0.02
WMC	0.57	1, 14	0.46	0.04

Note. * significant at $p < 0.05$.

Although, from Table 47, it appears that high WMC participants have shorter eye fixation sequence lengths than low WMC participants, this difference does not reach significance at $p < 0.05$. The interactions of WMC*complexity and WMC*Equation were also not significant, indicating that the eye fixation sequence length of participants with high and low WMC were not significantly different.

Of note was the significant interaction between complexity and equation. The graph of the interaction is given in Figure 37.

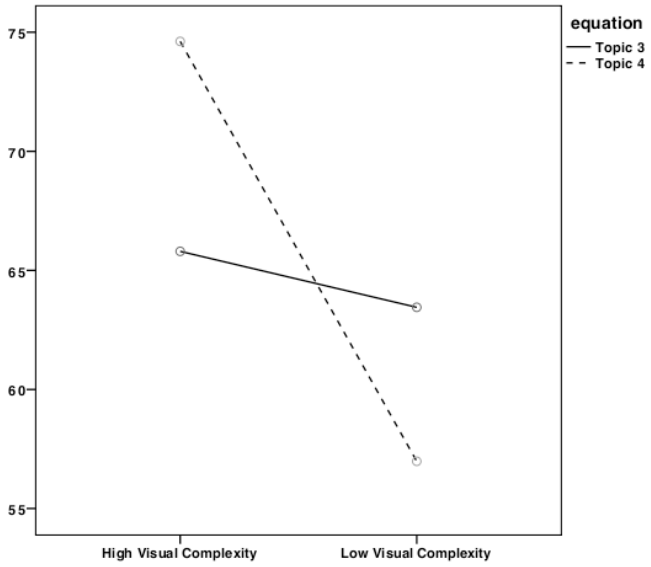


Figure 37. Interaction of complexity and equation on the eye fixation sequence lengths in ROIs across 3-molecule equations.

From the graph, it can be seen that there is no real difference in eye fixation sequence lengths for HVC and LVC equations for Topic 3. However, for Topic 4, the HVC equation has a significantly longer eye fixation sequence length ($M = 74.62$, $SE = 7.22$) than the eye fixation sequence lengths for the LVC equation ($M = 56.98$, $SE = 6.48$). This

indicates that the influence of complexity on eye fixation sequence length may be topic specific.

Expertise. To determine if there were significant differences in eye fixation sequence length between experts and novices, exploratory data analysis was conducted for normality and homogeneity of variance. Two-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test was not significant ($p > 0.05$) for all equations under both stimuli types, indicating a normal distribution of eye fixation sequence lengths for expert and novice participants. Levene's test for equality of variances was not significant ($p > 0.05$) for all but one equation, Topic 2 HVC ($F(1,19) = 5.16$, $p = 0.04$).

Two-molecule equations. For the 2-molecule equations there were unequal ns for the participants when considering AOIs (experts, $n = 7$; novices, $n = 14$) and ROIs (experts, $n = 7$; novices, $n = 14$). A 2x2x3 mixed factor ANOVA (expertise (expert and novice) x complexity of equation (HVC and LVC) x equation topic (Topic 1, Topic 2, and Topic 5)) was used to compare the eye fixation sequence lengths of participants while they read 2-molecule equations. The mean eye fixation sequence length for each equation, broken down by specificity, topic, complexity and working memory capacity is given in Table 50.

Table 50

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and Expertise for 2-Molecule Equations

			Expert		Novice	
Specificity	Topic	Complexity	Mean (*SD*)	*n*	Mean (*SD*)	*n*
AOI	1	HVC	43.71 (15.59)	7	40.07 (19.84)	14
		LVC	32.43 (22.20)		32.93 (17.99)	
	2	HVC	61.00 (10.76)	7	65.57 (38.74)	14
		LVC	44.71 (14.19)		48.00 (27.16)	
	5	HVC	29.43 (13.97)	7	32.14 (14.58)	14
		LVC	28.86 (12.64)		26.64 (10.06)	
ROI	1	HVC	46.86 (15.06)	7	42.07 (21.05)	14
		LVC	35.71 (23.59)		36.71 (19.07)	
	2	HVC	63.57 (10.44)	7	68.29 (39.74)	14
		LVC	46.57 (13.54)		51.21 (27.38)	
	5	HVC	32.43 (15.11)	7	35.50 (16.21)	14
		LVC	28.86 (12.64)		26.64 (10.06)	

The results from the ANOVA for AOI fixations, presented in Table 51, do not indicate a significant effect of expertise on the sequence lengths for participants. Although there appears to be a difference in the eye fixation sequence lengths for experts and novices, this difference did not reach the level of significance at $p < 0.05$. The interactions of expertise*complexity and expertise*equation were not significant.

Table 51

Summary of ANOVA on Eye fixation Sequence Lengths in AOIs of 2-Molecule Equations - Expertise

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	18.81*	1, 19	0.00	0.50
Equation	25.05*	2, 38	0.00	0.57
Complexity*Equation	3.13	2, 38	0.14	0.14
Complexity*Expertise	0.02	1, 19	0.88	0.00
Equation*Expertise	0.29	2, 38	0.75	0.02
Complexity*Equation*Expertise	0.34	2, 38	0.72	0.02
Expertise	0.01	1, 19	0.91	0.00

Note. * significant at $p < 0.05$.

The main effects for complexity and equation are significant at $p < 0.05$. Eye fixation sequences for HVC equations ($M = 45.32$, $SE = 4.55$) are significantly longer than LVC equations ($M = 35.60$, $SE = 3.59$). Regardless of the level of complexity, different topics also have significantly different eye fixation sequence lengths. Pairwise comparisons adjusted using the Bonferroni correction indicated that Topic 2 ($M = 54.82$, $SE = 6.08$) had the longest mean eye fixation sequence, followed by Topic 1 ($M = 37.29$, $SE = 4.55$) and Topic 5 ($M = 45.32$, $SE = 4.55$).

The eye fixation sequence lengths for the ROI fixations were compared also compare using the 2x2x3 ANOVA. Results are given in Table 52.

Table 52

Summary of ANOVA on Eye Fixation Sequence Lengths in ROIs of 2-Molecule Equations - Expertise

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	18.42*	1, 19	0.00	0.49
Equation	27.57*	2, 38	0.00	0.59
Complexity*Equation	2.13	2, 38	0.13	0.10
Complexity*Expertise	0.00	1, 19	0.98	0.00
Equation*Expertise	0.42	2, 38	0.66	0.02
Complexity*Equation*Expertise	0.49	2, 38	0.13	0.03
Expertise	0.02	1, 19	0.90	0.00

Note. * significant at $p < 0.05$.

Again, the results indicate that level of expertise does not influence the eye fixation sequence length of the participants viewing equations of varying complexity. The interactions of expertise x complexity and expertise x equation were not significant.

As in the AOI comparison, we see that the main effects for complexity and equation are significant at this level of specificity. For this dataset, the HVC equations ($M = 48.12$, $SE = 4.81$) have significantly longer eye fixation sequences than the LVC equations ($M = 37.62$, $SE = 3.73$). Regardless of the complexity, there is also a significant difference in the eye fixation sequences among topics. Pairwise comparison with Bonferroni adjustment showed that Topic 2 had the longest eye fixation sequence ($M = 57.41$, $SE = 6.18$), followed by Topic 1 ($M = 40.34$, $SE = 4.30$) and Topic 5 ($M = 30.86$, $SE = 2.77$). This same effect was seen in the AOI comparison.

Three-molecule equations. The sample sizes for the participants were also unequal in the 3-molecule comparisons. For AOIs (experts, $n = 8$; novices, $n = 16$) and ROIs (experts, $n = 8$; novices, $n = 16$) there were more novices than experts. A 2x2x3 mixed factor

ANOVA (expertise (expert and novice) x complexity of equation (HVC and LVC) x equation topic (Topic 1, Topic 2, and Topic 5) was used to compare the eye fixation sequence lengths of participants while they read 3-molecule equations. The mean eye fixation sequence length for each equation, broken down by specificity, topic, complexity and working memory capacity is given in Table 53.

Table 53

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and Expertise for 3-Molecule Equations

			Expert		Novice	
Specificity	Topic	Complexity	Mean (*SD*)	n	Mean (*SD*)	n
AOI	3	HVC	53.75 (16.61)	8	65.56 (32.25)	16
		LVC	46.38 (15.81)		61.5 (31.44)	
	4	HVC	65.75 (22.12)	8	74.87 (33.27)	16
		LVC	51.50 (19.51)		49.00 (27.43)	
ROI	3	HVC	57.75 (17.53)	8	67.06 (32.77)	16
		LVC	63.50 (34.97)		68.56 (33.86)	
	4	HVC	68.25 (23.53)	8	77.63 (33.88)	16
		LVC	53.75 (19.45)		52.19 (28.36)	

The results from the ANOVA for AOI fixations, given in Table 54, do not indicate a significant effect of expertise on the scan lengths for participants for 3-molecule equations. Although there appears to be a difference in the eye fixation sequence lengths for experts and novices, this difference does not reach the level of significance at $p < 0.05$. The interactions of expertise*complexity and expertise*equation are not significant at $p > 0.05$.

Table 54

Summary of ANOVA on Eye Fixation Sequence Lengths in AOIs of 3-Molecule Equations - Expertise

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	18.83*	1, 22	0.00	0.46
Equation	0.92	1, 22	0.35	0.04
Complexity*Equation	6.37*	1, 22	0.02	0.23
Complexity*Expertise	0.49	1, 22	0.49	0.02
Equation*Expertise	1.96	1, 22	0.18	0.08
Complexity*Equation*Expertise	1.73	1, 22	0.07	0.07
Expertise	0.61	1, 22	0.44	0.03

Note. * significant at $p < 0.05$.

As expected from the analysis of WMC for intramolecular ROIs, I saw the same significant interaction of complexity*equation ($p < 0.05$) for this dataset (see Figure 38), indicting the influence of complexity on eye fixation sequence was topic specific. Inspection of the graph indicates the same interaction as with WMC where there is a slight difference in eye fixation sequence lengths between HVC and LVC equations for Topic 3. However, for Topic 4, the HVC equation had a significantly longer eye fixation sequence length ($M = 70.31$, $SE = 6.53$) than the eye fixation sequence lengths for the LVC equation ($M = 50.25$, $SE = 5.45$).

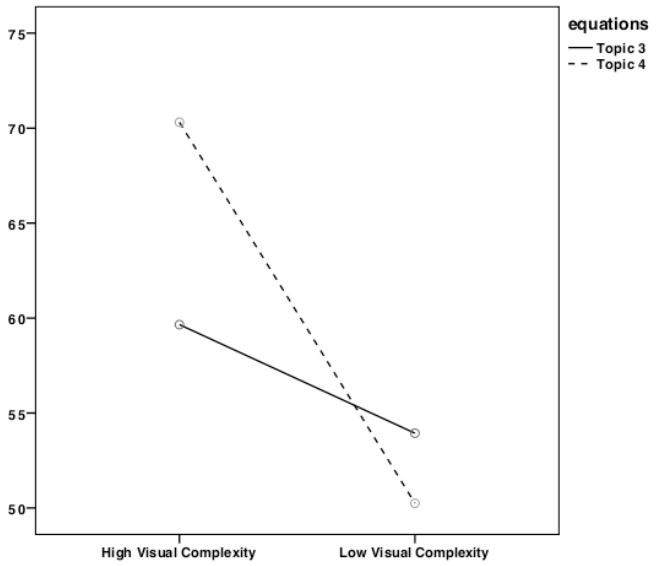


Figure 38. Interaction of complexity and equation on the eye fixation sequence lengths in AOIs across all 3-molecule topics.

The 2x2x3 ANOVA was also used to compare the eye fixation sequence distances of experts and novices viewing 3-molecule equations at the ROI level of specificity. Results are given in Table 55.

Table 55

Summary of ANOVA on Eye Fixation Sequence Lengths in ROIs of 3-Molecule Equations - Expertise

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	4.78*	1, 22	0.04	0.18
Equation	0.07	1, 22	0.79	0.00
Complexity*Equation	12.61*	1, 22	0.00	0.36
Complexity*Expertise	1.03	1, 22	0.32	0.05
Equation*Expertise	0.12	1, 22	0.73	0.01
Complexity*Equation*Expertise	0.25	1, 22	0.62	0.01
Expertise	0.25	1, 22	0.62	0.01

Note. * significant at $p < 0.05$.

There is no significant interaction between expertise*complexity and expertise*equation ($p > 0.05$). This indicates that expertise does not influence the eye fixation sequence length of the participants viewing equations of varying complexity.

Just as in the AOI comparison, there is a significant interaction of complexity*equation (see Figure 39), confirming the indication that the influence of complexity on eye fixation sequence is topic specific. Inspection of the graph (Figure 39) indicates the same interaction as with WMC where there is a slight difference in eye fixation sequence lengths between HVC and LVC equations for Topic 3. The difference for Topic 4 shows that the HVC equation has a significantly longer eye fixation sequence length (M = 72.94, SE = 6.70) than the eye fixation sequence length for the LVC equation (M = 52.97, SE = 5.60).

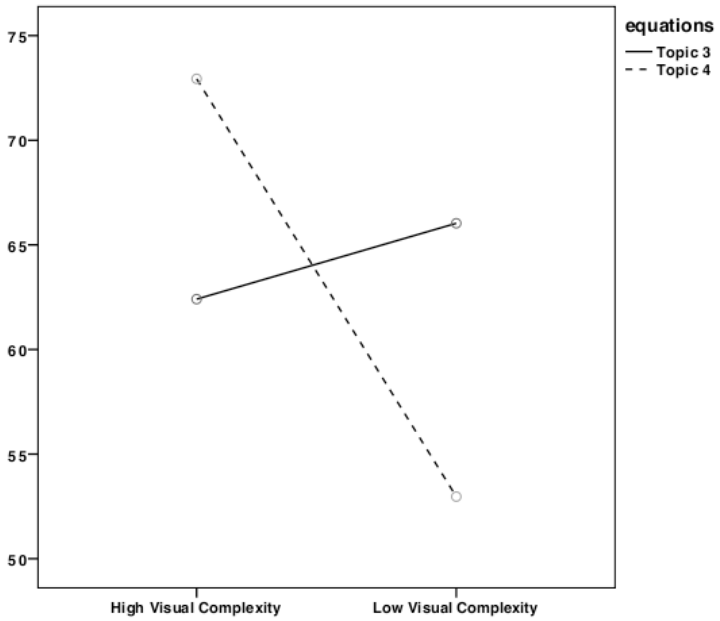


Figure 39. Interaction of complexity and equation on the eye fixation sequence lengths in ROIs across all 3-molecule topics.

Spatial ability. To determine if there are significant differences in eye fixation sequence length between participants of differing spatial ability, exploratory data analysis was conducted for normality and homogeneity of variance. Two-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test was not significant ($p > 0.05$) for all equations, indicating a normal distribution of eye fixation sequence lengths for high SA and low SA participants. Levene's test for equality of variances was not significant ($p > 0.05$) for all equations, except Topic 1 HVC for the AOI analysis ($F(1,13) = 5.93$, $p = 0.03$).

Two-molecule equations. For the 2-molecule equations, there are unequal sample sizes for the participants when considering AOIs (high spatial ability, $n = 9$; low spatial ability, $n = 5$) and ROIs (high spatial ability, $n = 8$; low spatial ability, $n = 5$). Incomplete data sets were seen as responsible for the reduced number of low SA participants. A 2x2x3 mixed factor ANOVA (SA (high SA, low SA) x complexity of equation (HVC and LVC) x equation topic (Topic 1, Topic 2, and Topic 5)) was planned for the analysis of 2-molecule AOIs and ROIs but could not be used. Limitations in the data (small, unbalanced sample size) prevented the computation of Box's test of equality of covariance matrices because there were fewer than 2 nonsingular cell covariance matrices.

A two-way mixed model ANOVA was used to compare the eye fixation sequence lengths of high SA and low SA participants reading each complexity pair of equations. The mean eye fixation sequence lengths for each equation, broken down by specificity, topic, complexity and spatial ability are shown in Table 56.

