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Patterns in Explanations of Organic Chemistry Reaction Mechanisms: A Text Analysis by Level of Explanation Sophistication

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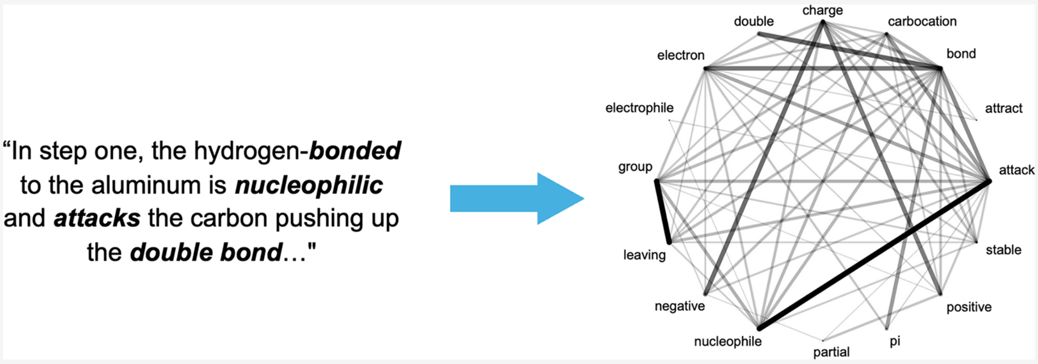

ABSTRACT: Learning the language of organic chemistry, i.e., how to describe reaction mechanisms, is crucial to success in any postsecondary organic chemistry course. However, it is well-known that learners struggle with reasoning about and explaining reaction mechanisms beyond surface-level features. Multiple studies have sought to aid learners in developing these skills. Investigating the connections that learners make regarding reaction mechanisms through their explanations provides insight into how we can better promote the development of learners' reasoning skills. In this study, we evaluate 20,000+ learner explanations of 90 reaction mechanisms. We use network analysis to explore patterns in keywords used by learners and visualize the word connections between them, based on their co-occurrence, within our entire data set, by reaction type, and by levels of explanation sophistication. Our results indicate that learners consistently rely on explicit surface-level features in their explanations with expected contextual variance by reaction type. This trend persists across the levels of sophistication, however, with improvements in the use of vocabulary and coherency as sophistication progresses. We hypothesize that this is evidence of learners actively working toward constructing understanding as they experiment with and refine their vocabulary until they are able to pare down their explanations in a coherent manner. This work offers insights for instructors seeking to promote the development of learners' reasoning skills and for researchers interested in the development of machine-learning models to assist in evaluating learner explanations of reaction mechanisms.

KEYWORDS: *Lower-Division Undergraduate, Organic Chemistry, Reaction Mechanisms, Explanations, Network Analysis, Chemical Education Research*

■ INTRODUCTION

Organic chemistry is ubiquitously touted as a difficult, if not the most difficult, postsecondary chemistry course for learners.[1−8] Learning reaction mechanisms is central to that difficulty; reaction mechanisms are a necessary learning component for success in the course. The scope of learning outcomes related to reaction mechanisms includes drawing reaction mechanisms, interpreting their meaning, and predicting the product of reactions.[9] Multiple studies show that learners struggle with reasoning about reaction mechanisms, particularly constructing explanations that extend beyond noting surface-level features of reaction mechanisms.[4,10−15] A large focus of the research on learning reaction mechanisms has centered on how learners develop an understanding of implicit features.[8,10−12,15−38] Many of these studies address the development of assessments,[8,15,21,23,24,27,29,31,32] rubrics,[10,12,21−23,29,31,32] and other tools or learning aids[24,33−38] to determine the type of reasoning learners are employing as well as how to promote higher levels of reasoning. Despite these efforts to promote learning, most learners still grapple

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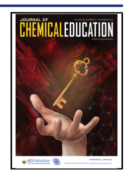

with understanding beyond identifying and describing explicit structural features of reactants, intermediates, and products of a given reaction mechanism. In our study herein, we ask: *what words are learners using in their explanations of reaction mechanisms and how does word use differ by reaction mechanism type?* Furthermore, *what differences in word use, if any, occur in differing levels of sophistication for learner explanations?*

In our study, learners in both semesters of a yearlong organic chemistry course sequence were asked to construct explanations for an array of reaction mechanisms.[10,12,15] Explanations were evaluated using a previously reported level of explanation sophistication rubric.[10,12] Network analysis is used to visualize the co-occurrence of words used in learner explanations, as well as to analyze the importance of keywords in the network graphs. Our results corroborate prior findings that learners mostly use words associated with surface-level, explicit features with observed differences by reaction type (e.g., aromatic versus reduction); our results extend research in this area by identifying that explanations at higher levels of explanation sophistication are associated with a more coherent use of terminology and with terminology associated with implicit-level features.

LEARNER REASONING IN CHEMISTRY

Several reasoning types are employed by learners in written explanations of chemical phenomena; these include, but are not limited to, teleological,[39−42] anthropomorphic,[43−46] and causal mechanistic reasoning.[21−23,47−49] In a review from Dood and Watts,[50] 19 studies were identified that evaluated or characterized levels of learner reasoning of organic chemistry reaction mechanisms. The review identified multiple, overlapping reasoning frameworks including teleological, anthropomorphic, mechanistic, causal, and causal mechanistic reasoning typologies.[4,10,12,16,21,29,34,47,50−52] One reviewed framework was focused on the level of explanation sophistication of learners' responses to prompts in the context of reaction mechanisms; the framework characterizes explanations into four levels from *Absent* to *Complex*.[10,12,34,52] While other frameworks presented in Dood and Watts' review,[21,51,53] including the level of explanation sophistication rubric, are applicable across various reaction mechanism contexts and assessment types (e.g., homework or examinations), the levels of explanation sophistication rubric was specifically developed for researchers and classroom use by instructors and learners.[10,34,52,54] To enhance accessibility, this rubric intentionally minimizes jargon, making it easier to interpret for those less familiar with the mechanistic reasoning terminology.

Previous studies have indicated that learners' abilities to explain reaction mechanisms varies depending on the specific components present, such as nucleophiles and electrophiles.[10,12,15] This suggests the importance of investigating beyond a broad evaluation of learner reasoning, focusing on these different components that comprise a reaction.[12,15] Studies show that learners tend to be cued toward, and more frequently mention, the nucleophile and its role in reaction mechanisms compared to electrophiles and their role.[12,15,55,56] When asking learners to describe what was occurring in various reaction mechanisms, Anzovino and Bretz[55,56] noted that only one of their 11 interviewees made any mention of an electrophile. Work by Frost et al.[12] reported a similar trend with higher levels of explanation sophistication observed for nucleophiles rather than electrophiles; however, in contrast to Anzovino and Bretz, descriptions of electrophiles were present within 80% of the 19,936 learner explanations evaluated and, on occasion, electrophiles were explained at a higher level of sophistication, especially when an explicit cue for the electrophile (e.g., a positive charge) was present.