Table 56

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and Spatial Ability for 2-Molecule Equations

			High		Low	
Specificity	Topic	Complexity	Mean (*SD*)	*n*	Mean (*SD*)	*n*
AOI	1	HVC	29.11 (9.55)	9	51.17 (21.89)	6
		LVC	26.22 (12.70)		36.00 (17.49)	
	2	HVC	49.40 (16.29)	10	67.00 (36.82)	7
		LVC	45.60 (22.75)		56.14 (33.20)	
	5	HVC	25.22 (16.47)	9	35.50 (17.04)	8
		LVC	24.56 (12.10)		34.38 (14.37)	
ROI	1	HVC	35.30 (14.29)	10	53.33 (23.77)	6
		LVC	30.50 (14.88)		46.50 (28.06)	
	2	HVC	52.30 (18.13)	10	70.57 (37.84)	7
		LVC	49.70 (24.59)		59.71 (33.15)	
	5	HVC	27.22 (17.43)	9	40.13 (17.53)	8
		LVC	24.56 (12.10)		34.38 (14.37)	

Results from the ANOVA for AOI fixations are given in Table 57.

Table 57

Summary of ANOVAs on Eye Fixation Sequence Lengths in AOIs of 2-Molecule Equations – Spatial Ability

Topic	Effect	*F*	*df*	*p*	Partial Eta Squared
1	Complexity	1.68	1, 14	0.22	0.11
	Complexity*SA	0.05	1, 14	0.82	0.00
	SA	3.59	1, 14	0.08	0.20
2	Complexity	1.70	1, 15	0.21	0.10
	Complexity*SA	0.64	1, 15	0.44	0.04
	SA	1.22	1, 15	0.29	0.08
5	Complexity	1.15	1, 15	0.30	0.07
	Complexity*SA	0.16	1, 15	0.70	0.01
	SA	3.13	1, 15	0.10	0.17

Note. * significant at $p < 0.05$.

There are no significant interactions between SA and complexity, indicating that the eye fixation sequences of high and low SA participants are not significantly different within a given topic. Complexity of the equations did not influence eye fixation sequence lengths.

These results are confirmed in the analysis of the ROIs. Again, the results indicate that there is no interaction between SA and complexity. Participants' eye fixation sequence lengths are not significantly different for each equation pair. Results of the ANOVAs for the ROI fixations are shown in Table 58.

Table 58

Summary of ANOVAs on Eye Fixation Sequence Lengths in ROIs of 2-Molecule Equations – Spatial Ability

Topic	Effect	*F*	*df*	*p*	Partial Eta Squared
1	Complexity	7.82*	1, 13	0.02	0.38
	Complexity*SA	3.62	1, 13	0.08	0.22
	SA	4.77*	1, 13	0.05	0.27
2	Complexity	2.34	1, 15	0.15	0.14
	Complexity*SA	0.54	1, 15	0.47	0.04
	SA	1.29	1, 15	0.27	0.08
5	Complexity	0.06	1, 14	0.82	0.00
	Complexity*SA	0.00	1, 14	0.95	0.00
	SA	2.57	1, 14	0.13	0.15

Note. * significant at $p < 0.05$.

Of note in these results are the significant, $p < 0.05$, main effects for the within-subject variable complexity and the between-subject variable SA in Topic 1. This indicates that for Topic 1, participants reading HVC equations exhibited a significantly longer eye fixation sequence ($M = 37.93$, $SD = 18.66$) than in LVC equations ($M = 30.13$, $SD = 15.03$).

Regardless of the complexity of the equation being read, the low SA participants exhibited significant longer eye fixation sequence lengths (M = 43.58, SE = 5.64) than the high SA participants (M = 27.67, SD = 4.61).

Three-molecule equations. For the 3-molecule equations, there were equal sample sizes for the participants when considering AOIs (high SA, n = 8; low SA, n = 8) and ROIs (high SA, n = 8; low SA, n = 8). The 2x2x3 mixed ANOVA, (SA (high SA and low SA) x complexity of equation (HVC and LVC) x equation topic (Topic 3 and Topic 4)) was used to compare the eye fixation sequence lengths of participants. Separate ANOVAs were carried out for AOI and ROI fixations. The mean eye fixation sequence length for each equation, broken down by specificity, topic, complexity and spatial ability is given in Table 59.

Table 59

Eye Fixation Sequence Length by Specificity, Equation Topic, Complexity and Spatial Ability for 3-Molecule Equations

			High		Low	
Specificity	Topic	Complexity	Mean (*SD*)	*n*	Mean (*SD*)	*n*
AOI	3	HVC	43.50 (18.42)	8	67.88 (30.84)	8
		LVC	53.75 (30.39)		54.38 (33.80)	
	4	HVC	49.13 (26.48)	8	78.75 (29.82)	8
		LVC	33.63 (18.45)		53.63 (30.10)	
ROI	3	HVC	44.75 (18.96)	8	72.00 (30.67)	8
		LVC	68.63 (45.03)		67.00 (34.89)	
	4	HVC	52.13 (28.63)	8	80.63 (30.29)	8
		LVC	36.37 (19.28)		57.13 (30.91)	

The results from the ANOVA for AOI fixations, given in Table 60, indicate that there is a significant effect of SA on the sequence lengths for participants. The interaction between complexity and SA is significant at $p < 0.05$. The graph of the interaction was examined to inform the analysis (Figure 40). As predicted, the high SA participants exhibit little difference in the eye fixation sequence lengths for HVC equations ($M = 46.31$, $SE = 8.78$) and LVC equations ($M = 43.69$, $SE = 9.28$). However, the low SA participants exhibited significantly longer eye fixation sequence for HVC equations ($M = 73.31$, $SE = 8.78$) than for LVC equations ($M = 54.00$, $SE = 9.28$).

Table 60

Summary of ANOVA on Eye Fixation Sequence Lengths in AOIs of 3-Molecule Equations – Spatial Ability

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	16.87*	1, 14	0.00	0.55
Equation	0.06	1, 14	0.81	0.00
Complexity*Equation	8.16*	1, 14	0.01	0.37
Complexity*SA	9.76*	1, 14	0.01	0.41
Equation*SA	1.94	1, 14	0.19	0.12
Complexity*Equation*SA	1.17	1, 14	0.30	0.08
SA	2.23	1, 14	0.16	0.14

Note. * significant at $p < 0.05$.

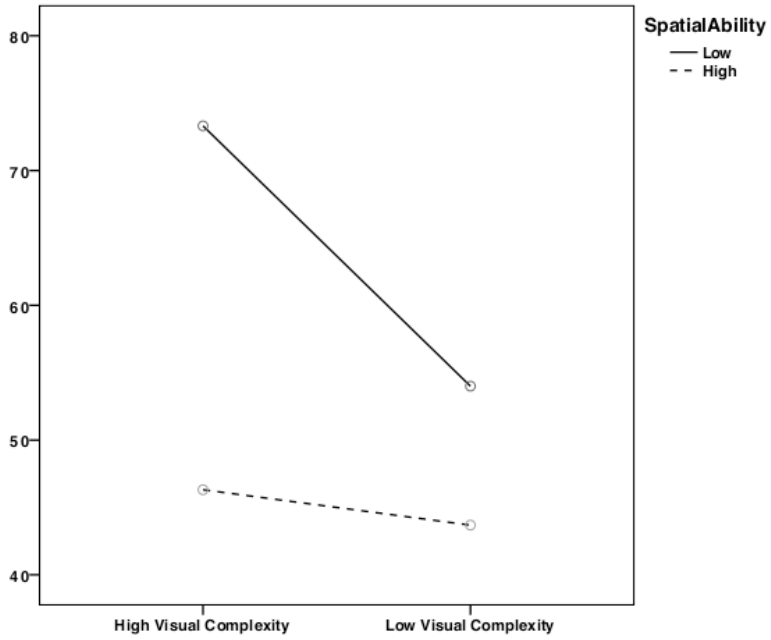


Figure 40. Interaction of complexity and spatial ability on the eye fixation sequence lengths in AOIs across all 3-molecule topics.

A second interaction, complexity*equation, was significant. This result confirms those found in previous analyses indicating that for some equations, complexity influences the eye fixation sequence length of participants. From the graph of the interaction given in Figure 41, there is not much difference in the eye fixation sequence length for HVC and LVC equations for Topic 3. There is a significant difference in the eye fixation sequence length in Topic 4. Participants exhibit significantly longer eye fixation sequence lengths for HVC equations (M = 63.94, SE = 7.05) than for LVC equations (M = 43.63, SE = 6.24).

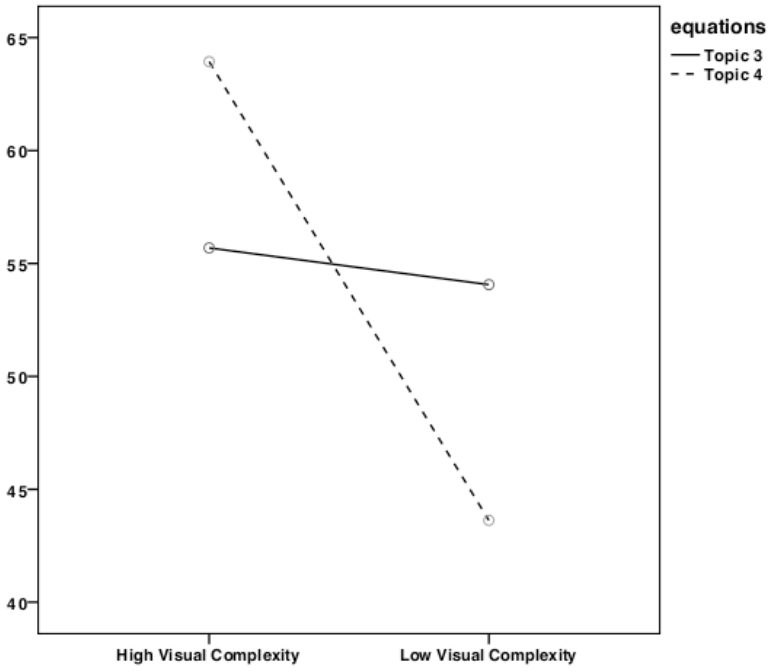


Figure 41. Interaction of complexity and equation on the eye fixation sequence lengths across AOIs

Finally, the eye fixation sequence lengths for the ROI fixations were compared. The results from the ANOVA are given in Table 61.

Table 61

Summary of ANOVA on Eye Fixation Sequence Lengths in ROIs of 3-Molecule Equations – Spatial Ability

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	1.66	1, 14	0.22	0.11
Equation	1.25	1, 14	0.28	0.08
Complexity*Equation	17.31*	1, 14	0.00	0.55
Complexity*SA	5.36*	1, 14	0.04	0.28
Equation*SA	1.02	1, 14	0.33	0.07
Complexity*Equation*SA	2.26	1, 14	0.15	0.14
SA	1.99	1, 14	0.18	0.13

Note. * significant at $p < 0.05$.

These results confirm those found in the previous study of SA for fixations in AOIs. There is a significant interaction between complexity and SA at $p < 0.05$. The graph of the interaction was examined to inform the analysis (Figure 42). As predicted, high SA participants exhibit little difference in eye fixation sequence lengths for HVC equations (M = 48.44, SE = 8.89) and LVC equations (M = 52.50, SE = 10.60). However, low SA participants exhibit longer eye fixation sequences for HVC equations (M = 76.31, SE = 8.89) than for LVC equations (M = 62.06, SE = 10.60).

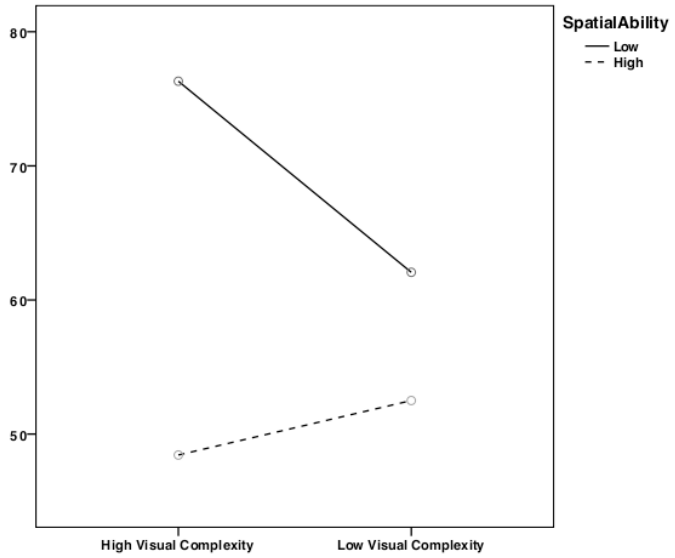


Figure 42. Interaction of complexity and SA on the eye fixation sequence lengths across ROIs

The second interaction, complexity*equation, is also significant. This confirms that, in some equations, complexity influences the eye fixation sequence length of participants. From the graph (Figure 43), we can see that there is not much of a difference in the eye fixation sequence length for HVC and LVC equations for Topic 3. But there is a significant difference in the eye fixation sequence length in topic 4. Participants exhibit a significantly

longer eye fixation sequence length for HVC equations (M = 66.38, SE = 7.37) than for LVC equations (M = 46.75, SE = 6.44).

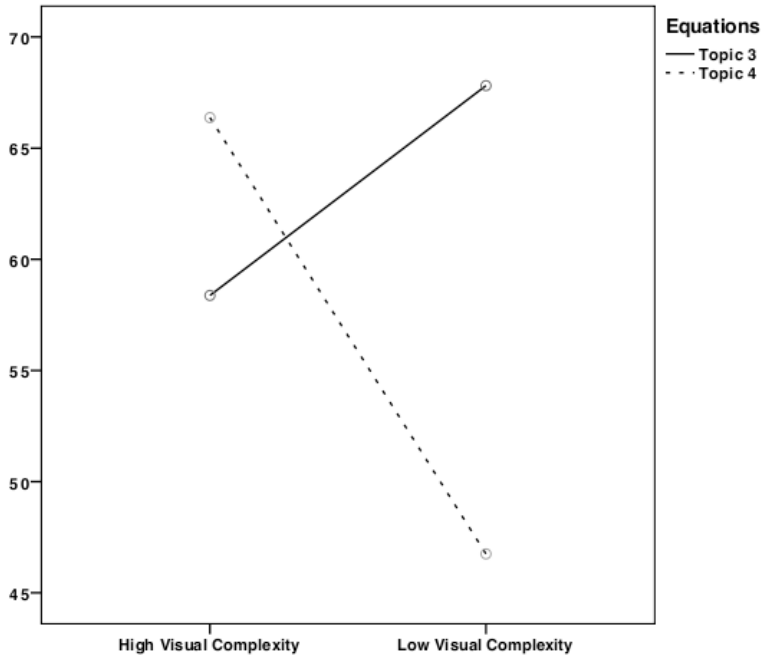


Figure 43. Interaction of complexity and equation on the eye fixation sequence lengths across ROIs.

Summary. Overall, the influence of WMC and SA on the fixation sequences appears to be topic dependent. Three-molecule equations are more susceptible to the influence of these participant characteristics. Participants with high WMC exhibit longer sequences of fixation for HVC equations than LVC equations, while low WMC participants exhibit the opposite effect. Low SA participant have longer fixation sequences than high SA participants when viewing 3-molecule equations. Expertise seemed not to play a significant role in the sequence of eye fixations.

Of note is the observed effect of complexity of the equation on the eye fixation sequences. Equations with HVC have significantly longer fixation sequences than LVC equations.

Eye fixation sequence analysis. Since the viewing of equations was self-paced, the total viewing time for each equation varied, leading to a high degree of variability in eye fixation sequences. To compare participants, the frequency of each fixation pattern was expressed as a percentage of the total fixation patterns observed. Percent fixation was calculated as follows: frequency of a fixation pattern / total frequency for all observed fixation patterns.

Eye fixation sequences in intermolecular AOIs for 2-molecule and 3-molecule equations were investigated separately since the number of AOIs was based on the number of molecules in the equation. Fixation patterns were aggregated across each type of equation. Table 62 provides a summary of the percentage fixation for the three fixation patterns identified in the analysis of AOI fixations. Successive fixation patterns are the most common pattern of fixation in both the 2-molecule and 3-molecule equations. There is a significant increase in the number of regressive and search fixations when the number of molecules in the equation increases from two to three molecules. Paired-samples t-tests indicate that the frequency of regressive fixations is significantly higher in 3-molecule equations than in 2-molecule equations ($t(26) = 4.27$, $p = 0.00$, $d = 0.41$) and the frequency of search fixations is also significantly higher in 3-molecule equations than in 2-molecule equations ($t(26) = 5.58$, $p = 0.00$, $d = 0.54$).

Table 62

Summary of AOI Fixation Patterns by Equation Type

	Percent Fixation Mean (SD)		
	Successive	Regressive	Search
2-Molecule	90.37 (3.55)	4.63 (2.13)	5.00 (2.17)
3-Molecule	85.00 (4.88)	6.48 (2.38)	8.52 (3.41)

Eye fixation sequences for intramolecular ROIs were isolated for each molecule. A total of 24 molecules were investigated. Since only transitions within a given molecule were considered for this portion of the study, data were aggregated across all equations. Table 63 provides a summary of the percentage fixation for the identified patterns of ROI fixations. Successive fixations on informative ROIs were the most common pattern, accounting for 65% of all fixations.