This tendency of learners to focus on nucleophiles over electrophiles mirrors a broader pattern in which learners can more easily identify, and are more likely to invoke explicit, surface-level features in their explanations of reaction mechanisms.[11,17,57] However, many of the important features of a reaction mechanism are implicit, requiring a learner (and practicing chemist!) to note and integrate those features with explicit features and prior knowledge in constructing a viable explanation; this deeper level of reasoning is often where learners struggle. Reliance on explicit features hinders a learner's ability to propose and explain mechanistic steps, and overall mechanisms, when those steps and mechanisms are unfamiliar (e.g., not explicitly taught in the course);[58,59] from the perspective of a practicing chemist, the ability to propose and explain the unexpected is essential to research.[60,61] Furthermore, learners may be misled by superficial features that are not wholly relevant to the task at hand or may only be able to make connections to certain concepts when prompted via visual features in different contexts, despite the relevancy being the same. For example, given several different heterogeneous bond-forming/breaking reaction mechanisms, learners may be able to identify an electrophile in a reaction mechanism only when a positive charge is explicit, despite the role of the electrophile in all such reactions.[55,56] This stance has been attributed to learners using rote-memorization techniques or applying simple associations rather than determining the relevance and correctness to select concepts in their problem-solving.[11,59,62−64]

THEORETICAL FOUNDATION

We employ constructivism, cognitive linguistics, and methodological interactionism to inform our work herein. The metaphor used by Nobel Laureate, Jean-Marie Lehn, "...atoms are letters, molecules are the words, super molecular entities are the sentences and the chapters and of course—science is the book", emphasizes the foundational role of language and structure in understanding of chemical concepts.[65,66] Piaget's constructivism emphasizes the importance of meaningful connections between concepts in the facilitation and transfer of knowledge and learning.[67] Cognitive linguistics further emphasizes the role of language in shaping thought processes and the understanding of concepts, proposing that learners' word choices can reflect their cognitive structures.[68] Methodological interactionism posits that language is influenced by social interactions;[69] this suggests that organic chemistry learners' language is shaped by their interactions and experiences with others (e.g., instruction, course materials, and peer discussion). The interplay between these frameworks provides a rich understanding of how learners construct knowledge and communicate their understanding regarding the reaction mechanisms.

Constructivism

Piaget's conceptualization of constructivism emphasizes that learned concepts are not isolated; even when memorized, these concepts are connected in ways that are fruitful and unfruitful to further learning and for transferability to new contexts.[67] Knowledge, however, must be connected in meaningful ways, and stored in well-organized structures to be useful in future

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applications.[70−72] As concepts are learned, those concepts must be assimilated into current knowledge structures or be the cause of knowledge reconstruction. Thus, learning can be conceptualized as a process of constructing and reconstructing a network of concepts and ideas.[73] As expertise increases, a learner's knowledge becomes increasingly more connected and more organized, with more points for accessing needed knowledge for a given task.[74,75]

Within the chemistry education research context, concept maps have been used to concretely depict and understand the "network" of conceptual connections for a given learner, for a given topic.[76−79] The benefit of concept maps as formative assessment tools has been repeatedly shown.[55,71,76−82] Multiple studies use "network analysis" techniques to understand collections of learner (and expert)-created concept maps. Such techniques have been used to understand how novices and experts organize organic chemistry reactions differently[75] and how undergraduate students make conceptual connections between organic chemistry reactions.[63] Network analysis techniques have also been used to examine learners' knowledge organization through written explanations. For example, Asmussen et al.[83] examined learner written responses to different chemical concepts applied while solving case comparison tasks on nucleophilic substitution reactions and compared the learner identified concepts with sample responses written by the organic chemistry professors, visualizing responses using network analysis. Derman et al.[76] investigated year eight and year 12 chemistry learners' cognitive structure of acid−base chemistry using a word association test and free writing techniques. Koponen et al.[84] explored preservice physics teacher learners' knowledge of electricity and magnetism via concept networks and written reports. This collection of research suggests that networks and network analysis techniques are viable means for visualizing and evaluating learners' organic chemistry conceptual connections.

Our work is informed by Piaget's constructivism. However, we deviate from a traditional view of concept maps as a tool for learners to explicitly show the connections between concepts. Our work focuses on learners' co-occurrence of words used in explanations of reaction mechanisms as evidence of their learning; this is in alignment with prior work[85,86] that analyzed co-occurrences of features to investigate how learners engage in reasoning and the combination of said features in their explanations.

Cognitive Linguistics

Mapping language onto concepts is key to understanding and acquiring language.[87] Cognitive linguistics offers the possibility to study cognition by examining language, informing the relationship of language to cognition in a systematic approach, and emphasizing how linguistic structures reflect underlying cognitive processes.[68,88] Cognitive linguistics suggests that language is not simply an arbitrary tool for communication but rather that language shapes thought processes and influences understanding of complex concepts. Cognitive linguistics also posits that linguistic structures or categories are not simply tools for communication but are integral components of cognition, affecting how individuals perceive, categorize, and reason about their experiences. This perspective highlights how learners use specific terminology to navigate complex topics and concepts.[89,90]

Within organic chemistry, learners' choice of words in their explanation of reaction mechanisms can reveal underlying cognitive structure and their understanding and highlight the interplay between context and conceptual understanding. Much of the organic chemistry education research literature has shown that learners often gravitate toward explicit, surface-level features in their explanations rather than implicit features, e.g.10, 12, 16, 55, 56, 86, and 91; this may reflect the perceived accessibility or fragmented ideas of certain concepts. As learners begin to engage with more implicit features, their shift in focus may serve as an indicator of their cognitive development; these concepts, once unconnected, are now well-integrated into their cognitive structure. This is not to suggest that learners who only mention surface-level features or "buzz" words demonstrate no evidence of learning. The ability to recognize and use words within the appropriate context reflects that learners are beginning to engage with the language of organic chemistry, even if their explanations remain somewhat superficial, a sentiment shared by Watts et al.[86] Our work employs principles of cognitive linguistics to examine how the language choices of organic chemistry learners reveal their conceptual understanding and reasoning processes regarding reaction mechanisms.

Methodological Interactionism

Scientific practice contributes to the development of language within a discipline through novel theories and research; in turn, language shapes the discipline itself, giving meaning to novel concepts and practices as new individuals enter the field. Methodological interactionism posits that learning practical skills within a domain (e.g., drawing reaction mechanisms) is closely tied to language.[69,92] Methodological interactionism assumes that knowledge is socially constructed, that learning or practicing a skill creates opportunities for discussion with others (e.g., instructors and peers), helping to deepen understanding.[93] On the individual level especially, language plays a crucial role in advancing the engagement in a practice as it is through talking or writing about the skill that learners connect concepts, refine their knowledge, and construct expertise.[69] In other words, to participate in practice, one must be able to communicate within the context of the domain (e.g., talk or write about reaction mechanisms).

For learners in organic chemistry, learning the language to explain reactions is important for learner success in the course.[94,95] This framework suggests that learners' explanations are not constructed in isolation; rather, they are shaped and influenced by their interactions with instructors, course materials, and peers. As they learn, learners adopt and refine language in their explanations, incorporating technical terms and concepts in a way that reflects their personal understanding as well as the collective learning experience. Therefore, as both our work and prior literature suggest,[8,10,12,16,21,26,28,31,57,86,96] organic chemistry instruction and assessment should focus on developing learners' skills to effectively communicate their understanding of reaction mechanisms (e.g., their written explanations), the development of which has the potential to further promote their understanding and comprehension of these concepts. Our work herein reflects the principles of methodological interactionism as we investigate the patterns of how learners use keywords in their explanations across different reaction types; these patterns offer insights not only into individual

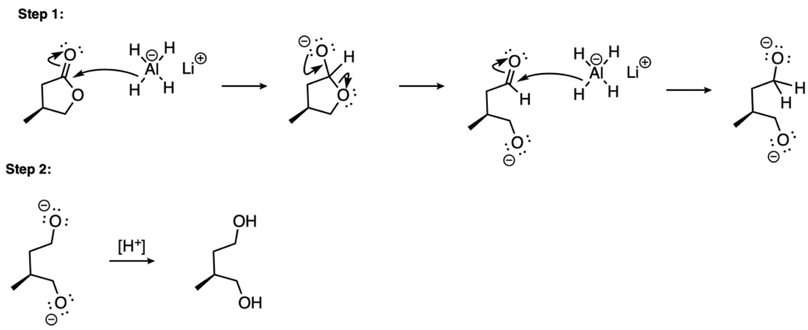

Figure 1. Exemplar original prompt. Further cued variations of this prompt are reported in Crowder et al., 2024.[15]

reasoning but also into the influence of instruction, course materials, and classroom or peer discourse.

RESEARCH QUESTIONS AND GOALS

Research suggests that learners struggle with constructing explanations of organic chemistry reaction mechanisms while also grappling with recognizing the importance of certain underlying concepts and features present in these reaction mechanisms. Prior work in this area has largely focused on understanding the reasoning learners employ as they construct their explanations and attempts to elicit certain types of reasoning;[10,12,15] our work extends prior work in considering the connections learners make with their explanations.

Our study answers two research questions:

1. What words are most prevalent in learners' explanations of organic chemistry reaction mechanisms? How are those words used in connection with each other?
2. What differences in word use or co-occurrence of word pairs in learner explanations are observed between levels of explanation sophistication?

We aim to use network analysis techniques to gain insight into learner explanations of reaction mechanisms through visualizing the co-occurrence of word use; our work points to key means for how instruction can further promote the development of learners' reasoning skills.

METHODS

Our work was carried out under application Pro#00028802, "Comprehensive evaluation of the University of South Florida's undergraduate and graduate chemistry curricula", as reviewed by the University of South Florida's Institutional Review Board (IRB) on December 13, 2016. Data are deidentified and are not linked by the learner per an IRB review.

Data Collection

Data were collected at the University of South Florida, a large, research-intensive, public university in the southeastern United States and an emerging Hispanic-serving institution. Data were collected in the first semester of a year-long postsecondary organic chemistry course over eight semesters (Fall 2017−Spring 2018, Spring 2019−Fall 2020, and Fall 2021−Spring 2022) and in the second semester of the same course sequence over two semesters (Spring 2020 and Fall 2021). Both courses were taught by four instructors over nine total semesters. The course used Solomons et al.'s *Organic Chemistry*, 12th ed.[97] (Fall 2017−Spring 2019), Klein's *Organic Chemistry*, 3rd ed.[98] (Fall 2019−Spring 2021), and Klein's *Organic Chemistry*, 4th ed.[99] (Fall 2021−Spring 2022).

Qualtrics was used to collect learners' explanations of reaction mechanisms. Constructed-response items used in our study varied based on the level of cueing (see Figure 1 for an exemplar prompt) and are reported in prior work.[15] The constructed-response item format we used was initially reported for a single-step proton transfer reaction[21] and asked learners to articulate "*what*" was occurring in a reaction mechanism and "*why*" it was occurring. The separation of the explanation into "*what*" and "*why*" prompts was found to elicit more causal mechanistic reasoning responses from learners.[21] Research suggests that learners only consider certain features in their explanations when explicitly prompted;[19,23] thus, further iterations and modifications to this constructed-response item have been made to provide explicit conceptual support (e.g., scaffolding and cueing) to help learners make further connections.[10,15,23,24] Dood et al.[24] modified the prompt by replacing the explicit Lewis structures with chemical names to assess fluency in converting between chemical names and structures. Crandell et al.[23] studied different prompt wordings to better understand in what ways the organic chemistry learner thought processes may be receptive to certain prompt wordings. The constructed-response item format underwent further modifications for use with acid−base reactions[22,24,33,37] and multistep substitution reactions.[10,12,15,23,34]

A total of 90 reaction mechanisms were used to collect data for our study (reported in Yik et al., 2023;[10] Frost et al., 2023;[12] Crowder et al., 2024[15]). A total of 22,015 responses were collected and evaluated. The 90 reaction mechanisms are categorized into five types: carbocation (n = 8,693 explanations, n = 19 reactions), S_N2 (n = 5,312 explanations, n = 20 reactions), nucleophilic addition (n = 3,264 explanations, n = 23 reactions), reduction (n = 3,165 explanations, n = 16 reactions), and aromatic (n = 1,581 explanations, n = 12 reactions). Learners had the opportunity to complete a maximum of three assessments at three to four points throughout a term for bonus points toward their midterm or final examination scores. All assessments occurred in the three days before a midterm or final examination.

Data Coding and Interrater Reliability

We used a previously published rubric for the evaluation of our explanations; the rubric consists of four levels of sophistication: *Absent*, *Descriptive*, *Foundational*, and *Complex*.[12] Responses designated as *Absent* are composed of statements such as "I don't know how to answer this", irrelevant descriptions of the reaction, or are unable to identify the electrophile and other relevant features. For *Descriptive* level responses, these explanations contain simplistic descriptions of general bond-forming processes, possibly identifying the electrophile with a

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primary focus on surface-level features. *Foundational* level responses include details about the role of electrons in the bond-forming processes with mention of some implicit features (e.g., attractions, lone pairs, pi bonds). Finally, *Complex* level responses include in-depth descriptions of electronic and implicit features (e.g., partial charges, polarity differences, and electron density), as well as how those implicit features are interrelated. Assignment of level of explanation sophistication, including interrater reliability of those assignments, has been previously reported with final agreement ranging from 86.5% to 93.3% (κ = 0.700 to 0.890), indicating strong agreement.[10,12,15]

Analysis

Analyses were conducted with R (version 4.3.3)[100] using RStudio (version 2023.12.1 + 402).[101] Network analysis packages used include ggraph[102] and igraph.[103]

Words within each explanation were limited to those central to reaction mechanisms; this is a practical choice we have made, as a network graph of *all* words within *all* explanations is unwieldy and uninterpretable. Word choice was based on relevancy and frequency of appearance, with English stopwords used to further limit and refine our important word list (e.g., words like "the" or "if" were not included in our study). Central words and associated co-occurrence were determined for the complete data set and by each reaction mechanism type (i.e., carbocation, S_N2, nucleophilic addition, reduction, and aromatic) and include the 16 most relevant and frequently occurring keywords: "attack", "attract", "bond", "carbocation", "charge", "double", "electron", "electrophile", "group", "leaving", "negative", "nucleophile", "partial", "pi", "positive", and "stable". Our keyword list originally included 32 words; however, we limited our report to 16 words for the sake of visualization purposes in the network graphs and for more focused analyses. Words were set to certain positions within the network graphs to allow for direct comparisons between the multitude of network graphs present in the study; however, this limited our ability to expand upon the spatial relationship between words; thus, the network graphs presented herein are used solely to visualize word co-occurrences.

A connection between words exists if those two words co-occur within a given explanation (e.g., "electrophile" and "positive"). The weight of a connection is relative to how many explanations contain those two words (e.g., 16,291 of 22,015 explanations contain both the words "nucleophile" and "attack"). Log transformations are used to visualize such connections; this allows for better depiction and thus interpretation of the relative weight (i.e., prevalence of two words found in an explanation) of a co-occurrence.