Table 63

Summary of ROI Fixation Patterns by Equation Type

	Percent Fixation Mean (SD)			
	Successive iROI	Successive dROI	Regressive	Search
ROI	65.41 (9.04)	16.43 (6.76)	13.53 (4.17)	4.62 (2.23)

Working memory capacity. To determine if there are significant differences in the usage of successive and regressive fixation patterns based on WMC, exploratory data analysis was conducted to assess the normality of the data. For the AOI analysis, 2-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test

results were significant ($p < 0.05$) only for the 2-molecule equations. Common transformations did not improve normality of the distribution, so a non-parametric Mann-Whitney test was used to compare pattern usage based on participant characteristics for this equation type. A 2x2 split-plot ANOVA was used to analyze the 3-molecule equations and the examination of fixations in ROIs within molecules.

First to be evaluated was the 2-molecule equations. Separate Mann-Whitney tests were conducted to evaluate the hypothesis that low WMC participants have more frequent successive fixations than high WMC participants in ROIs from HVC and LVC equations. The results of the test indicated that, for LVC equations, low WMC participants make a greater number of successive fixations than high WMC participant ($U = 11.00$, $p = 0.04$). Low WMC participants have an average rank of 11.67, while high WMC participants have an average rank of 6.60. There is no significant difference between low WMC and high WMC participants for HVC equations ($U = 16.00$, $p = 0.13$). The hypothesis that low WMC participants have more frequent regressive fixation in LVC and HVC equations was also evaluated using separate Mann-Whitney tests. The results suggest that the frequency of regressive fixations is not significantly different for low WMC and high WMC participants ($U = 16.00$, $p = 0.13$). Unexpectedly, the results indicated that high WMC participants make more regressive fixations than low WMC participants in ROIs in LVC equations ($U = 5.00$, $p = 0.01$). Low WMC participants have an average rank of 4.33, while high WMC participants have an average rank of 11.00.

For 3-molecule equations, separate 2x2 ANOVAs were used to compare the frequency of successive fixations and regressive fixations. The within-subject factor was WMC (high WMC and low WMC) and the between-subject factor was complexity (HVC and LVC). The results, summarized in Table 64, indicate that high WMC participants make the same number of successive and regressive fixations as the low WMC participants when viewing equations, regardless of the complexity.

Table 64

Summary of the ANOVAs on Successive and Regressive Fixations in AOIs of 3-Molecule Equations – Working Memory Capacity

Variable	Source	*F*	*df*	*p*	Partial Eta Squared
Successive Fixation	Complexity	0.12	1,14	0.74	0.01
	Complexity*WMC	0.79	1,14	0.39	0.05
	WMC	2.85	1,14	0.11	0.17
Regressive Fixation	Complexity	0.00	1,14	0.98	0.00
	Complexity*WMC	0.54	1,14	0.48	0.04
	WMC	0.11	1,14	0.74	0.01

Finally the intramolecular successive and regressive fixation patterns of high WMC and low WMC participants were compared to identify differences when participants read HVC and LVC equations. A 2x2x2 mixed factorial ANOVA was used to compare the successive fixation patterns. The between-subject factor was WMC (high WMC and low WMC). The within-subject factors were complexity (HVC and LVC) and content (iROIs and dROIs). A summary of the results is given in Table 65. These results indicate that a participant's WMC does not play a significant role in the frequency of successive fixation patterns.

Table 65

Summary of ANOVA on Successive and Regressive Fixations in ROIs of 3-Molecule Equations – Working Memory Capacity

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	24.16*	1,14	0.00	0.63
Content	184.04*	1,14	0.00	0.93
Complexity*Content	9.49*	1,14	0.01	0.40
Complexity*WMC	0.40	1,14	0.54	0.03
Content*WMC	1.05	1,14	0.32	0.07
Complexity*Content*WMC	0.02	1,14	0.90	0.00
WMC	1.30	1,14	027	0.09

Note. * significant at $p < 0.05$.

There is a significant interaction between complexity and content. The graph for the interaction is given in Figure 44. Successive fixations in informative ROIs are more frequent than successive fixations in distractor ROIs. While there is no significant difference in the frequency of successive fixations in iROIs between HVC equations ($M = 65.21$, $SE = 3.00$) and LVC equations ($M = 69.27$, $SE = 2.10$), participants engaged in more frequent successive fixations on dROIs for HVC equations ($M = 20.45$, $SE = 2.86$) than LVC equations ($M = 9.22$, $SE = 1.41$). This indicates that complexity plays a significant role in how participants view important and unimportant information within a molecule.

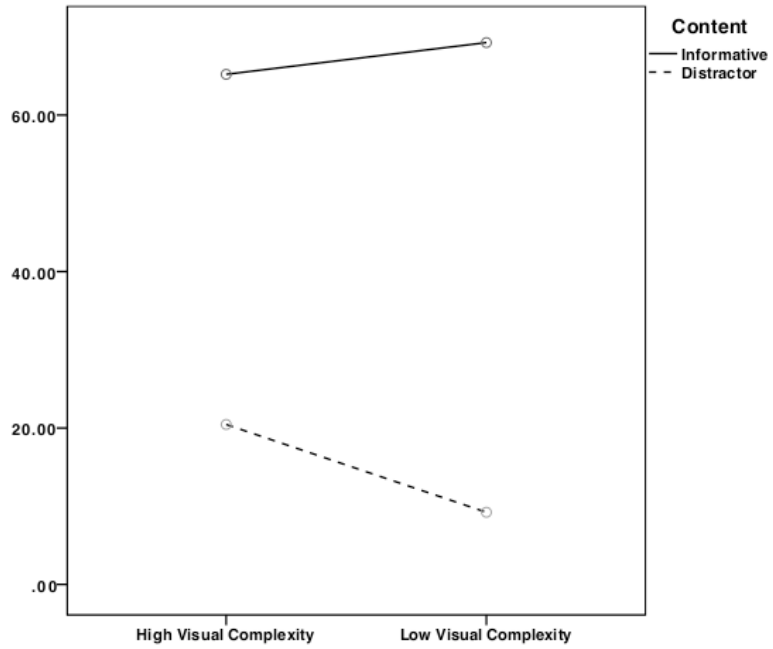


Figure 44. Interaction between complexity and content for successive fixations within molecules.

Lastly, I considered the effect WMC has on the regressive fixations in ROIs from HVC and LVC equations. The frequency of the regressive fixations was entered into the 2x2 mixed ANOVA with WMC (high WMC and low WMC) as the between-subject factor and complexity (HVC and LVC) as the within-subject factor. There is no significant main effect for WMC ($F(1,14) = 0.44$, $p = 0.52$, partial eta squared = 0.03) and the interaction between WMC and complexity is also not significant ($F(1,14) = 0.08$, $p = 0.78$, partial eta squared = 0.01). These results indicate that a participant's WMC does not play a role in the frequency of regressive fixations on molecules for either type of equation. There is a strong significant main effect for complexity ($F(1,14) = 35.27$, $p = 0.00$, partial eta squared = 0.72) suggesting that participants make significantly more regressive fixations on molecules in

LVC equations ($M = 18.14$, $SE = 1.54$) than on those in HVC equations ($M = 9.42$, $SE = 1.03$).

Expertise. To determine if there were significant differences in the usage of successive and regressive fixation patterns based on expertise, exploratory data analysis was conducted to assess the normality of the data. For the AOI analysis, 2-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test results were significant ($p < 0.05$) only for the 2-molecule equations. Common transformations did not improve normality of the distribution, so a non-parametric Mann-Whitney test was used to compare pattern usage based on participant characteristics in this equation type. A split-plot ANOVA was used to analyze the 3-molecule equations and fixations in ROIs for each molecule.

For 2-molecule equations, separate nonparametric Mann-Whitney tests was used to compare the effect of expertise on the successive and regressive fixation frequencies. Equations with HVC and LVC were investigated separately. The results indicate that there is no significant difference in the frequency of successive fixation patterns for HVC equations ($U = 59.00$, $p = 0.37$, $d = 0.17$) and LVC equations ($U = 73.00$, $p = 0.87$, d = 0.03). There is also no significant difference in the frequency of regressive fixation patterns for HVC equations ($U = 45.00$, $p = 0.10$, $d = 0.31$) and LVC equations ($U = 71.50$, $p = 0.81$, d = 0.05). Expertise of the participant does not affect the frequency of successive or regressive fixation patterns for 2-molecule HVC or LVC equations.

Next, the frequency of successive and regressive fixations in AOIs of 3-molecule equations was investigated. Frequency of successive fixations and regressive fixations were entered into two separate 2x2 mixed ANOVAs with expertise as the between-subject factor and complexity of the equation as the within-subject factor. A summary of the results is given in Table 66. There are no significant main effects or interactions for either ANOVA. These results indicate that expertise does not significantly influence the successive or regressive fixation patterns for 3-molecule equations.

Table 66

Summary of ANOVAs on Successive and Regressive Fixations in AOIs of 3-Molecule Equations - Expertise

Variable	Source	*F*	*df*	*p*	Partial Eta Squared
Successive Fixation	Complexity	0.88	1,25	0.36	0.03
	Complexity*Expertise	3.65	1,25	0.07	0.13
	Expertise	0.10	1,25	0.76	0.00
Regressive Fixation	Complexity	0.12	1,25	0.73	0.01
	Complexity*Expertise	4.05	1,25	0.06	0.14
	Expertise	0.07	1,25	0.80	0.00

Next, the frequencies of successive and regressive fixations were investigated for intramolecular ROIs. A 2x2x2 mixed factorial ANOVA was used to compare the frequency of successive fixations of expert and novice participants. The within-subject factor was expertise (expert and novice). The between-subject factors were complexity of the equation (HVC and LVC) and content of the ROIs (iROIs and dROIs). Results are given in Table 67.

Table 67

Summary of ANOVA on Frequency of Successive Fixation Patterns in ROIs of Molecules - Expertise

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	18.62*	1,25	0.00	0.43
Content	443.96*	1,25	0.00	0.95
Complexity*Content	11.01*	1,25	0.00	0.45
Complexity*Expertise	0.07	1,25	0.79	0.00
Content*Expertise	20.45*	1,25	0.00	0.31
Complexity*Content*Expertise	12.42*	1,25	0.00	0.33
Expertise	1.11	1,25	0.30	0.04

Note. * significant at $p < 0.05$.

The 3-way interaction (complexity x content x expertise) is statistically significant. The graph for this interaction is given in Figure 45.

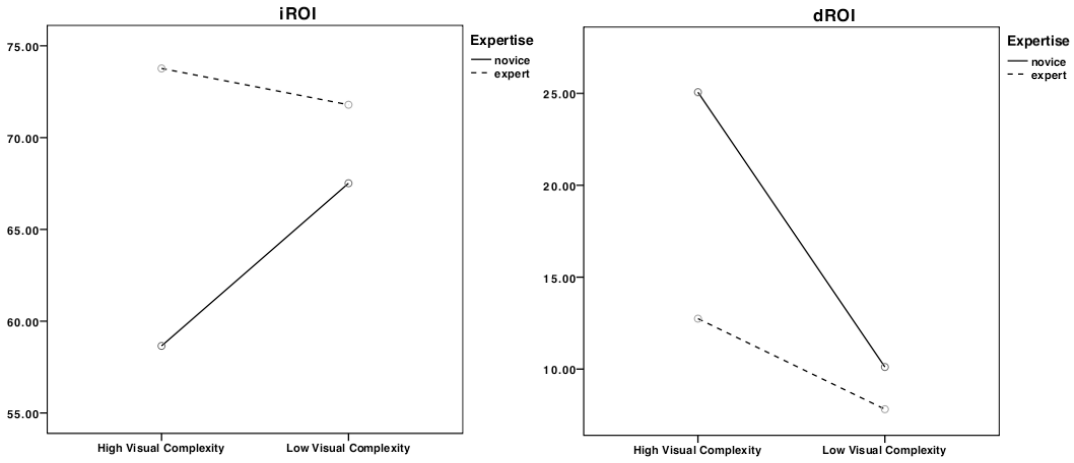


Figure 45. Three-way interaction between complexity and expertise across content.

Simple effect analysis, with Bonferroni adjustment (Gamst, Meyers, & Guarino, 2008), was carried out and the results indicate that experts make significantly more successive fixations on iROIs than novices for molecules in HVC equations. However, the frequency is not significantly different between experts and novices for the molecules in

LVC equations. Novices have a significantly higher frequency of fixation on dROIs than the experts for molecules in HVC equations, but there was no significant difference in fixations for the molecules in LVC equations.

Regressive fixation patterns on iROIs and dROIs for molecules in HVC and LVC equations were also examined. A 2x2 mixed ANOVA with expertise as the between-subjects factor and complexity of the equation as the within-subjects factor was carried out on the frequency of regressive fixations. Results indicate that there is no significant main effect for expertise ($F(1,25) = 1.26$, $p = 0.273$, partial eta squared = 0.05) and no significant interaction between expertise and complexity ($F(1,25) = 0.51$, $p = 0.02$, partial eta squared = 0.05). This indicates that expertise did not significantly affect the frequency of regressive fixations in ROIs of molecules with HVC or LVC. As seen in the previous analysis, there is a significant main effect for complexity ($F(1,25) = 42.24$, $p = 0.00$, partial eta squared = 0.63). Participants have a higher frequency of regressive fixations on molecules from LVC equations ($M = 17.79$, $SE = 1.21$) than on molecules from HVC equations ($M = 9.45$, $SE = 0.99$).

Spatial ability. To determine if there were significant differences in the usage of successive and regressive fixation patterns based on expertise, exploratory data analysis was conducted to assess the normality of the data. For the AOI analysis, 2-molecule and 3-molecule equations were tested separately. The Kolmogorov-Smirnov test results were significant ($p < 0.05$) only for successive fixations in 2-molecule equations. Common transformations did not improve normality of the distribution, so a non-parametric Mann-

Whitney test was used to compare pattern usage based on participant characteristics for this equation type. The planned split-plot ANOVA was used to analyze the 3-molecule equations and ROI fixations within molecules.

For 2-molecule equations, there is no significant difference in the frequency of successive fixations in AOIs in HVC equations ($U = 34.00$, $p = 0.59$) or LVC equations ($U = 40.00$, $p = 1.00$). High SA and low SA participants do not differ significantly in the frequency of successive fixations on intermolecular AOIs.

The results of the 2x2 mixed ANOVA indicate no significant main effect for complexity ($F(1,16) = 0.13$, $p = 0.72$, partial eta squared = 0.01) and no significant interaction between complexity of the equation and the SA of the participant ($F(1,16) = 0.54$, $p = 0.47$, partial eta squared = 0.03). There is no significant main effect for SA of the participant ($F(1,16) = 1.21$, $p = 0.29$, partial eta squared = 0.07). These results indicate that the SA of participants does not significantly influence their use of regression fixation patterns.

For 3-molecule equations, the spatial ability of participants also does not significantly influence their use of successive or regression fixation patterns. Percent frequency of successive fixation patterns was entered into a 2x2 mixed ANOVA with SA as the between-subject factor and the complexity of the equation as the within-subject factor. The results indicate that there is no significant main effect for SA ($F(1,16) = 0.09$, $p = 0.77$, partial eta squared = 0.06) and no main effect for complexity ($F(1,16) = 0.78$, $p = 0.39$, partial eta squared = 0.05). The interaction between SA and complexity is also not

significant ($F(1,16) = 0.03$, $p = 0.87$, partial eta squared = 0.00). Similar results are seen when the percent fixation of regressive fixation patterns was entered into the same ANOVA. There is no significant main effect for SA ($F(1,16) = 0.71$, $p = 0.41$, partial eta squared = 0.04), no main effect for complexity ($F(1,16) = 0.00$, $p = 0.95$, partial eta squared = 0.00), and no significant interaction between SA and complexity ($F(1,16) = 0.32$, $p = 0.58$, partial eta squared = 0.01).

Next, intramolecular transitions were examined. A 2x2x2 mixed factorial ANOVA was used to investigate the frequency of success fixations on iROIs and dROIs in molecules from HVC and LVC equations. Table 68 summarizes the results of the ANOVA. There is a significant main effect for SA, indicating that participants with high spatial ability ($M = 42.01$, $SE = 0.73$) make significantly more successive fixations than participants with low spatial ability ($M = 39.16$, $SE = 0.82$). This effect is evident regardless of the type of regressive fixation (dROIs and iROIs) or the complexity of the equation.

Table 68

Summary of ANOVA on Frequency of Successive Fixation Patterns in ROIs of Molecules – Spatial Ability

Effect	*F*	*df*	*p*	Partial Eta Squared
Complexity	15.51*	1,16	0.00	0.49
Content	395.18*	1,16	0.00	0.98
Complexity*Content	59.30*	1,16	0.00	0.79
Complexity*SA	1.04	1,16	0.32	0.06
Content*SA	3.91	1,16	0.07	0.20
Complexity*Content*SA	4.16	1,16	0.06	0.21
SA	6.74*	1,16	0.02	0.30

Note. * significant at $p < 0.05$.

As expected from the previous analysis, there is a significant interaction between complexity and content. From the graph in Figure 46, participants make significantly fewer fixations in dROIs in the molecules of HVC (M = 23.94, SE = 1.81) and LVC equations (M = 9.27, SE = 1.30) than in iROI for these equations.

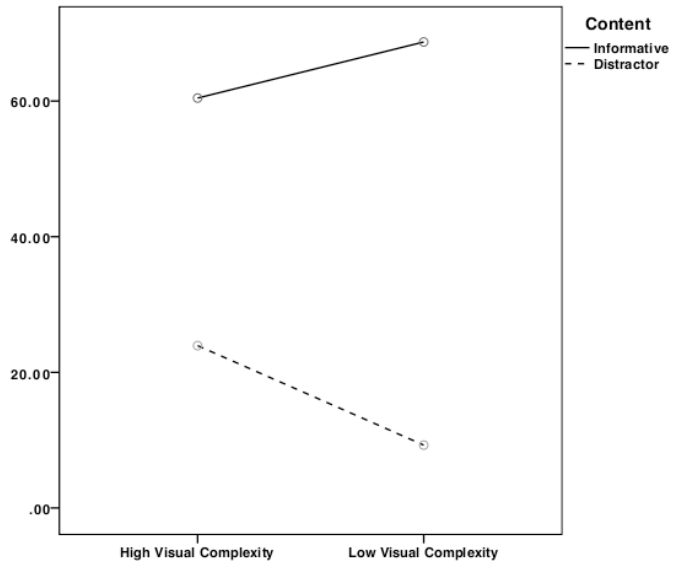


Figure 46. Interaction between complexity of the chemical equation and the content of ROIs (iROI and dROI)

Pairwise comparisons, corrected using the Bonferroni adjustment, indicate that the frequency of successive fixations on the informative regions of the molecules in HVC (M = 60.43, SE = 1.81) equations are significantly more frequent than in molecules from LVC (M = 68.70, SE = 1.40) equations. Successive fixations on distractor information are more frequent in molecules from HVC equations (M = 23.94, SE = 1.72) than in molecules from LVC equations (M = 9.27, SE = 1.30).

Finally, regressive fixations patterns within molecules were examined. Percent frequency of regressive fixation patterns was entered into a 2x2 mixed ANOVA with SA (high SA and low SA) as the between-subject factor and the complexity of the equation (HVC and LVC) as the within-subject factor. There is a significant main effect for SA ($F(1,16) = 5.42$, $p = 0.03$, partial eta squared = 0.25), indicating that low SA participants ($M = 16.28$, $SE = 1.47$) make more frequent regressive fixations in ROIs within molecules than high SA participants ($M = 11.68$, $SE = 1.32$). However, there is no significant interaction between SA and complexity ($F(1,16) = 0.22$, $p = 0.65$, partial eta squared = 0.01) which indicates that the complexity of the equation does not significantly affect the frequency of regressive fixations. There is a strong main effect for complexity, confirming the results from the WMC analysis. Regardless of SA, the frequency of regressive fixations in molecules from LVC equations ($M = 39.16$, $SE = 0.82$) is significantly lower than the frequency of these regressions in HVC equations ($M = 42.01$, $SE = 0.73$).

Summary. This analysis investigated the frequencies of two fixation patterns in AOIs and ROIs. Successive patterns of fixation make up a large share of the 3-fixation patterns in eye fixation sequences. Regressive and search fixation patterns together make up less than 15% of 3-fixation patterns. There is no influence of WMC on the use of either successive or regressive fixation patterns. The expertise of the participant does not seem to affect the frequency of successive and regressive patterns in the 2-molecule equations. In 3-molecule equations, expertise plays a significant role in the frequency of successive fixation patterns. Experts make significantly more successive fixations in iROIs, while novices

make significantly more fixations in dROIs. Spatial ability does not significantly influence the frequency of fixation patterns for 2 or 3-molecule equations. Complexity of the equations is shown to have a significant effect again - this time on the frequency of fixation specific fixation patterns.

Conclusion

The results from Study 2 provide evidence for the process model for the comprehension of organic chemistry notation. Evidence from eye tracking data supports the proposed stages of the model.

The results also suggest that the complexity of equations plays a significant role in the eye movements of participants. The effects of WMC, expertise, and SA are not as consistent, and the data seems to suggest that their effects may be topic specific.

Chapter 5 - Conclusion

In this dissertation, eye movements were used to develop and validate a novel reading comprehension model for organic chemistry equations and to explore other factors, such as the visual complexity of the equation that influence how these equations are read. This research was composed of two studies. The first study validated a rubric to score the visual complexity of organic structural formulas used to write chemical equations. The second study, the validation of a process model for the comprehension of organic chemistry equations, used the rubric to classify equations that participants read during eye tracking. As part of this second study, effects of participant variables and visual complexity of the chemical equation on eye movements were investigated to determine their effects on viewing patterns during reading comprehension.

This chapter will discuss the conclusions based on the results presented in Chapter 4. Limitations of the study, suggestions for future research, and educational implications will also be discussed.

Conclusions

From this research, there are three main conclusions that can be drawn from the data collected. The first conclusion is that it is possible to quantify the visual complexity of molecular formulas based on the number of visual elements in the molecule. This visual complexity of molecular formulas has a significant effect on how people read and understand organic chemistry equations, as illustrated by the viewing patterns of participants during reading comprehension. The second conclusion is that based on eye tracking data, it is

possible to develop and validate a process model for reading and understanding organic chemistry equations. Finally, expertise plays a significant role in how participants read chemical equations. These conclusions are discussed below.

Role of Visual Complexity

The visual complexity of chemical equations plays a vital role in how they are read. The literature suggested that, for diagrams such as molecular structures and chemical equations, as the number of elements in a diagram increases, the ability of a reader to locate and process relevant information decreases (Larkin & Simon, 1987; Koedinger & Anderson, 1990; Halford et al., 1998; Halford, Baker, McCredden, & Bain, 2005). Since chemical equations are written using molecular formulas for the reactants and products, it is important to first develop a systematic way to classify molecules according to the number of visual elements in order to quantify the visual complexity of the equation. In Study 1, a rubric was developed for this purpose. The rubric took into account both the number of elements in the molecule and the interconnectedness or "geography" of these elements in the final molecule. The development of the rubric allowed for the differentiation of high and low visual complexity equations.

This rubric was used in Study 2 to categorize the equations as high or low visual complexity. By studying the average reading times for these equations, it was found that high visual complexity (HVC) equations had significantly longer reading times than low visual complexity (LVC) equations. Since there is more visual information to process in the

HVC equations, it is expected that the reading times would be longer. It was hypothesized that experts would be able to process molecules with high visual complexity faster than novices due to the experts' ability to identify meaningful patterns in the equations (Chi et al., 1982). However, there were no significant statistical interactions between expertise and complexity, meaning that the effect of visual complexity on reading time was the same for experts and novices in this study.

In terms of the number of fixations, participants viewing HVC equations exhibited significantly more fixations and had longer fixation times than with the LVC equations. HVC equations also exhibited longer fixation sequences when the fixation patterns were analyzed. I believe that both the longer fixation times and longer sequences of fixations are due to the more complex relationships that are considered in analyzing larger, more complicated equations containing a variety of visual elements. This belief is supported by the increase in the number of Off Content fixations in HVC equations verses LVC equations. These Off Content fixations provide participants with time to integrate the larger amount of visual information in the HVC equations and to check for inconsistencies in developing internal representations.

Process Model for Reading Organic Chemistry Equations

Using eye-tracking data, a model was developed for the comprehension of organic chemistry equations that accounted for the cognitive processes used during reading

comprehension. The model consisted of six major stages or "processes" that are mediated by working memory and require additional input from long term memory.

In the ***Get Input*** stage of the process model, the eye fixates on a specific element of the equation. Information about that region is located, encoded, and initially processed. To validate this stage of the model, eye tracking data was analyzed for a series of eye fixations on the equation that systematically focused on different features of the equation. It was hypothesized that equations are processed like written English text, from left to right. This means that when a reader reads a chemical equation, he/she reads the reactant(s), then the conditions, and finally the product. To test this hypothesis, Levenshtein distances were used. The Levenshtein distance is the minimum number of deletions, additions, or replacements that must be made to a particular sequence so that it matches another sequence. Thirty-five percent of the participants' scanpaths follow the left to right reading pattern of reactant to condition to product. This means that sixty-five percent of the participants' scanpaths follow a pattern other than the hypothesized left-to-right reading pattern.

Stage two, ***Intramolecular search***, provides for the systematic intramolecular search of a given structure of an organic molecule. To validate the existence of this stage, eye fixation sequences were analyzed to identify sequential, repeating patterns of eye fixations. Ninety-six percent of the participants (n = 26) exhibited a 4-fixaiton repeating pattern in the eye fixation pattern, where the participant fixated on a molecule and then fixated on a

different area within the that molecule. This indicates that most participants perform some sort of intramolecular search process at some point in the reading process.

During the ***Encoding and access lexicon*** stage of the model, an internal representation of the equation is built in the mind of the reader. When the reader encounters repeated instances of the same functional group or rereads a portion of the equation, subsequent fixations were found to be significantly shorter. Eye fixations are directly linked to the processing of visual information, i.e., when the eye is fixated on an object, information is being processed. Once the eye moves, processing ceases until the next fixation (Just & Carpenter, 1980). During this stage, the reader created an internal representation of the equation, activating chunks of information in LTM. When the reader re-encounters the same feature, the chunk activation for that feature is higher due to recency effects. This, in turn, increases the speed and accuracy of processing for that feature during subsequent fixations.

In the ***Intramolecular relationships*** stage, relationships between features in the molecules in the chemical equation are established. During fixations, the reader processes and assigns relationships to features in the molecule. To confirm this stage of the process model, cluster analysis was used to statistically group fixations into clusters. These clusters were assigned a designation of "informative ROI" if the content played a signification role in the reaction or "distractor ROI" if the content played no role in the reaction. It was found that there was a significant difference in the fixations for the informative and distractor ROIs within the same molecule. This means that viewers process these regions differently.

Informative ROIs had fixations that were almost twice as long as the ROIs that contained distractor information. Participants spent more time processing information that was key to understanding the role of particular regions of a molecule in the chemical reaction than they spent processing information considered unimportant to understanding the chemical reaction.

Like intramolecular relationships, participants must assign relationships to molecules within the reaction equation. This is done in the ***Intermolecular relationships*** stage of the process model. An analysis of the fixation patterns confirmed that participants view ROIs (both informative ROIs and distractor ROIs) across all molecules in the equations. When reading times were considered for fixations on the intermolecular ROIs, it was found that fixations on informative ROIs were significantly longer than those on distractor ROIs. Participants spent more time viewing the ROIs that contained information key to understanding the relationships of molecules to the overall reaction than those ROIs that that did not provide insight into the complete chemical reaction.

In the final stage of the process model, ***Reaction Wrap-up***, final fixation durations were analyzed to determine if the readers paused at the end of the reading to integrate their internal representations of the equations and check for inconsistencies. The last fixation, before the novices indicated that they understood the reaction, was significantly longer than the average of all other fixations. This indicated that the novices fixated on a region of the screen before indicating that they understood the chemical equations. There was no significant difference for experts in this study. This is not unexpected considering that the

equations selected for the experiment are part of an introductory organic chemistry curriculum. Since these equations are familiar to the experts through of their teaching, they would require less time to check for inconsistencies and do not exhibit an increase in the duration of the final fixation.

When the content of the final fixations was analyzed, no patterns emerged. Unlike sentences, where the last fixation tends to occur on the final punctuation (Just & Carpenter, 1980), it appears that chemical equations have no such standard pause for integration. While the longer fixation duration supports the ***Reaction Wrap-up*** stage of the process model, it appears that there is no region of the chemical equation that is analogous to the final punctuation of an English sentence.

This model provides a basis for understanding the reading process for organic chemistry equations from the time the participants' eyes first fixate on the equation until the participants indicate the chemical reaction is understood. By relying on eye tracking data, I was able to show specific viewing patterns that were characteristic of different cognitive processes that occurred during reading.

Reading Differences Based on Participant Characteristics

As part of the validation of the process model for the comprehension of organic chemistry notation, the effects of three participant variables (working memory capacity, spatial ability, and expertise) on viewing patterns were investigated. No consistent significant effects of spatial ability and working memory capacity on viewing patterns were seen. This may be due to small sample sizes for both variables. However, significant

differences in the viewing patterns were observed when the sample was analyzed based on the expertise of the participants. Overall viewing patterns for experts are significantly different from those of novices. Significantly shorter fixation times are reported for experts than novices for AOIs and ROIs.

Viewing patterns of specific features of the equation (ROIs) were also significantly different for novices and experts. At the start of the study, I hypothesized that experts would have a greater number of fixations and spend significantly more time than novices on informative ROIs while having a lower frequency of fixations and spend less time than novices on distractor ROIs. Evidence from the study indicates that this is true for 3-molecule equations. Novices have a greater number of fixations on the dROIs and spend longer times looking at these ROIs. Since novices lack the declarative knowledge needed to identify meaningful patterns in the chemical equations (Chi et al., 1982), they tend to engage in general search processes (Gick, 1986; Gick & Holyoak, 1980; Larkin et al., 1980). These search processes distribute the fixations across both iROIs and dROIs. This effect was pronounced in the HVC equations.

The three main conclusions of this study extend our understanding of how chemical equations are read and understood. First, the visual complexity of molecular formulas, which can be quantified using the rubric developed in this study, plays a significant role in how people read chemical equations. Second, eye movement data indicates that there exists an organized set of cognitive processes that occur during the reading of organic chemistry equations. Finally, expertise plays a significant role in how people read chemical equations.

These conclusions provide valuable information for the development of interventions to address the needs learners in organic chemistry.

Limitations and Future Study

Further research is needed to address several limitations of this study. In Study 1, the three-part validation of the rubric used to score the visual complexity of the chemical equations, it was found that the rubric worked well for differentiating molecules of low visual complexity (complexity score from 0 – 19) from those with high visual complexities (complexity score from 40 – 59). However, the rubric failed to adequately differentiate molecules with mid-level complexities (complexity score from 20 – 39) from either extreme. The scores on the mid-level stimuli and the written comments of the participants suggested that there was a factor that was not accounted for in the rubric. These mid-level stimuli either contained a single cyclic element or a repeat of the same cyclic element. Upon analysis of the written comments of the participants, a theme emerged in which participants were using geometric and spatial terms to order structures from least complex to most complex. This indicates to me that they use prior knowledge from geometry, a domain outside of chemistry, to chunk structures in working memory. This type of chunking is not accounted for in the rubric.

A small-scale study was carried out to explore the use of "geometric chunking", which I define as the use of geometric terms to group together sets of bonded atoms and thus reduce cognitive load. Ten interviews were held where students were briefly shown a series

of molecules containing substituted ring structures and asked to immediately recall what they had seen. In 80% of the interviews, students used geometric terms to recall the structures, such as "pentagon", "vertex", and "hexagon". Consider the structure of 1-chloro-3-methylcyclopentane (Figure 47).

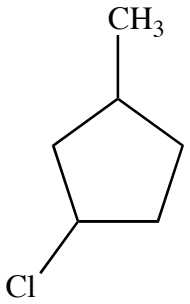


Figure 47. Small-scale study stimulus containing a pentagon

Eight of the ten participants were able to correctly recall the structure of 1-chloro-3-methylcyclopentane, using the word "pentagon" at least once in their description of the molecule viewed. Seven of the ten used "vertex" or "vertices" and three used the word "point" or "corner" to describe the point of attachment for the methyl ($-CH_3$) and the chloride (-Cl) groups. All participants used phrases like "up", "down", "bottom" and "left" to describe the placement of the chloride and methyl groups. According to the rubric, this ring contains 5 single bonds, and 5 implicit atoms (4 secondary carbon atoms and 1 tertiary carbon atom). This five-membered ring would have a *Organic Chemistry Notation Complexity score* of 26. The participants' descriptions suggest that, instead of encoding as a set of discrete elements, they chunked the bonded atoms into a familiar pattern - a pentagon.