Descriptive statistics were used to investigate the unique number of words within an average learner's explanation and are reported as median, minimum (i.e., min), and maximum (i.e., max). Unique words are counted based on whether they appear within a response or not for each of the 16 keywords (e.g., an explanation may include the word "attack" three times but is only counted once for analysis purposes). Histograms are used to visualize the number of unique words used by the frequency at which they appear in explanations.

Descriptive statistics, histograms, and network graphs are reported for the complete data set, by level of explanation sophistication, by reaction type, and by level of explanation sophistication by reaction type.

RESULTS AND DISCUSSION

Results of our study suggest that explicit, surface-level features (e.g., "nucleophile" and "attack") are among the most prevalent words and pairs of words used in learner explanations regardless of reaction type. Many of these explicit features are central to learner explanations (e.g., "attack", "bond", and "group"). There are, however, words and pairs of words that are more closely associated with certain reaction mechanism types more so than with other reaction mechanism types; for example, the pair "negative" and "charge" is prevalent in the reduction mechanism network but not nearly as prevalent in the aromatic reaction mechanism network. Furthermore, we observe a progression in the words and pairs of words that learners use across levels of sophistication, where learners move from using surface-level "buzz" words (i.e., at the *Descriptive* level) to mainly consisting of implicit features (i.e., at the *Complex* level). This highlights the shift from a more fragmented, scattered, and unconnected knowledge base toward a stronger, stable, and organized knowledge base.

Research Question 1: What Words Are Most Prevalent in Learners' Explanations of Organic Chemistry Reaction Mechanisms? How Are Those Words Used in Connection with Each Other?

An array of words are used and used in combination in explanations of reaction mechanisms (see Figure 2); for parsimony, only the most prevalent words (n = 16) and associated co-occurrences are shown. The pairs of words used most prevalently are "leaving" and "group", "nucleophile" and "attack", and "double" and "bond"; this is depicted in Figure 2 as the boldest lines connecting those word pairs. These words and co-occurring word pairs are associated with explicit, surface-level features. Co-occurring words less common in the explanations include "partial" with "positive", "negative", and/or "charge" and "attract" with "charge", i.e., words associated with more implicit features of molecules and reaction mechanisms.

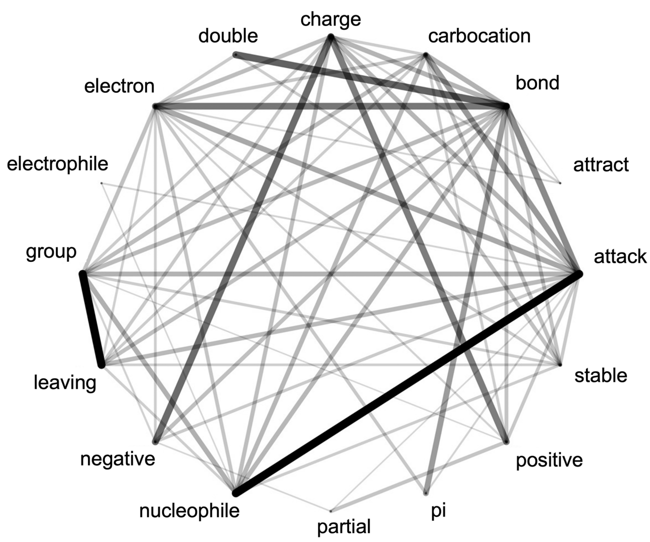

Figure 2. Full network of word use and co-occurrence of word use for all data (N = 22,015 explanations). Limited to connections that occur at least 850 times. Connections are reported on a log scale.

Quantitative measures further illuminate what words an average explanation might contain (see Table 1). Typically,

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Table 1. Descriptive Statistics of Words Used in Explanations of Reaction Mechanisms for All Data and for the Reaction Mechanism Type

Reaction Type	Median	Min	Max	*n*
Complete	6	0	16	22,015
Carbocation	6	0	15	8,470
S_N2	5	0	15	4,982
Nucleophilic Addition	6	0	16	3,817
Reduction	5	0	15	3,165
Aromatic	5	0	15	1,581

learners used an average of five to six of the 16 keywords within their explanations; at most, 15 to 16 of the keywords were used within a single explanation. Our results (see Figure 3) suggest a normal-like distribution of the number of keywords used in a single explanation response. This indicates that high word use (i.e., 15 to 16) is an extreme. This trend holds for each of the five reaction types (i.e., carbocation, S_N2, nucleophilic addition, reduction, and aromatic; see Table 1), not only for the median word use but also for the general distributions of these words (see histograms reported in Figure 4). From these results, we hypothesize that learners, in general, are not using words simply for the sake of using them in their responses (e.g., "gaming" the system) but rather using words perceived as meaningful or important for their reaction mechanism explanations. While some learners may be attempting to "game" the system, we would expect to see a higher frequency of keywords in their explanations if this were widespread instead of something we observed only to a limited extent. We hypothesize, however, that low-performing learners (e.g., at the *Absent* level) may still use these "buzz" words superficially.

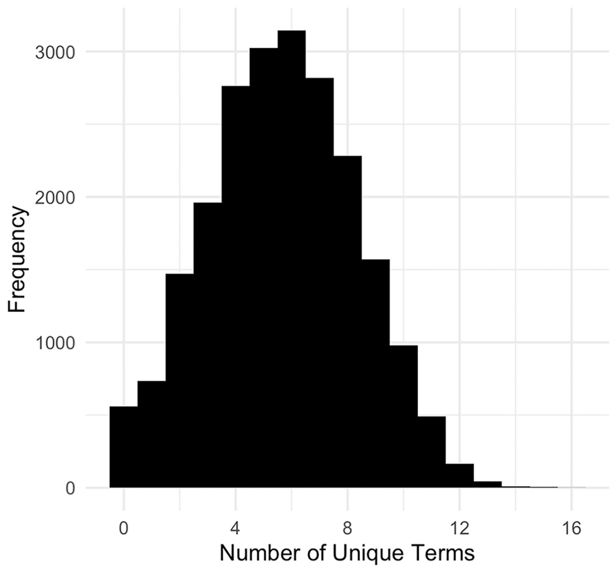

Figure 3. Histogram of unique words used in reaction mechanism explanations for all data (N = 22,015 explanations).

While the five reaction mechanism types have similar average word usage within learner responses (see Table 1), we hypothesize that the prevalence of these words and co-occurring word pairs is not consistent across reaction mechanism types. For example, "double" and "bond" is a word pair more associated with the reduction mechanism type compared to the S_N2 mechanism type, or the "leaving" and "group" word pair is more associated with the carbocation mechanism type compared to the aromatic mechanism type. Figure 5 contains the network graphs for the five reaction types; note that the same words are in each network graph and in the same location to facilitate direct comparison between the network graphs. As expected, particular word pairs are more prevalent by reaction mechanism type.

For example, within the network graph for the carbocation reaction type, "leaving" and "group", as well as "nucleophile" and "attack", are frequently co-occurring word pairs; for this reaction mechanism type, a substituent typically "leaves" early in the reaction mechanism either prior to, or in tandem with, a "nucleophile" "attacking". For the S_N2 reaction type, the two most prominent word pair co-occurrences are also "leaving" and "group" as well as "nucleophile" and "attack"; though the pair "negative" and "charge" is also common as the negative charge on the nucleophile is sometimes explicit within the S_N2 mechanism type. Within the nucleophilic addition reaction type, there is one word pair consistently co-occurring: "double" and "bond", a common explicit feature for all the reactions within this reaction mechanism type. Mechanisms within the reduction reaction type all feature an explicit negative charge on the reducing agent and the double bond; the most common pairs of co-occurring words include "negative" and "charge", "double" and "bond", and "nucleophile" and "attack". Double bonds are the key structural feature of mechanisms within the aromatic reaction type and are thus easily recognized by learners, even more so than a "nucleophile" "attack", and as such are often described at a surface-level in their responses.