This effectively reduced the visual complexity of the molecule for them by relating it to a familiar object.

Participants in this small-scale study were also presented with a molecule containing a less familiar geometric shape - a seven-sided heptagon (Figure 48):

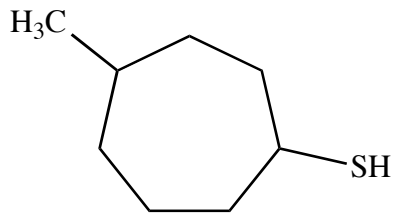


Figure 48. Small-scale study stimulus containing a heptagon

For this stimulus, only three of the participants were able to successfully recall the entire structure viewed. Only one participant used the phrase "heptagon" and "heptagonal" to describe the ring structure. The other participants used more descriptive phrases for the ring, such as "seven-sided shape" and "seven lines in a circle". These descriptions break the ring down into simpler elements (lines or sides) joined together, much in the way that the rubric calculates the visual complexity of the structure. The results from the analysis of this stimulus suggest that there are cases where geometric chunking may not have as big an effect. Additional research is needed to study the extent of "geometric chunking" and refine the rubric scoring to account for this observed phenomenon.

Aware of the limitations caused by "geometric chunking", the rubric was used judiciously to classify the stimuli used in Study 2, the validation of the process model for

the reading comprehension of organic chemistry equations. It is important to note that six of the ten equations used in Study 2 contain one or more familiar geometric shapes, including hexagons and pentagons (see Appendix H). This inclusion of geometric shapes introduced another limitation to the study that will be addressed with further development of the rubric to account for the inclusion of these shapes.

After informally surveying two commercially available textbooks for the 2-semester organic chemistry sequence, it became apparent that the inclusion of the ring structures was unavoidable. The alternative for the high visual complexity (HVC) equations (average complexity score of 50 – 90) would be equations with molecules that include large hydrocarbons (with at least 12 carbons in the chain) and highly branched and/or substituted molecules. These types of molecules 1) would be atypical for a two-semester organic chemistry course sequence, 2) may have notation that would suggest to the novice features that confound results, such as spurious spatial interactions between groups, 3) have a relatively small area that would contain informative content (iROI) compared to the area that would contain distractor content (dROI), and 4) would be extremely large, offering technical challenges for rendering on the eye tracker.

The overall goal of this study was to better understand how people, and in particular undergraduate students, read and understand chemical equations. To this end, I chose to use examples similar to those typically found in a two-semester organic chemistry sequence. Since limitations were already known for how the rubric scored molecules that contained ring

structures, decisions were made to try and mitigate the effects of these limitations in Study 2. Two equations were used for each chemical reaction, one with molecules of LVC (average *Organic Chemistry Notation Complexity score* of 18-25) and one with molecules of HVC (average *Organic Chemistry Notation Complexity score* of 52-89). To further ensure that there was a difference in visual complexity between the structures, I chose reaction pairs that had a difference in average complexity scores of 30 or greater. Informally surveying the sections of the textbooks that covered the chemical reactions of interest, it was noted that the HVC reactions were similar to the most visually complex reactions presented and the LVC reactions were similar to the least visually complex molecules presented in the textbook.

A second limitation to Study 2 is the sample size. Recruitment from the eligible populations occurred over the summer and two consecutive semesters (six separate recruiting sessions, flyers, and signs). A total of 36 people volunteered for the study (novice $n = 25$; expert $n = 11$). One expert participant withdrew from the study, so his/her data was excluded from analysis. The remaining participants ($n = 35$) were eye-tracked and useable reading time data was collected from all 35 participants. Data errors on the hard drive of the eye-tracker propagated into the backups prevented access to other useable eye movement data (fixation duration and scanpath) from both the first expert and the first six novices. Of the remaining 28 participants, only 19 novices and eight experts yielded useable eye tracking data. The remaining expert could not be successfully eye tracked. Although overall reading

time data was collected for this participant, high error rates in the eye movement data (fixation duration and frequency) caused this data to be discarded. The resulting eye movement data that was analyzed was small (novice, $n = 19$; expert, $n = 8$). The small number of participants limited the analysis. Small sample size reduces the power of analyses such as ANOVA, increasing the likelihood of Type II error. Results in this study that were found to not be significant may be significant with a larger population. The sample size limited the type of statistical analyses that could be reliably used. A sample size of 30 or more of each subgroup would be ideal.

A third limitation to this study is the level of expertise of the participants. For this study, expertise in reading and comprehending organic chemistry equations was based on years of experience in organic chemistry. Expert participants were drawn from teaching pools at three separate institutions. Although all the experts had experience teaching organic topics for at least 3 years at the undergraduate level, these experts were not at the same level of education. Six participants had PhDs in chemistry, one had a Masters degree, and two were advanced graduate students in organic chemistry. Their area of specialization in chemistry included organic chemistry ($n = 4$), bioorganic chemistry ($n = 2$), inorganic chemistry ($n = 1$), physical chemistry ($n = 1$), and analytical chemistry ($n = 1$). When first fixation patterns within the AOIs (reactant(s), conditions, and product) were analyzed, differences in the sequence of the fixations were evident. Most of the experts with a strong background in organic and bioorganic chemistry tended to look at the reaction conditions first

followed by the product. The literature suggests that this type of synthetic thinking, focusing on how organic compounds are synthesized and characterized, develops from experience in the research lab (Bhattacharyya, 2006). Through years of laboratory and synthetic work that focuses on organic compounds and how they are made, these experts developed highly organized of systems of prior knowledge that is centered on the conditions under which particular chemical transformations occur. These experts develop strategies for reading chemical equations that focus on conditions as a means for classifying a chemical reaction that they are processing and aids in the retrieval of prior knowledge from their highly organized long-term memory. Therefore, it makes sense that their first fixation is on the conditions. This behavior was not as evident for experts from outside the organic and bioorganic specializations. While these experts have read a lot of organic chemistry and are instructors in the domain, their knowledge lacks a highly structured organization focused on reaction conditions and the synthesis of organic products that years of research in organic chemistry creates. These experts do not develop similar specialized reading strategies as their colleagues in organic and bioorganic develop. Therefore, differences in the reading patterns are evident. These experts tend to follow a pattern of first fixations that is similar to reading English text, from left to right (reactant(s) to condition to product).

These differences are also seen in the educational level of the experts. Experts with higher levels of education tend to have more opportunities to work in synthetic and research laboratories during their educational career. These experiences also help to build the highly

structured organization of declarative knowledge. Again, we see a trend in the focus on reaction conditions as a first fixation for chemists with more education experience than their less educated colleagues. Unfortunately this study, with such a small sample size (n = 9), can do little more than look for trends in the data and make observations about this particular population. The findings of this study need to be explored in a larger study focusing on viewing patterns by level of education or area of expertise to more fully investigate the differences observed in this study.

The fourth limitation of this study relates to the spatial arrangement of molecules in two of the chemical equations used as stimuli in the eye tracking. An inadvertent mismatch of orientations was made in the equation pairs for the Grignard equations (see Figure 49 and Figure 50)

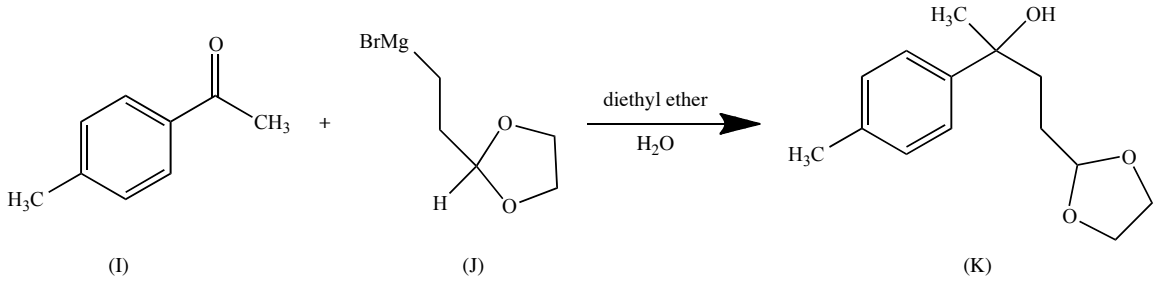
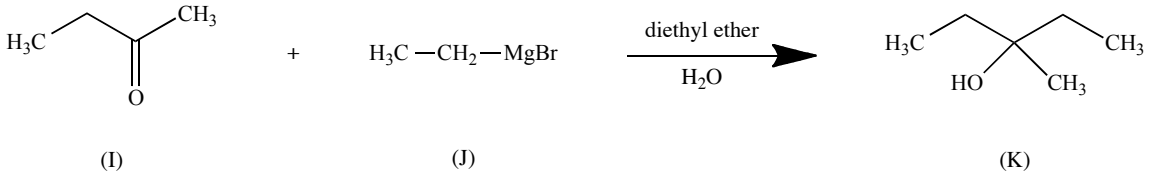


Figure 49. Low visual complexity Grignard equation



(I) (J) (K)

Figure 50 High visual complexity Grignard equation

In the low visual complexity equation (Figure 49), the magnesium-bromide (MgBr) is located on the right side of the molecule. This location is oriented 180° away from the site of the reaction with the double bonded oxygen. In the high visual complexity equation (Figure 50), the magnesium-bromide is located on the left side of the molecule, close to the site of the chemical reaction. An informal analysis of two current commercially published organic chemistry textbooks, was carried out to determine if these two different molecular orientations were associated with the Grignard reaction as presented in a typical organic chemistry course. In both textbooks, equations containing both specific orientations were found in sections related to the Grignard reaction. It was concluded that participants were likely to have read similar equations, containing both orientations, during their initial training in organic chemistry. The data from these equations were retained for the study but the results are treated with some caution. It is unclear from the data collected what effect, if any, this mismatch in orientation had on the participants' reading times of these chemical reactions. It would be necessary to carry out a systematic study of the orientation of molecules in a bimolecular reaction on eye movements to address this question. Such a follow-up was outside of the scope of this study.

Despite these limitations, this study provides valuable insight into how organic chemistry equations are read for comprehension. It is among the first to use eye-tracking data to describe how individuals read organic chemistry equations, and it proposes a model of cognitive processes that occur during reading of those equations. It is also the first attempt to quantify visual complexity of the structural formulas used in organic chemistry. The additional studies proposed in this section would strengthen this line of research and be a valuable addition to our understanding of teaching and learning in organic chemistry.

Educational Implications

This study has shown that different cognitive processes are used during the reading of organic chemistry equations and that there exists individual differences in processing of organic chemistry equations based on expertise of the reader. This is an important finding for organic chemical educators to keep in mind when designing situations where individuals are given a finite time to read and process organic chemistry equations (i.e. instruction, testing, computer application development, animation/video production). Novices and experts exhibit similar viewing patterns for simple equations containing molecules with few visual elements. Therefore, the amount of time needed to read and understand this type of equation is roughly the same for experts and novices. However, as the visual complexity of the equations increases, the differences in the amount of time these two populations need to read an equation becomes apparent. While both experts and novices can interpret the chemical symbols that are written in the equation, novices require more time than experts to process the additional visual elements and determine the information central to

understanding the chemical equation. In equations with high visual complexity, novices spend more time looking at irrelevant information and less time looking at important regions of the molecules.

In terms of instruction, when more visually complex molecules are presented, the instructor should provide additional time for the students to process the written equation before moving on with instruction. Computer-paced applications and animations, where the learner does not have control over the advancing program need to also take into account time requirements for student to read and process the visual information before advancing. In the development of assessments, adequate time should be allocated for students just to read, process, and comprehend all chemical equations on the assessment. Reading is a prerequisite for problem solving, and, without consideration of the cognitive demands of reading the equations presented, inadequate time for testing can confound achievement results. Students may simply not have enough time to read all the equations on the assessment, locate the necessary information, apply their problem solving strategies, and answer the questions. It is important to consider the processes that take place during reading, being mindful of the cognitive demands on the learner as he/she reads different types of equations. By providing adequate time for reading and comprehending the organic chemistry equations presented, chemical educators can better develop classroom practices, educational interventions, and assessments to meet the needs of their learners.

Chemical equations are the language of organic chemistry. Chemists use this language in instruction, professional communications, and research. Reading these

equations is a fundamental part of problem solving and instruction in organic chemistry. By understanding the processes involved in reading chemical equations, instructional practices can be developed that better address the cognitive demands placed on novice learners.

Appendix A

Complexity Rubric for Organic Chemistry Notation

Directions:

For each item in the rubric (Table 69), 1 point is given for each instance of that feature. Each item is described in Table 70. If a specific item does not appear in the molecule, a 0 is entered in the table below. Multipliers are applied to each given instance of a feature where indicated.

Table 69

Complexity Rubric for Organic Chemistry Notation

Item	Count	Total
Structure		
Bonds		
Carbon atoms		
Non carbon atoms		
Numeric subscripts		
Numeric superscripts		
Charges		
Radicals		
Lone pairs	X 2	
Assignment		
Primary assignment (x1)	X 1	
Secondary assignment (x2)	X 2	
Tertiary assignment (x3)	X 3	
Quaternary assignment (x4)	X 4	
Geometry		
Chiral centers (specified geometry)		
Rings		
Bridges		
Fused rings (number of shared sides)		
	Chemical Notation Complexity Score	

Table 70

Description of Rubric Items

Rubric Item	Definition
Bonds	Total number of bonds. This a count of the number of bars used in the representation of the molecule. Single bond = 1; Double bond = 2; Triple bond = 3
Carbon atoms	Count of all carbon atom contained in molecule. This includes both explicit (symbolic notation – "C") and implied by the line drawing (vertices and intersections of lines).
Non-carbon atoms	Count of all non-carbon atoms explicitly noted in the structure. For elements with single character symbols (C, N, I, etc), each non-carbon atoms is +1. For those elements which contain symbols with two characters (Si, Cl, Br, etc), each non-carbon atom is +2.
Numeric subscripts	Count of all numeric subscripts used to denote more than on atom of the same element. For example: NH_3 or CH_3 would both have a 1 entered into the column.
Numerical superscripts	Count of all numeric subscripts used to denote magnitude of the charge on a molecule. This count does not include the signs associated with the charge.
Charges	Count of all the sign designations (+/-) used in the notation. This count does not include the magnitude of the charge.
Radicals	Count of all the lone electrons (free radicals) designated in the structure.
Lone pairs	Count of all electron pairs (lone pairs) designated in the structure. Multiply by 2.

(continued)

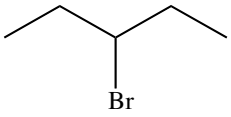
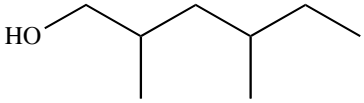
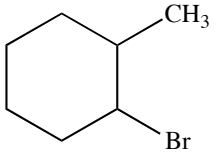
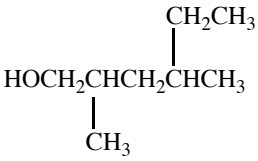
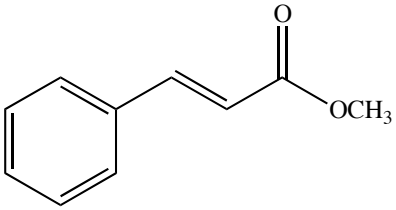
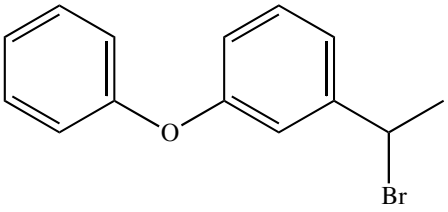
Rubric Item	Definition
Primary assignment	Count of all carbons (explicit and implicit) and nitrogen atoms attached to one other carbon atom. Multiply by 1.
Secondary assignment	Count of all carbons (explicit and implicit) and nitrogen atoms attached to two other carbon atoms. Multiply by 2.
Tertiary assignment	Count of all carbons (explicit and implicit) and nitrogen atoms attached to three other carbon atoms. Multiply by 3.
Quaternary assignment	Count of atoms attached to four other carbon atoms. Multiply by 4.
Chiral centers	Count of atoms that have four different substituents. Visual cuing is used to denote the chirality of the center. Most common are the "wedge" and the "broken wedge" notation.
Rings	Cyclic or heterocyclic structures. Assign a value equal to the total number of atoms in ring structure(s). If there is more than one ring in the structure, this is equal to the sum of all the carbons in each ring.
Bridges	Number of carbons in the least substituted carbon bridge.
Fused rings	Polycyclic compounds contain more than one ring joined together. A value of +1 is assigned for each shared bond in the molecule.