These results are expected, in that expert-level explanations should contain the expected prevalent words and co-occurring word pairs; the differences observed for the five reaction mechanism types further confirm expected differences in how those reaction mechanisms should be explained. Given that these explanations were written by learners, it is reassuring that students are using, at a minimum, the words associated with reaction mechanisms and each reaction mechanism type. This suggests that most concepts seem to be available at the cohort level, an expected observation proposed by Asmussen et al.[83] However, it should be noted that within the full and individual mechanism networks (see Figures 2 and 5), the word "electrophile" is rarely used, whereas "nucleophile" is consistently one of the most used words. Moreover, for reaction mechanisms with more explicit, surface-level cues of the electrophile, learners are observed using "carbocation" in their explanations to indirectly identify the electrophiles. This observation is not entirely novel,[12,55,56,91] rather it has been suggested that a potential cause of this difference between learner usage of the words "nucleophile" and "electrophile" may be due to the active voice that chemists give the nucleophile regarding its role in bond formation (e.g., nucleophile or nucleophilic attack)[91] and a reliance on explicit structural features to be able to identify a nucleophile or electrophile within the reaction mechanism (e.g., charges and lone pairs).[55,56]

Though the keywords are generally present and prevalent in learner explanations overall, an area for further exploration is which words and co-occurring pairs of words persist or (dis)appear by each level of learner explanation sophistication.

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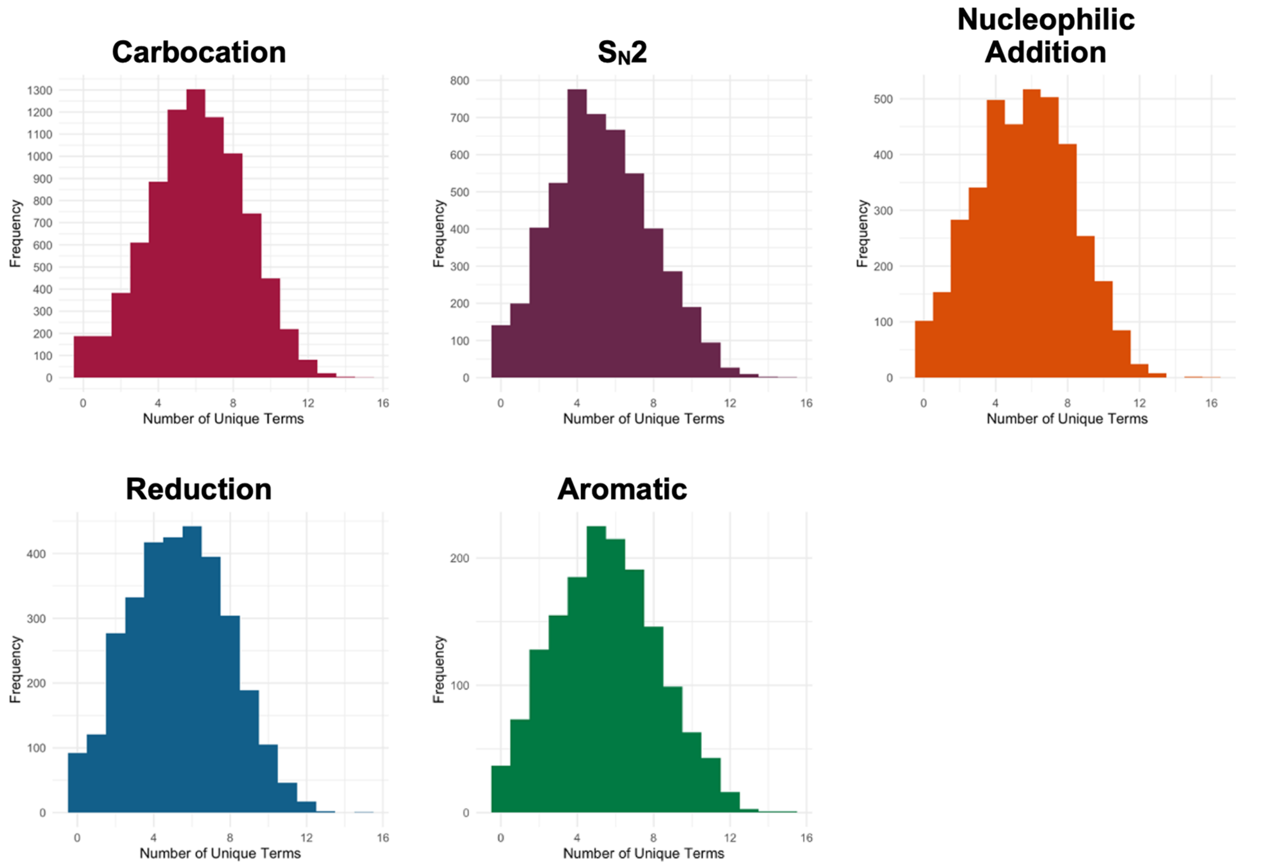

Figure 4. Histogram of unique words used in reaction mechanism explanations by reaction mechanism type

Research Question 2: What Differences in Word Use or Co-occurrence of Word Pairs in Learner Explanations Are Observed between Levels of Explanation Sophistication?

Our data are largely comprised of *Descriptive* level explanations (n = 13,065 or 59% of all explanations; see Table 2), which are, by definition, indicative of a focus on surface-level features and general bond-forming processes; this level of explanation sophistication distribution holds for each reaction mechanism type. Given the majority of explanations are categorized at the *Descriptive* level, the network graphs shown previously in Figure 5 may be skewed toward that level, and thus, we sought to determine whether learner explanations at different levels of sophistication show differences in their prevalent words and word pairs.

Descriptive statistics better illuminate word use frequency by level of explanation sophistication for the 16 keywords (see Table 3) for all data and by reaction mechanism type. As expected, we observe that the number of keywords used is associated with the level of explanation sophistication categorization, with a higher level of explanation sophistication associated with using more of the central words. We observe, as well, a large range of the central words used with explanations categorized at all levels ranging from zero or one word through more than ten words used. Histograms depicting the frequency of central word usage by level of explanation sophistication (see Figure 6) suggest that there is a normal-like distribution with few explanations containing ten or more of the central words. These trends (i.e., more central words used in explanations categorized at greater levels of sophistication and normal-like distributions with few explanations containing ten or more central words) hold for each reaction mechanism type (see Table 3 and Figure 6).

In comparison to the network in Figure 2 (i.e., the network graph for all explanations), there are notable differences between the words commonly used in each of the levels of explanation sophistication (Figure 7) and by reaction type.

At the *Absent* level, only a handful of words are used concurrently; this suggests that learners constructing such explanations have a limited set of available words from which to describe what is happening and why for the reaction mechanisms. These explanations may simply include keywords sparingly if at all, for example, "···In this reaction it seems that the OH is taking a hydrogen from the molecule. The oxygen in the molecule is then *attacking* the CL and it rearranges with the oxygen···" (emphasis added; an explanation constructed for an S_N2 epoxidation reaction). Oftentimes explanations categorized at this level simply state the reaction type, for example, "On the molecular level there is an *electrophilic* reaction to chlorinate the ring which will lose aromaticity and then regain it at the end of the reaction···"emphasis added; an explanation constructed for an electrophilic aromatic chlorination reaction). We hypothesize that, overall, these learners exhibit a superficial familiarity, but do not necessarily have the "fluency" to construct coherent explanations.