Appendix B

Figures for visual sorting task

Table 71

Molecules for Visual Sorting Task for Part 1: Content Validity

Name	Structural Formula	Chemical Notation Complexity Score
2 bromopentane		19
2,4-dimethyl-1-hexanol		24
1-bromo-2-methylcyclohexane		38
2,4-dimethyl-1-hexanol		40
Methyl 3-phenylpropenoate		55
m-(α-Bromoethyl)diphenyl ether		79

Appendix C

Figures for recall task

Table 72

Molecules for Recall Task for Part 2: Construct Validity

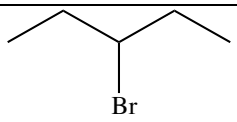
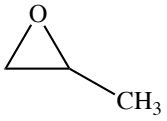
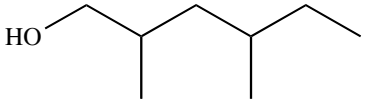
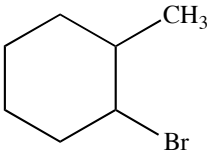
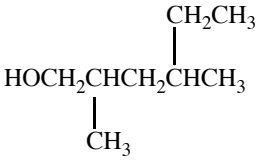
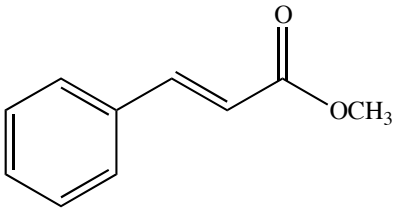
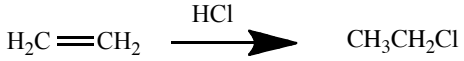
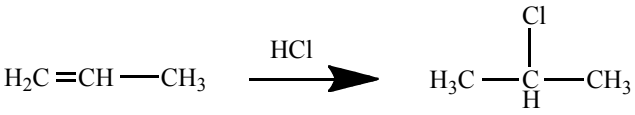
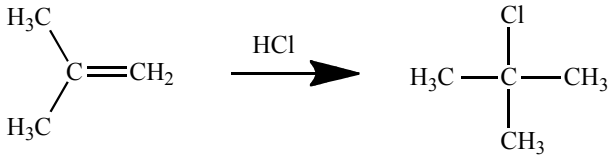
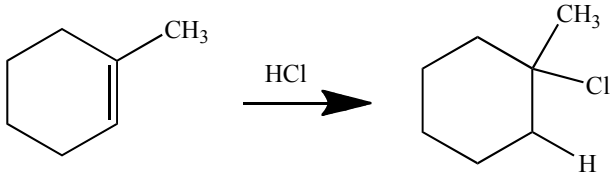
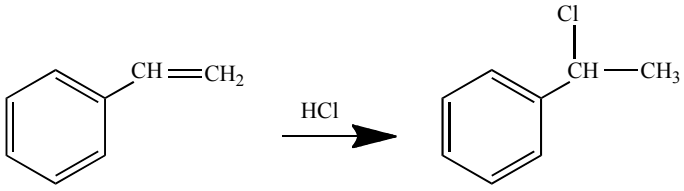
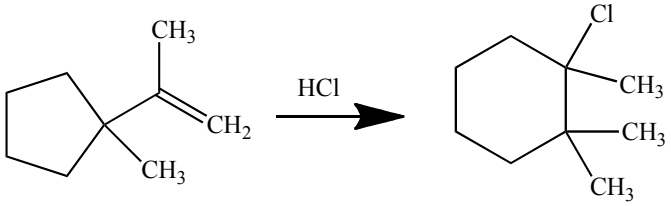
Level of Complexity	Molecule		Chemical Notation Complexity Score
	Letter	Structural Formula	
	A		19
Low (0-19)			
	B		14
	C		24
Medium (20-39)			
	D		38
	E		40
High (40-59)			
	F		55

Table 73

Equations for Recall Task for Part 2: Construct Validity

Level of Complexity	Letter	Structural Equation	Average Notation Complexity Score
	G		9.5
Low (0-19)	H		15.5
	I		20.5
Medium (20-39)	J		38.5
	K		45.5
High (40-59)	L		48.5

Appendix D

Survey for ordering task

The following is a copy of the task used in Part 3: Predictive validity. The task was delivered via paper-and-pencil.

ID Number: _____

1.3 Predictive Validity

1. This semester, have you participated in another study concerning the visual complexity of organic chemistry molecules or equations? (Please circle)

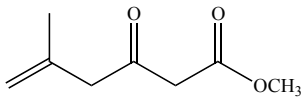
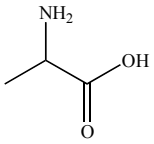
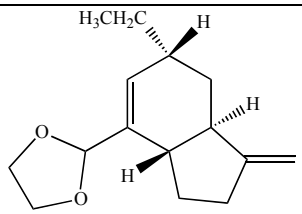
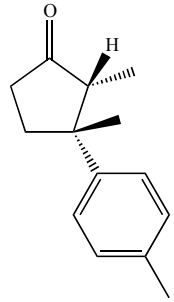
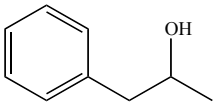
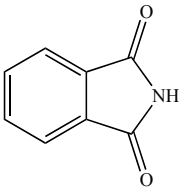
Yes No

2. Select the statement that best describes your highest level of instruction in organic chemistry. (Place an "X" in the box next to your selection)

	a. I have never taken a class covering topics in organic chemistry.
	b. In high school, I took a class that provided a brief introduction to organic chemistry (for example, general chemistry or AP chemistry).
	c. In high school, I took a class that provided significant instruction to organic chemistry (for example, general chemistry or AP chemistry).
	d. In high school, I took one or more classes that were devoted to the study of organic chemistry.
	e. I am currently taking a course at CUA that includes topics related to organic chemistry.
	f. I have taken one or more organic chemistry courses at a community college, college, or university.

Below are six organic chemistry molecules of varying complexity.

1. Arrange the six molecules (A-F) in order from least complex to most complex by writing the letters on the blanks provided.

 **A**	 **B**	 **C**
 **D**	 **E**	 **F**

_____ _____ _____ _____ _____ _____

Least complex Most complex

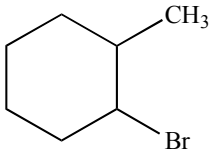
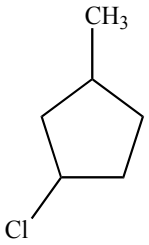
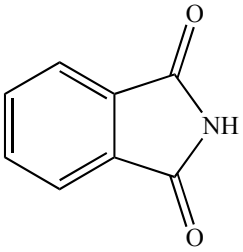
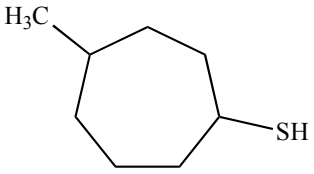
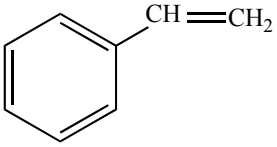
2. Please provide a brief explanation for how you ordered the molecules.

Appendix E

Structural formulas for Investigation of Geometric Chunking

Table 74

Structural Formulas for Interviews

Letter	Structural Formula
A	
B	
C	
D	
E	

Appendix F

Demographic survey for novices

The following survey was delivered to novices via email and returned to the researcher during the eye-tracking session.

ID Number: _____

2.1 Preliminary Survey

Undergraduate/Graduate/Academic Staff

This survey is a part of a study to develop a model of reading comprehension for organic chemical equation. As part of this study, we will be looking at how expertise is related to reading comprehension. Your responses will be kept completely confidential. Information will be reported using an alias and/or a randomly assigned identification number.

Name: _____

Gender: (circle) Male Female

Are you at least 18 years of age? (Circle) YES NO

Are you 24 years of age or older? (Circle) YES NO

Eye tracking can be sensitive to corrective eyewear.

Do you wear contacts? (Circle) YES NO

Do you wear prescription glasses? (Circle) YES NO

Current status (enter number): _____

1. Freshman
2. Sophomore
3. Junior
4. Senior
5. Graduate student
6. Academic staff
7. Other: (please specify) _____

Undergraduate Major: _____

Highest degree earned: (enter number): _____

1. High school
2. Some graduate work
3. Masters: (specify area of specialization) _____
4. PhD: (please specify area of specialization) _____

Chemistry courses completed at CUA (Place an X in the box of all that apply):

	Chem 103/113 General Chemistry I (lecture/lab)
	Chem 104/114 General Chemistry II (lecture/lab)
	Chem 203/213 Organic Chemistry I (lecture/lab)
	Chem 204/214 Organic Chemistry II (lecture/lab)
	Chem 311 Analytical Chemistry
	Chem 351/353 Physical Chemistry I (lecture/lab)
	Chem 352 Physical Chemistry II
	Chem 501 Advanced Inorganic Chemistry
	Chem 508 Instrumental Analysis and Chemical Spectroscopy
	Chem 518 Chemical Instrumentation Lab
	Chem 525 Synthetic Organic Chemistry I
	Chem 526 Synthetic Organic Chemistry II
	Chem 571 Biochemistry I
	Other Chemistry courses: (Please Specify)

Chemistry courses currently enrolled in at CUA (Place an X in the box of all that apply):

	Chem 103/113 General Chemistry I (lecture/lab)
	Chem 104/114 General Chemistry II (lecture/lab)
	Chem 203/213 Organic Chemistry I (lecture/lab)
	Chem 204/214 Organic Chemistry II (lecture/lab)
	Chem 311 Analytical Chemistry
	Chem 351/353 Physical Chemistry I (lecture/lab)
	Chem 352 Physical Chemistry II
	Chem 501 Advanced Inorganic Chemistry
	Chem 508 Instrumental Analysis and Chemical Spectroscopy
	Chem 518 Chemical Instrumentation Lab
	Chem 525 Synthetic Organic Chemistry I
	Chem 526 Synthetic Organic Chemistry II
	Chem 571 Biochemistry I

	Other Chemistry courses: (Please Specify)

Have you taken a chemistry course from an institution other than CUA? (Circle) YES NO

If Yes, please select all courses completed at another institution (Place an X in the box of all that apply):

	General Chemistry I (lecture/lab)
	General Chemistry II (lecture/lab)
	Organic Chemistry I (lecture/lab)
	Organic Chemistry II (lecture/lab)
	Analytical Chemistry
	Physical Chemistry I (lecture/lab)
	Physical Chemistry II
	Advanced Inorganic Chemistry
	Instrumental Analysis and Chemical Spectroscopy
	Chemical Instrumentation Lab
	Synthetic Organic Chemistry I
	Synthetic Organic Chemistry II
	Biochemistry I
	Other Chemistry courses: (Please Specify)

Did you study organic chemistry in High school? (Circle) YES NO

Have you participated in a chemistry research project outside of your coursework? (Circle) YES NO

If Yes, please describe your project.

Have you had an internship or employment working in a chemistry lab? (Circle) YES NO

If Yes, please describe your internship or employment.

Do you read any chemistry journals outside of normal coursework? (Circle) YES NO

If Yes, which statement(s) best describe your chemical journal usage over the last 12 months: (Place an X in the box of all that apply)

	I read only the journals within my chemical specialty.
	I read journal that cover a broad range of chemistry topics (JACS, Science).
	I read journals that specialize in biochemistry.
	I read journals that specialize in organic chemistry.
	I read scholarly chemical magazines (C&E news).
	I read scholarly articles online sources.

On a scale from 1 – 5, where 1 completely disagree and 5 is completely agree, please rate the following statements.

1	Completely disagree
2	Somewhat disagree
3	Neither disagree or agree
4	Somewhat agree
5	Completely agree
0	Not applicable

Rating	Statement
	I am confident in my ability to identify chemical elements based on their symbols.
	I am confident in my ability to read chemical equations used in general chemistry.
	For general chemistry, I am confident in my ability to understand a chemical reaction when it is presented as an equation.
	I am confident in my ability to read chemical equations used in organic chemistry.
	For organic chemistry, I am confident in my ability to understand a chemical reaction when it is presented as an equation.
	If given the name of an organic compound, I can draw its structural formula.
	If given the structural formula of an organic compound, I can write the name of the compound.

Appendix G

Demographic survey for experts

The following survey was delivered to experts via email and returned to the researcher during the eye-tracking session.

ID Number: _____

2.2 Preliminary Survey

Instructor Survey

This survey is a part of a study to develop a model of reading comprehension for organic chemical equation. As part of this study, I will be looking at how expertise is related to reading comprehension. Your responses will be kept completely confidential. Information will be reported using an alias and/or a randomly assigned identification number.

Gender: (circle) Male Female

Highest degree earned: (Circle) PhD Masters Some graduate work

Specialization in Chemistry: _____

Eye tracking can be sensitive to corrective eyewear.

Do you wear contacts? (Circle) YES NO

Do you wear prescription glasses? (Circle) YES NO

Years teaching at the post-secondary level: (including as a TA) _____

Current teaching institution: _____

Years teaching at your current institution: _____

Chemistry courses you have taught in the past 5 years (Place an X in the box of all that apply):

Lecture	Lab	Course
		General Chemistry I
		General Chemistry II
		General, Organic, and Biochemistry for the Health Sciences (GOB)/ Nursing Chemistry
		Chemistry for Non-Science Majors
		Organic Chemistry I
		Organic Chemistry II
		Analytical Chemistry
		Physical Chemistry I
		Physical Chemistry II
		Advanced Inorganic Chemistry
		Instrumental Analysis and Chemical Spectroscopy
		Chemical Instrumentation Lab
		Synthetic/Advanced Organic Chemistry I
		Synthetic/Advanced Organic Chemistry II
		Biochemistry I
		Biochemistry II
		Other Chemistry courses: (Please Specify)

Chemistry courses you are currently teaching (Place an X in the box of all that apply):

Lecture	Lab	Course
		General Chemistry I
		General Chemistry II
		General, Organic, and Biochemistry for the Health Sciences (GOB) / Nursing Chemistry
		Chemistry for Non-Science Majors
		Organic Chemistry I
		Organic Chemistry II
		Analytical Chemistry
		Physical Chemistry I
		Physical Chemistry II
		Advanced Inorganic Chemistry
		Instrumental Analysis and Chemical Spectroscopy
		Chemical Instrumentation Lab
		Synthetic/Advanced Organic Chemistry I
		Synthetic/Advanced Organic Chemistry II
		Biochemistry I
		Biochemistry II
		Other Chemistry courses: (Please Specify)

Have you conducted laboratory research in chemistry or biochemistry? (Circle) YES NO

If YES, number of years working in a research lab. _____

Are you currently engaged in laboratory research? YES NO

If YES, does your research involve the synthesis of organic compounds? YES NO

If YES, does your research involve the use of organic compounds?
(i.e. solvents, analytes, etc) YES NO

If YES, under which general specialization(s) would you classify your research? (Place an X in the box of all that apply):

	Organic Chemistry
	Biochemistry
	Medicinal Chemistry
	Physical Chemistry
	Analytical Chemistry
	Chemical Education
	Computational Chemistry
	Inorganic Chemistry
	Other (please specify):

What are the top three journals you read on a regular basis?

1. _____

2. _____

3. _____

Which statement(s) best describe your journal usage of the last 12 months?
(Place an X in the box of all that apply)

	I read only the journals within my chemical specialty.
	I read journal that cover a broad range of chemistry topics (JACS, Science).
	I read journals that specialize in biochemistry.
	I read journals that specialize in organic chemistry.
	I read scholarly chemical magazines (C&E news).
	I read scholarly articles online sources.

Appendix H

Digit Span Backwards (DSB) test

Procedure

The following is the procedure for the DSB:

1. The participant is given a response sheet.
2. The following instructions are read aloud by the tester:

I am trying to find out more about factors that may influence how you read chemical equations, and this test will give me useful information about your working memory. The computer is going to say some numbers. You must not write as it speaks. When it stops reading the numbers, the computer will say "write". Write down the numbers in the same order as they were read. Please write your responses in the boxes on your sheet as quickly as possible and write from left to right. For example, if the computer read "4 1 9", you write 4 then 1 then 9 in the boxes provided. When the computer says "Next", stop writing. It will then read another set of numbers. Write your responses in the next row of the table provided.

The computer will start by reading three sets of 2 numbers. Then it will read three sets of 3 numbers and so on and so on, ending with three sets of 10 numbers. Try you best to recall the numbers in the order that they were read. When you miss 2 sets of numbers in the same group, this portion of the test will end.

Do you have any questions?

[Pause. Answer questions.]

Let's begin.

3. The tester starts the automated verbal presentation. Numbers are read at the rate of one per second. A male computerized "accessibility voice" available on the Mac OS 10.5.8 reads the following:

    a. "Listen"

    b. "8"

    c. "3"

    d. "Write"

    e. [delay x = 2 s]

    f. "Next"

    The participant is given x seconds write his/her response, where x is the number of stimuli read. In the example above, the participant is given 2 seconds to write down his/her response.