Explanations categorized at the *Descriptive* level have more co-occurring word pairs; this suggests that learners are "learning" how to use language to construct an explanation, albeit with little focus on what words are appropriate for a given reaction mechanism. Generally, these explanations focus on more surface-level features, for example, "In step one, the hydrogen-*bonded* to the aluminum is *nucleophilic* and *attacks*

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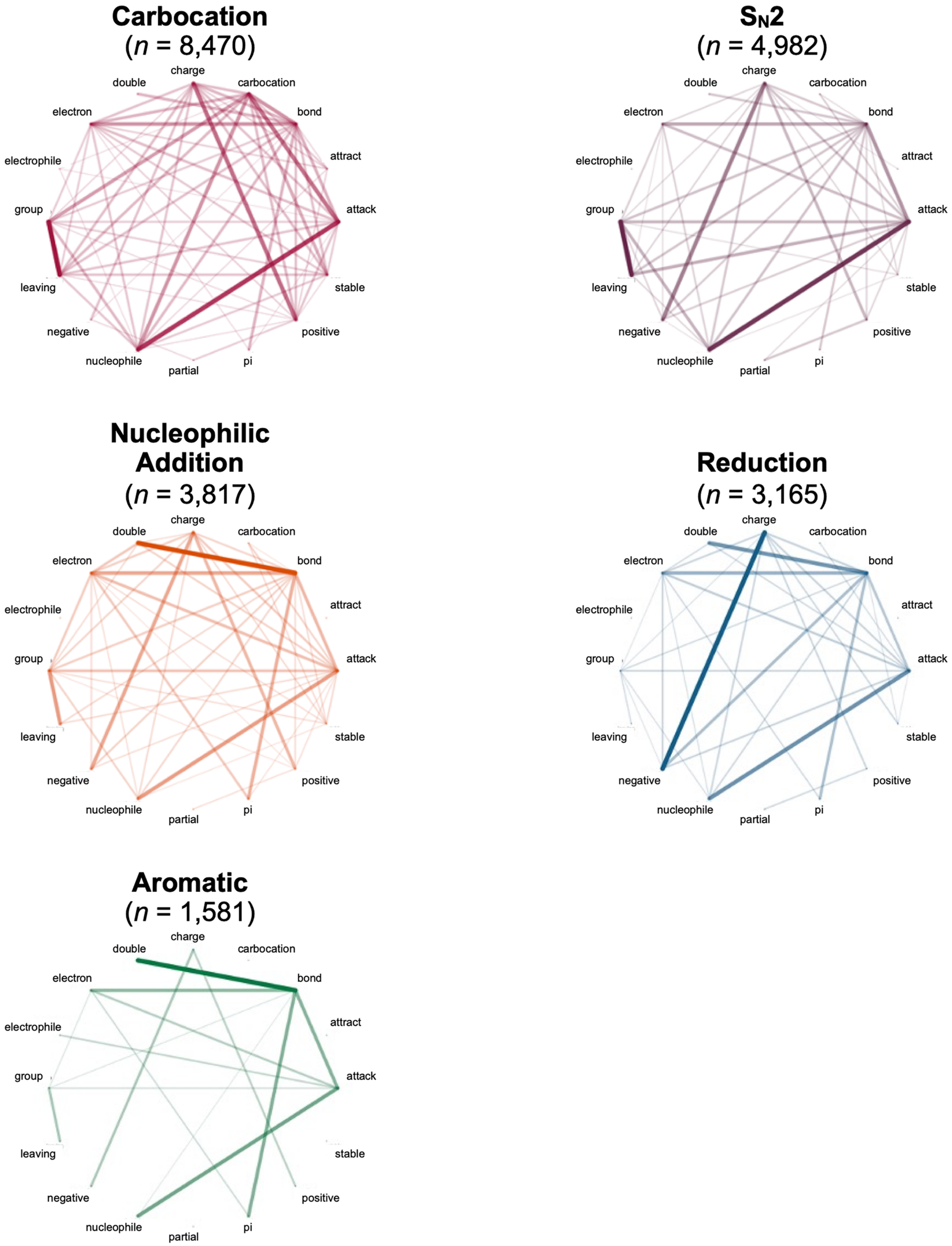

Figure 5. Full network of word use and co-occurrence of word use by reaction mechanism type. Limited to include connections that occur at least 250 times, connections are reported on a log scale.

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Table 2. Distribution of Reaction Mechanism Explanations by Level of Explanation Sophistication for All Data and by Reaction Mechanism Type[a]

Reaction Type	Absent	Descriptive	Foundational	Complex	Total
Complete	4,036 (18.34)	13,065 (59.34)	3,186 (14.47)	1,728 (7.85)	22,015 (100)
Carbocation	1,360 (16.06)	4,614 (54.47)	2,017 (23.81)	479 (5.66)	8,470 (100)
S_N2	881 (17.68)	3,140 (63.03)	447 (8.97)	514 (10.32)	4,982 (100)
Nucleophilic Addition	726 (19.02)	2,485 (65.10)	326 (8.54)	280 (7.34)	3,817 (100)
Reduction	724 (22.87)	1,818 (57.44)	287 (9.07)	336 (10.62)	3,165 (100)
Aromatic	345 (21.82)	1,008 (63.76)	109 (6.89)	119 (7.53)	1,581 (100)

[a]Row percentages are reported in parentheses.

Table 3. Descriptive Statistics of Words Used in Reaction Mechanism Explanations by Level of Sophistication for All Data and by Reaction Mechanism Type

	Absent			Descriptive			Foundational			Complex		
Type	Median	Min	Max	Median	Min	Max	Median	Min	Max	Median	Min	Max
Complete	3	0	11	6	0	14	8	1	16	9	1	15
Carbocation	3	0	9	6	0	12	7	1	14	9	2	15
S_N2	3	0	9	5	0	12	7	1	12	9	2	15
Nucleophilic Addition	3	0	11	6	0	12	7	1	16	9	2	15
Reduction	3	0	10	5	0	13	7	2	11	8	1	15
Aromatic	3	0	10	6	0	14	8	2	13	9	2	15

the carbon pushing up the *double bond*..." (emphasis added; an explanation constructed for a $LiAlH_4$ reduction of a carbonyl). However, they may sparingly mention implicit features or the role of electrons, for example, "The N is the *nucleophile attacking* the hydrogen, the proton from the hydrogen moves to where the *double bond* is, and the Cl *bond* breaks and the Cl takes those *electrons* with it⋯"" (emphasis added; an explanation constructed for an addition−elimination aromatic reaction). We observe that learners constructing such explanations (i.e., *Descriptive* level) know just enough to say a lot about a reaction mechanism but not yet necessarily how to communicate this in a clear, coherent, and efficient explanation.

We argue that a more coherent set of the central words is used at the *Foundational* explanation sophistication with stabilization at the *Complex* level; this suggests that learners are more cognizant of the relevant explanatory words and have learned how to combine those words in constructing appropriate explanations. Explanations categorized at the *Foundational* level may feature the attraction of charges, for example, "The bromine *leaves* creating a *carbocation*. the *electrons* on the OH *group* are then *attracted* to the *positive charge*..." (emphasis added; an explanation constructed for an S_N1 reaction). Additionally, they explicitly make the connection between charges and electron density; for example, "...the *negative* ion that makes up lithium aluminum hydride is *electron* rich as [*sic*] is able to act as a *nucleophile*. The carbon *double bonded* to the *electron* rich oxygen is *electron* poor..." (emphasis added; an explanation constructed for a $LiAlH_4$ reduction of a carbonyl). Explanations categorized at the *Complex* level further build upon these features as well as include other electronic properties, though partial charges are the most notably mentioned, for example, "...The H- group performs a *nucleophilic attack* on the *partially positive* carbon atom, and the *double bond* of the oxygen is broken...The *partially positive* carbon *attracts* the H-..." (emphasis added; an explanation constructed for a $LiAlH_4$ reduction of a carbonyl) or "...The enolate anion then *attacks* itself at the other carbonyl carbon because this carbon atom has a *partial positive charge*, *attracting* the *negative charge* of the enolate anion..." (emphasis added; an explanation constructed for a Dieckmann cyclization nucleophilic addition reaction). Overall, there is a shift in learner focus in explanations at these higher levels of sophistication toward the role of implicit features, this is in contrast to the focus of explicit surface-level features observed in explanations at lower explanation sophistication levels.

There are several important trends in word use and co-occurrence of word pairs by level of explanation sophistication and by reaction mechanism type. First, there are more co-occurring word pairs for the carbocation reaction mechanism type; based on the wide diversity of reaction mechanisms within this type (e.g., acid-catalyzed hydration of methylenecyclohexane, bromination of cyclohexene, and unimolecular nucleophilic substitution reaction of t-butyl bromide with ethanol), the number and frequency of co-occurrences is expected. The carbocation and S_N2 reaction mechanism types are the first mechanisms introduced in the first-semester of organic chemistry and were primarily administered to first-semester learners. As foundational mechanisms, they shape how learners initially learn to communicate about reactions, which may explain the greater variety in word use, even at higher levels of sophistication, as learners are still developing and organizing their understanding. In contrast, nucleophilic addition and aromatic reaction mechanism types were mostly given to second-semester learners, who are expected to have a more organized knowledge structure and greater fluency with the language of organic chemistry, a trend that is reflected at the higher levels of sophistication in Figure 7.

Next, at all levels of explanation sophistication, but particularly at the *Complex* level, we observe that the relevant word pairs for each reaction mechanism type are most frequent; for example, "nucleophile" and "attack" for the S_N2 mechanism type, "double" and "bond" for the nucleophilic addition and aromatic mechanism types, and "charge" for the reduction type. However, the context in which these words were used is important too. For example, the word pair "negative" and "charge" appears at every level of sophistication for the reduction reaction mechanism type, yet it is not used

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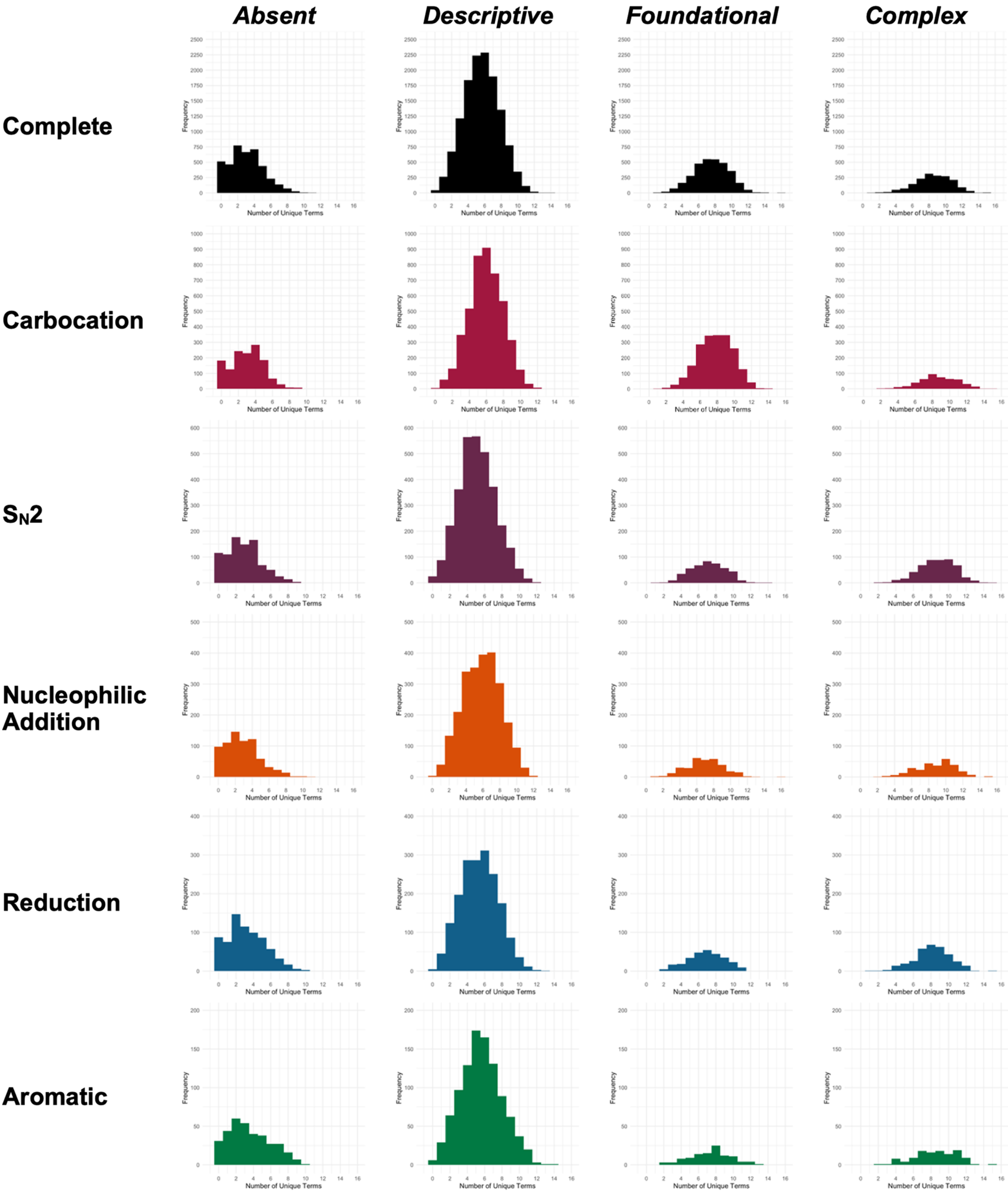

Figure 6. Histograms of unique words used in reaction mechanism explanations by level of sophistication for the complete data set and by reaction mechanism type.

the same at each level. At more novice levels, this word pair may only refer to the explicit structural feature present, unable to grasp the underlying meaning: an area of electron density on the molecule. An explanation categorized at the *Absent* level may recognize what the name of the negative sign on a molecule is, but lacks understanding of the deeper, underlying significance; a concept that becomes clearer as learners gain fluency and grasp the nuance of the concept. Additionally, by reaction mechanism type, the co-occurrence word pair frequencies associated with implicit features increases with