4. Step 3 is repeated for all the number sequences in the table below:

Stimuli set	A	B	C
Set of 2	8 3	5 4	2 7
Set of 3	8 2 9	6 8 7	8 7 1
Set of 4	6 2 4 1	1 3 7 2	5 3 1 6
Set of 5	8 4 1 3 2	8 5 2 9 3	7 9 5 1 4
Set of 6	5 8 7 2 6 1	4 9 2 6 1 7	1 4 8 2 3 9
Set of 7	2 9 4 1 3 7 8	6 2 9 7 8 6 5	1 8 9 7 5 6 2
Set of 8	6 5 1 4 8 2 7 9	2 8 6 5 3 1 9 7	8 5 7 2 9 1 3 6
Set of 9	6 7 9 1 7 4 3 8 2	2 3 9 8 7 4 6 1 5	5 3 9 7 4 8 2 1 6
Set of 10	4 9 8 2 1 7 6 4 5 3	2 8 5 3 9 6 7 6 2 4	2 9 1 4 9 8 4 3 5 7

When a participant cannot accurately recall 2 of the 3 sequences (A, B, and/or C) in any stimuli set, the test proceeds to step 6.

5. One minute break.

6. The following instructions are read aloud by the tester:

Ready to continue?

[Pause for participant response. If participant needs more time, pause.]

Now the computer is going to read another set of numbers. You must not write as it speaks. When it stops reading the numbers, the computer will say "write". This time there is a twist. When the computer finish saying the numbers, I want you to write them down in reverse order. Please write your responses in the boxes on your sheet as quickly as possible and write from left to right. For example, if the computer says "7, 1, 3", you will write down 3 then 1 then 7. Do not write the numbers down backwards on the sheet. Instead, turn the number around in your head and write them down normally.

Any questions?

[Pause. Answer questions.]

Let's begin.

7. The tester starts the automated verbal presentation.
8. The numbers are read at the rate of one per second. A male computerized "accessibility voice" available on the Mac OS 10.5.8 reads the following:
    a. "Listen"
    b. "2"
    c. "8"
    d. "Write"
    e. [delay x = 2 s]
    f. "Next"

    The participant is given x seconds write his/her response, where x is the number of stimuli read. In the example above, the participant is given 2 seconds to write down his/her response.

9. Step 8 is repeated for all the number sequences in the table below:

Stimuli set	A	B	C
Set of 2	2 8	3 7	9 1
Set of 3	1 3 2	3 5 6	2 5 1
Set of 4	2 3 5 9	7 3 9 2	4 8 1 5
Set of 5	6 2 1 4 3	9 1 6 3 5	8 2 6 9 1
Set of 6	2 6 1 3 8 4	2 4 7 6 8 1	4 2 3 8 9 6
Set of 7	1 2 8 5 3 9 4	8 2 4 3 1 6 7	3 1 8 5 6 2 4
Set of 8	1 8 4 7 2 9 1 3	6 5 7 9 2 3 8 1	7 6 5 9 1 2 4 3
Set of 9	7 4 6 2 3 1 9 5 8	8 6 7 9 3 4 6 1 2	5 1 3 9 8 5 2 6 7
Set of 10	5 7 3 1 2 9 8 4 2 6	9 7 8 1 7 3 4 8 2 6	6 9 8 3 2 8 5 1 4 9

When a participant cannot accurately recall 2 of the 3 sequences (A, B, and/or C) in any stimuli set, the test proceeds to step 10.

10. The following instructions were read aloud by the tester:

This is the end of the Digit span test.

Thank you for participating in this part of the study.

The next part of the study will be the eye tracking.

Scoring

The digit span is equal to the length of the last stimuli set that the participant correctly recalled at least 2 of the 3 trials.

ID Number: _____

2.3 DSB

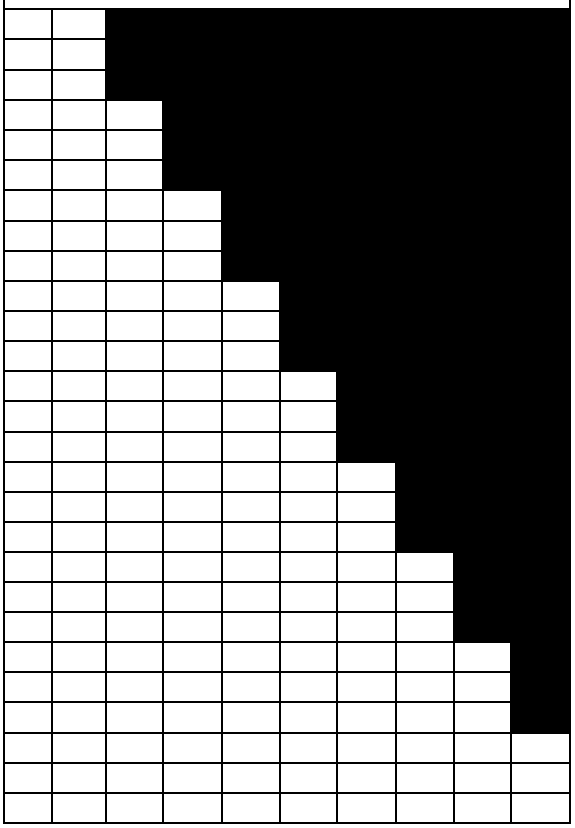
Response Sheet

Digital Span Test

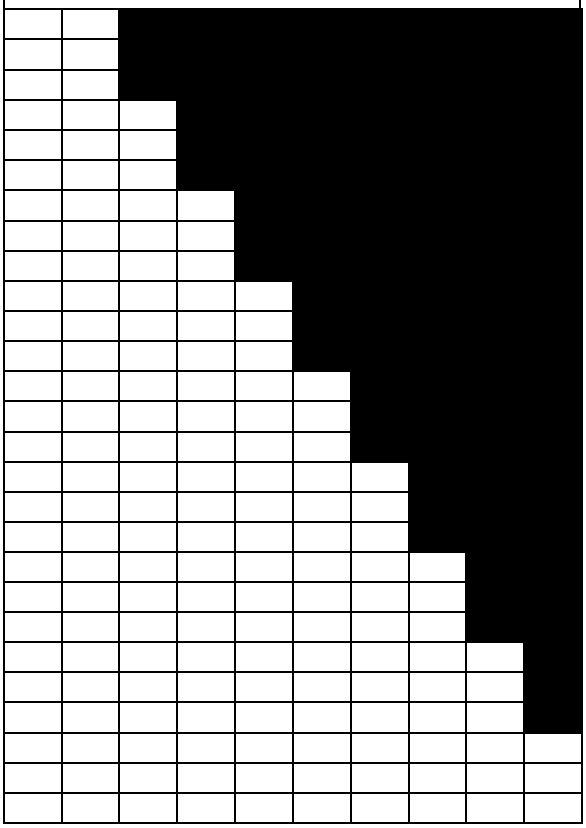
This test is a part of a study to develop a model of reading comprehension for organic chemical equation. As part of this study, we will be looking at how working memory capacity is related to reading comprehension. Your responses will be kept completely confidential. Information will be reported using an alias and/or a randomly assigned identification number. Write numbers in the boxes below.

Do not write anything until you are instructed to do so.

NUMBER TEST FORWARDS



NUMBER TEST BACKWARDS



Appendix I

Purdue Visualization of Rotations test (ROT)

Do NOT make any marks on this exam.
Mark your answers on the separate answer sheet

DIRECTIONS

This test consists of 20 questions designed to see how well you can visualize the rotation of three-dimensional objects. An example of the type of question included in this test is shown below.

IS ROTATED TO

AS

IS ROTATED TO

A B C D E

For each question, you should:

Study how the object in the top line of the question is rotated.

Picture in your mind what the object shown in the middle line of the question looks like when rotated in exactly the same manner.

1. Select from among the five drawings (A, B, C, D, or E) given in the bottom line of the question the one that looks like the object rotated in the correct position

That is the correct answer to the example shown above?

Answers A, B, C, and E are wrong. Only drawing D looks like the object after it has been rotated. Remember that each question has only one correct answer.

Now look at the example shown below and try to select the drawing that looks like the object in the correct position when the given rotation is applied.

IS ROTATED TO

AS

IS ROTATED TO

A B C D E

Note that the rotation in this example is more complex. The correct answer for this example is B.

Do NOT make any marks in this booklet.
Mark your answers on the separate answer sheet.
You will be told when to begin

1
IS ROTATED TO
AS
A
B
C
D
E
2
IS ROTATED TO
AS
A
B
C
D
E
3
IS ROTATED TO
AS
A
B
C
D
E
4
IS ROTATED TO
AS
A
B
C
D
E

5
IS ROTATED TO
AS
A
B
C
D
E
6
IS ROTATED TO
AS
A
B
C
D
E
7
IS ROTATED TO
AS
A
B
C
D
E
8
IS ROTATED TO
AS
A
B
C
D
E

9
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
E
11
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
E
10
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
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12
IS ROTATED TO
AS
IS ROTATED TO
A
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13
IS ROTATED TO
AS
A
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D
E
14
IS ROTATED TO
AS
A
B
C
D
E
15
IS ROTATED TO
AS
A
B
C
D
E
16
IS ROTATED TO
AS
A
B
C
D
E

17
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
E
19
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
E
18
IS ROTATED TO
AS
IS ROTATED TO
A
B
C
D
E
20
IS ROTATED TO
A6
IS ROTATED TO
A
B
C
D
E

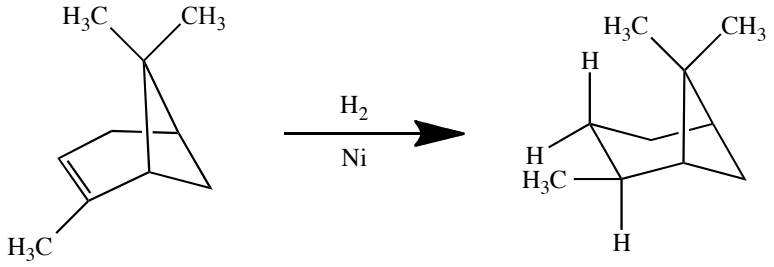
Appendix J

Eye tracking stimuli

The Average Chemical Notation Complexity (ACNC) was calculated for each equation in this study. The equations, ACNC, and the complexity scores for each molecule are presented below.

Topic 1: Hydrogenation of an alkene using a nickel (Ni) catalyst

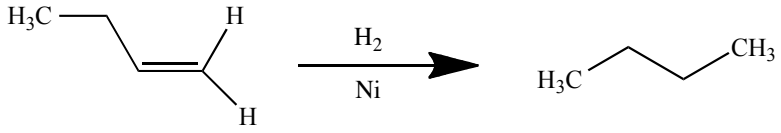
HVC: ACNC = 61



(A) (B)

Molecule	Complexity score
A	59
B	63

LVC: ACNC = 18.5

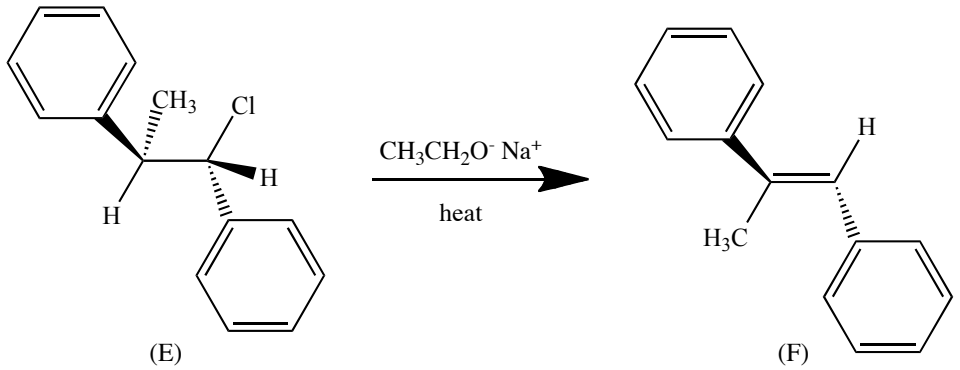


(C) (D)

Molecule	Complexity score
C	20
D	17

Topic 2: Elimination of HX

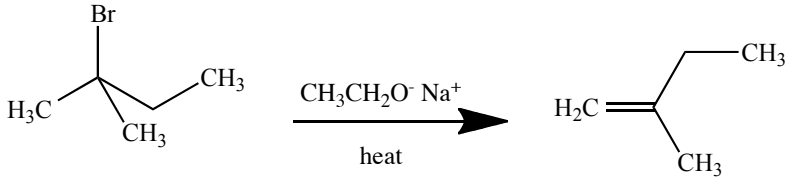
HVC: ACNC = 89



(E) (F)

Molecule	Complexity score
E	92
F	86

LVC: ACNC = 25

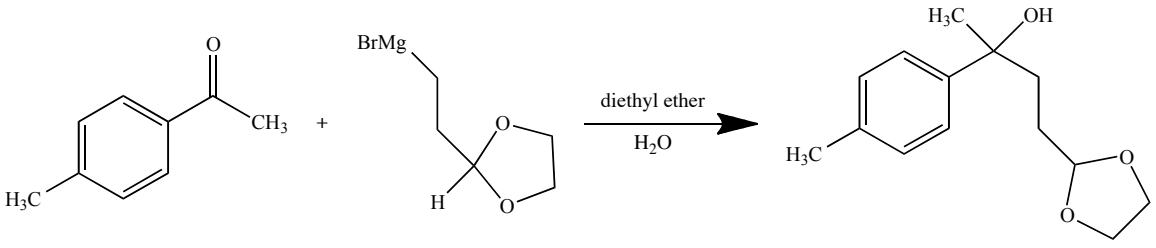


(G) (H)

Molecule	Complexity score
G	26
H	24

Topic 3: Grignard reaction with a ketone

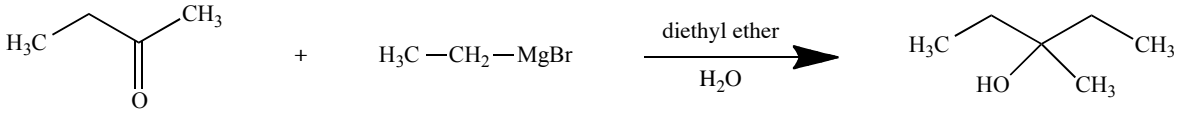
HVC: ACNC = 53



(I) (J) (K)

Molecule	Complexity score
I	52
J	27
K	80

LVC: ACNC = 21.33

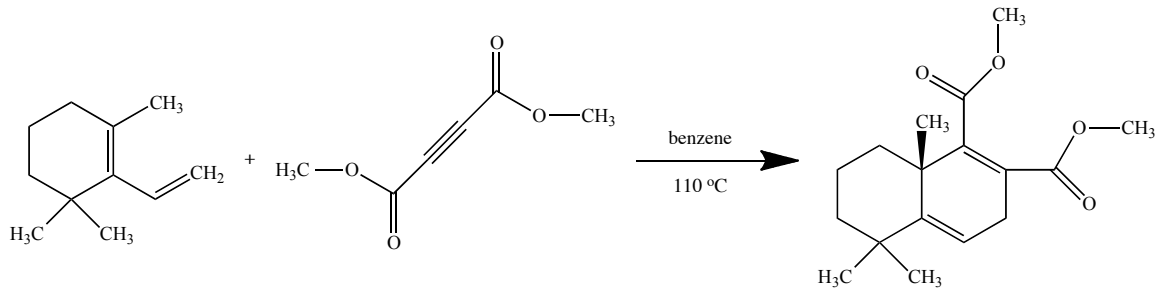


(I) (J) (K)

Molecule	Complexity score
L	20
M	14
N	30

Topic 4: Diels-Alder reaction

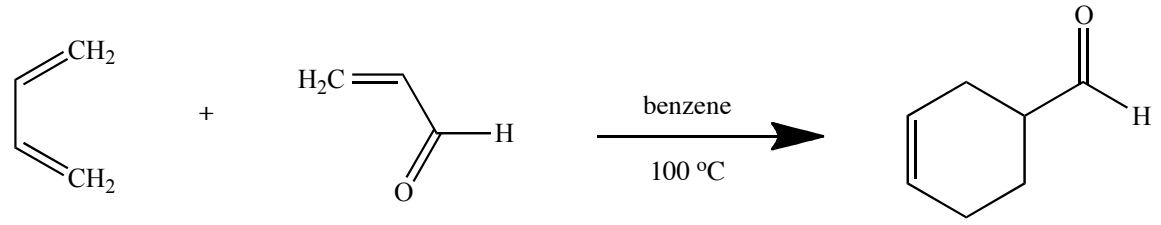
HVC: ACNC = 65.33



(O) (P) (Q)

Molecule	Complexity score
O	60
P	33
Q	103

LVC: ACNC = 24.67

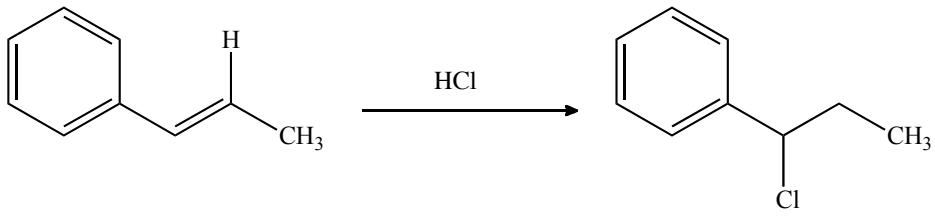


(R) (S) (T)

Molecule	Complexity score
R	17
S	17
T	40

Topic 5: Addition of HCl

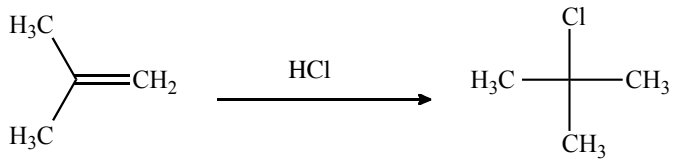
HVC: ACNC = 52



(U) (V)

Molecule	Complexity score
U	54
V	50

LVC: ACNC = 21



(W) (X)

Molecule	Complexity score
W	20
X	22

Appendix K

Eye-tracking procedure

Procedure

The following procedure was used for the eye-tracking session after a participant is seated at the eye tracker and his/her calibration is stored.

1. The following instructions are read aloud by the tester:

We are trying to find out how you read organic chemistry equations. Today, you will be shown a series of chemical equations, one at a time. Please do not memorize the equations. Instead, read them as naturally as possible. Once you have finished reading the equation on the screen and understand the reaction, press the spacebar to continue.

At the end of the session, you will be asked a series of questions about what you have read.

Any questions?

[Pause. Answer any questions.]

Let's begin.

Please focus on the spot on the screen and press the space bar.

2. Once the space bar is struck, data collection commences. A white dot appears on the screen.
    a. The dot corresponds to the center, upper third of the display, located above the chemical equation. The purpose of focusing on a dot on the screen is to start all participants fixated on the same location on the screen.
    b. The dot is displayed for 30 seconds.
3. A static organic chemistry equation is displayed.
    a. The first equation displayed is the low complexity equation for Topic 1.
    b. Subsequence equations are displayed in random order using the randomize feature on the eye-tracker.
4. The participant reads the equation for comprehension at his/her own pace, pressing the space bar to indicate that he/she understands the equation.
    a. After the first equations, the participant is instructed to complete the first two pages of the Post-test (Appendix L).
        i. Upon completion of the Post-test, the participant is reseated at the eye tracker.
        ii. The participant is instructed to press the space bar when they are ready to proceed.
    b. For all other equations, proceed to step 5.
5. A white dot appears on the screen.

a. The participant is instructed to focus on the spot on the screen.

b. The dot is displayed for 15 seconds.

6. Repeat steps 3-5 for the remaining equations.
7. Immediately after viewing the ten chemical equations (five high/low complexity pairs), the participant completes the remainder of the Post-test questions (Appendix L).

    a. No eye tracking data was collected during the Post-test

    b. The post –test was delivered via paper-and-pencil.

8. The following instructions were read aloud by the tester:

    This is the end of the eye tracking.

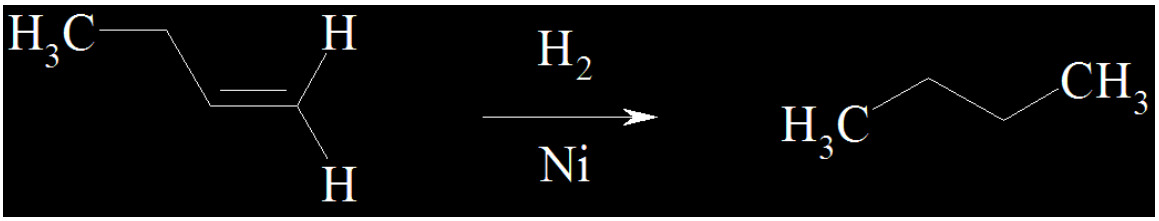
    We're almost done. The part of this study will be the Purdue Visualization of Rotations test.

Appendix L

Post-test for Study 2

The following questions were used to follow-up on the eye-tracking session. This information was *used* to inform the analysis.

Consider the following chemical equation that was displayed during this eye tracking session:



1. Have you ever seen this exact equation before today? Yes No I don't know
2. Have you ever seen an example of this reaction using different molecules?

   Yes No I don't know
3. Are there any functional groups in the reactant that are unfamiliar to you?

   Yes No
4. Are there any functional groups in the product that are unfamiliar to you?

   Yes No

Please do not look back at the previous page to answer the questions below.

Comprehension

1. Could the reaction on the previous page take place as written?

   Yes No I don't know

2. In the equation given on the previous page, an alkene was hydrogenated. Was the addition to the double bond on the same side or on opposite sides of the double bond?

3. Which of the following were the conditions for the reaction:

   a. H_2 / Ni
   b. H_2O / Ni
   c. H_2 / Pt
   d. H_2O / Pt
   e. H_2

4. If you were to propose a mechanism for the reaction on the previous page, how many steps would be in the mechanistic scheme? _____

5. Using the scale below, rate your confidence in the answer for question 4? _____

   0 = No confidence

   1 = Very low confidence

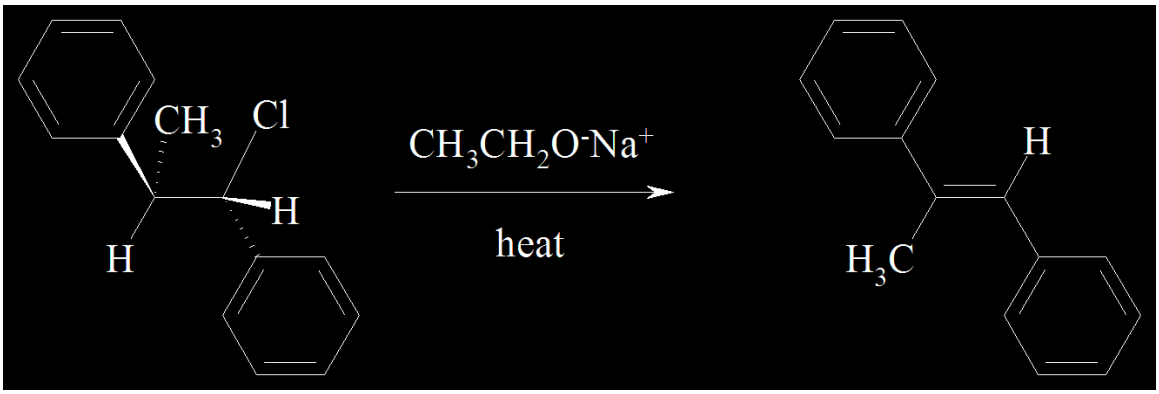
   2 = Some confidence

   3 = Reasonable confidence

   4 = Sufficient confidence

   5 = Very high confidence

Consider the following chemical equation that was displayed during this eye tracking session:



1. Have you ever seen this exact equation before today? Yes No I don't know

2. Have you ever seen an example of this reaction using different molecules?

   Yes No I don't know

3. Are there any functional groups in the reactant that are unfamiliar to you?

   Yes No

4. Are there any functional groups in the product that are unfamiliar to you?

   Yes No

Please do not look back at the previous page to answer the questions below.

Comprehension

6. Could the reaction on the previous page take place as written?

Yes No I don't know

7. The equation given on the previous page is an elimination reaction. Were the groups that were eliminated on the same side of the C-C single bond (as drawn) or on opposite sides of the C-C single bond?

8. Which of the following were the conditions for the reaction:

a. CH_3CH_3 / heat
b. $CH_3CH_2O^-$ / heat
c. $CH_3CH_2O^-Na^+$ / heat
d. $CH_3CH_2O^-Li^+$ / heat
e. $CH_3CH_2O^-Ca^{2+}$ / heat
f. I don't know

9. If you were to propose a mechanism for the reaction on the previous page, how many steps would be in the mechanistic scheme? _____

10. Using the scale below, rate your confidence in the answer for question 9? _____

0 = No confidence

1 = Very low confidence

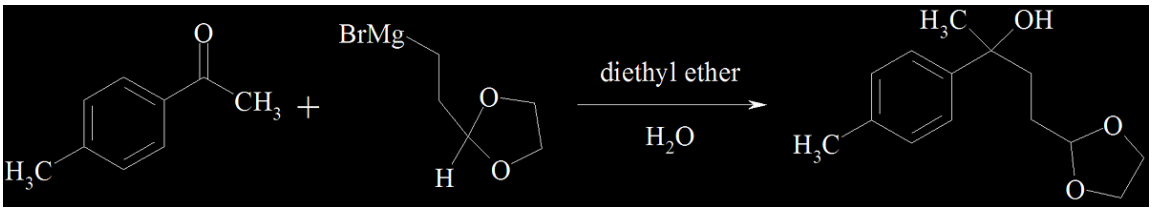
2 = Some confidence

3 = Reasonable confidence

4 = Sufficient confidence

5 = Very high confidence

Consider the following chemical equation that was displayed during this eye tracking session:



5. Have you ever seen this exact equation before today? Yes No I don't know
6. Have you ever seen an example of this reaction using different molecules?

   Yes No I don't know
7. Are there any functional groups in the reactant that are unfamiliar to you?

   Yes No
8. Are there any functional groups in the product that are unfamiliar to you?

   Yes No

Please do not look back at the previous page to answer the questions below.

Comprehension

11. Could the reaction on the previous page take place as written?

    Yes No I don't know

12. The equation given on the previous page is a Grignard reaction. What type of alcohol was formed in this reaction?

    a. primary
    b. secondary
    c. tertiary
    d. I don't know

13. If you were to propose a mechanism for the reaction on the previous page, how many steps would be in the mechanistic scheme? _____

14. Using the scale below, rate your confidence in the answer for question 18? _____

    0 = No confidence

    1 = Very low confidence

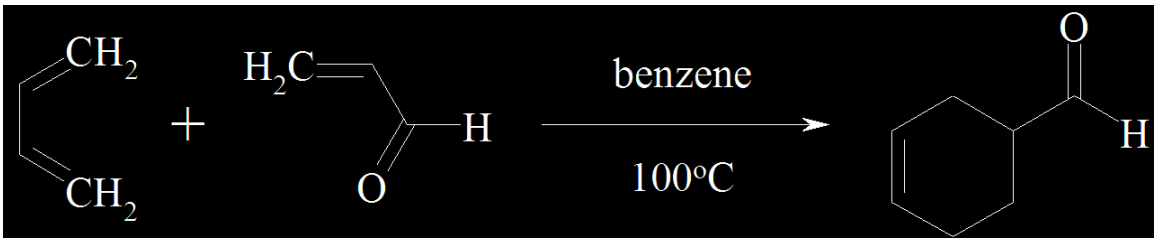
    2 = Some confidence

    3 = Reasonable confidence

    4 = Sufficient confidence

    5 = Very high confidence

Consider the following chemical equation that was displayed during this eye tracking session:



9. Have you ever seen this exact equation before today? Yes No I don't know

10. Have you ever seen an example of this reaction using different molecules?

Yes No I don't know

11. Are there any functional groups in the reactant that are unfamiliar to you?

Yes No

12. Are there any functional groups in the product that are unfamiliar to you?

Yes No

Please do not look back at the previous page to answer the questions below.

Comprehension

15. Could the reaction on the previous page take place as written?

Yes No I don't know

16. In the equation given on the previous page , the product that is formed is a:

a. alkane
b. alkene
c. cycloalkane
d. cycloalkene
e. substituted benzene
f. I don't know

17. If you were to propose a mechanism for the reaction on the previous page, how many steps would be in the mechanistic scheme? _____

18. Using the scale below, rate your confidence in the answer for question 22? ____

0 = No confidence

1 = Very low confidence

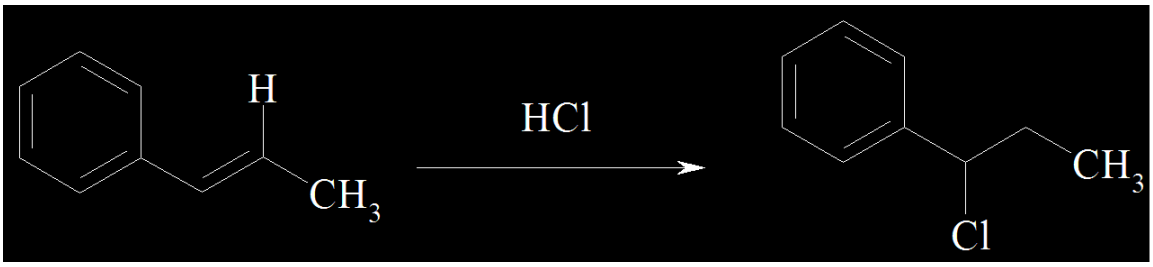
2 = Some confidence

3 = Reasonable confidence

4 = Sufficient confidence

5 = Very high confidence

Consider the following chemical equation that was displayed during this eye tracking session:



13. Have you ever seen this exact equation before today? Yes No I don't know

14. Have you ever seen an example of this reaction using different molecules?

Yes No I don't know

15. Are there any functional groups in the reactant that are unfamiliar to you?

Yes No

16. Are there any functional groups in the product that are unfamiliar to you?

Yes No

Please do not look back at the previous page to answer the questions below.

Comprehension

19. Could the reaction on the previous page take place as written?

Yes No I don't know

20. The equation given on the previous page is what type of reaction?

a. addition
b. elimination
c. substitution
d. rearrangement
e. redox
f. I don't know

21. If you were to propose a mechanism for the reaction on the previous page, how many steps would be in the mechanistic scheme? _____

22. Using the scale below, rate your confidence in the answer for question 22? ____

0 = No confidence

1 = Very low confidence

2 = Some confidence

3 = Reasonable confidence

4 = Sufficient confidence

5 = Very high confidence

Appendix M

Three-fixation patterns for 2-molecule and 3-molecule equations

Occurrence of 3-Fixation Patterns for AOIs in 2-Molecule Equations

Patterns	N	Occurrence (%)
RRR	1591	95%
PPP	831	92%
PPR	462	93%
RPP	435	85%
RRP	433	82%
PRR	424	86%
CCC	380	49%
RRC	301	86%
CRR	232	74%
RCC	218	69%
CPP	205	70%
CCR	151	49%
CCP	136	52%
PPC	136	53%
RCP	91	43%
RCR	77	33%
PCC	74	32%
PRP	70	31%
RPR	66	28%
PCR	60	27%
PRC	46	24%
PCP	44	22%
CRC	43	20%
CRP	43	22%
CPR	38	22%
RPC	35	18%
CPC	23	14%

Occurrence of *3-Fixation Patterns for AOIs in 3-Molecule Equations*

Patterns	N	Occurrence (%)	Patterns	N	Occurrence (%)
SSS	727	90	SCP	49	36
RRR	702	89	PRS	47	34
PPP	701	88	RRC	46	31
RSS	261	90	SPS	41	25
PPS	252	82	RCC	40	26
RRS	245	87	CPC	30	21
SPP	219	75	CSR	28	22
SRR	217	83	PSP	28	17
SSR	215	76	RPR	27	18
SSP	210	73	CCR	25	21
PPR	203	72	PSC	23	17
PSS	193	64	SPR	23	19
RPP	191	70	SRC	23	19
CCC	189	54	PCP	21	16
PRR	177	64	RCP	19	16
RRP	155	64	CPR	16	13
CPP	136	68	RPC	16	14
SSC	130	68	RPS	16	13
CCP	111	64	CPS	14	11
SRS	110	54	SPC	14	11
SCC	106	60	RCS	12	10
CSS	86	49	CSP	10	9
PCC	71	49	SCR	10	7
PPC	70	47	CRS	7	6
PSR	68	47	PRC	7	5
CCS	67	40	CRP	5	5
RSR	60	34	PCR	5	5
SRP	58	36	RCR	5	4
RSP	57	37	CRC	3	3
SCS	55	29			
CSC	36	22			
PRP	33	22			
CRR	32	22			
RSC	32	24			
PCS	31	23			

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