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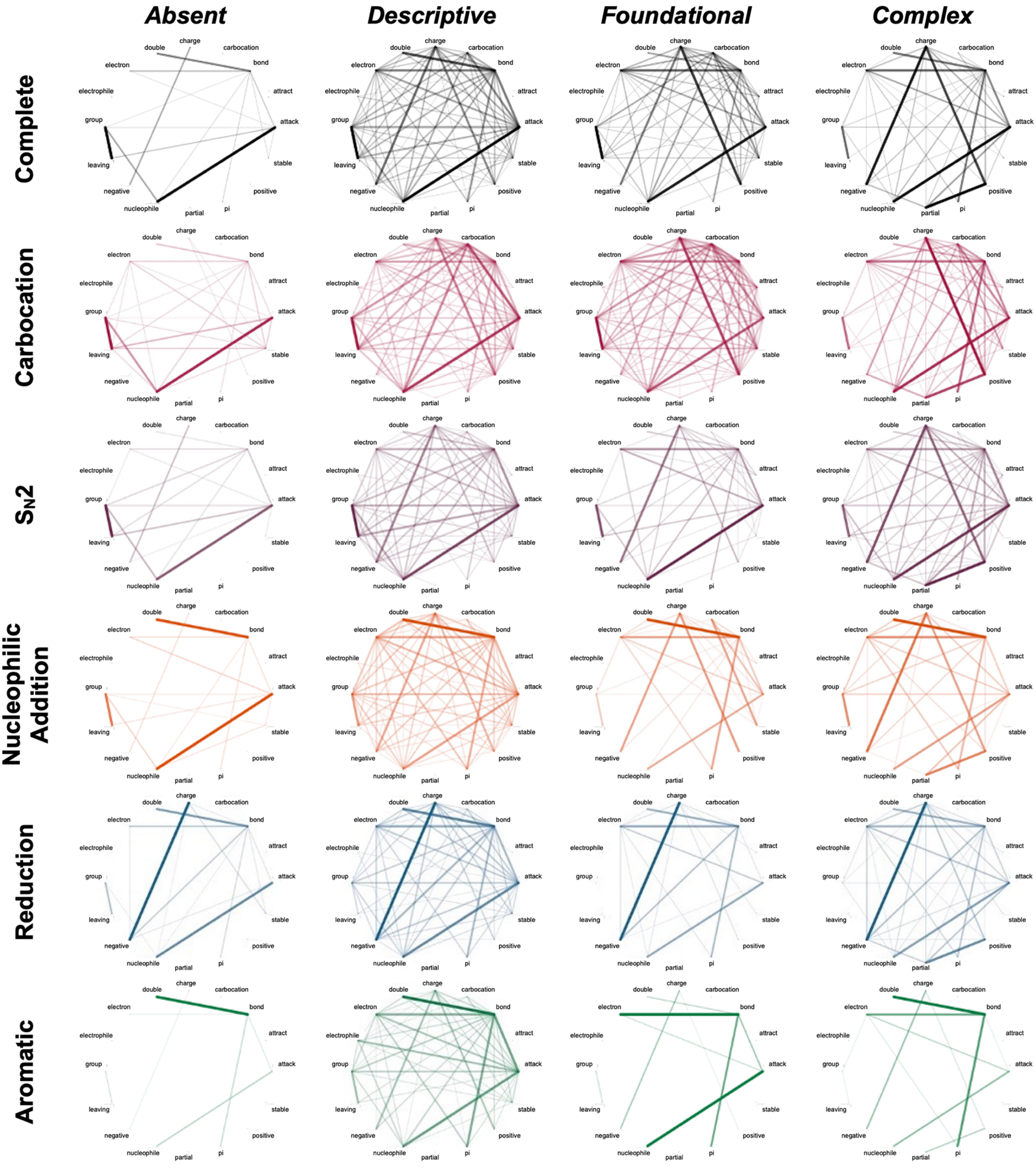

Figure 7. Network graphs of word use and co-occurrence of word use by level of explanation sophistication for all data and each reaction mechanism type. Limited to include connections that occur at least 250 times for the complete data set and at least 50 times for each reaction type, connections are reported on a log scale

level of explanation sophistication; for example, "partial" and corresponding "positive" or "negative" charges are much more prevalent in explanations categorized at higher levels of sophistication. From the premise that language use reflects underlying cognitive structures, the limited depth in vocabulary indicates that learners with explanations categorized at the *Absent* level are at an early stage in their cognitive development. This contrasts with those at higher levels of sophistication, with progression reflecting an evolving cognitive structure as these learners increasingly engage with the nuance of the language of organic chemistry.

Regardless of reaction type, the word "electrophile" was rarely used, whereas "nucleophile" was one of the most prevalent at all levels of sophistication, mirroring a result from

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Research Question 1. Though learners were able to discuss relevant features of electrophiles in their explanations, they rarely explicitly identified them. Even for explanations categorized at the *Foundational* and *Complex* levels, learners rarely explicitly identified the electrophile, opting to describe surface-level features (e.g., a positively charged carbon) or implicit features (e.g., partial positive or electron poor) instead.

Summary of Results and Discussion

Our work corroborates a foundational theme in the chemical education research literature: when we, as educators, ask learners to describe and explain, we come to understand that our expectations for learning are not always met as desired. This is reflected in our results, where learners frequently used explicit, surface-level terms (e.g., "nucleophile" and "attack") in their explanations, but rarely used more implicit features (e.g., "attract" or "partial" charges) or consistently omitted other relevant features (e.g., "electrophile"). This is corroborated by work by Asmussen et al.,[83] that indicated that some concepts were seldom applied by learners despite being relevant in multiple tasks. This highlights an important aspect of learners' cognitive development; the use of surface-level features in explanations suggests that learners are engaging with the language of organic chemistry; however, it also indicates that learners are still at an early stage of conceptual integration. Though learners can recognize and use appropriate words, reflecting initial engagement in the discipline, it does not necessarily equate to a deep understanding. It is known that a learner's ability to draw a reaction mechanism does not equate with that learner's ability to describe what is happening in the reaction mechanism they have drawn, nor explain why the reaction they have drawn occurs.[9] The literature supports this claim, though the results are often muddied depending on whether the learner drew a "correct" reaction mechanism or not. Our work herein, and work from prior studies,[10,12,15,28,34,86,96,104,105] minimizes the "correctness" confounding variable and has learners explain a "correct" reaction mechanism that is provided to them. Whether drawn by the learner, or a correct reaction mechanism provided to the learner, we continue to observe that all learners' explanations are not at the highest level of reasoning. We might argue, though, that the distribution of responses (rather than all correct) in the context of our research is more illuminating as to how we can facilitate and create meaningful learning experiences.

The learning objectives and instructional goals at our institution primarily focus on bringing learners at least to the *Descriptive* level. From the perspective of methodological interactionism, the way that content is taught and discussed in the classroom (shaped by these goals and expectations) plays a significant role in how learners construct their understanding of reaction mechanisms, a result reflected in our data, as the majority of learner explanations were categorized at the *Descriptive* level (~59%). Despite the skew toward this level, trends observed for the complete data set mirror those at each level of explanation sophistication, albeit with a progression in the number of words used and the use of more implicit features in explanations across the spectrum of levels and levels by reaction mechanism type. This suggests that there is a hierarchical ordering of words and concepts necessary for engaging in more complex reasoning, reflecting findings reported in the literature.[21,51,85,106] Although there is little that can be drawn out from *Absent* level responses due to how little learners conveyed in explanations categorized at the *Absent* level, learners who attempt to construct these explanations and use relevant words are at least beginning to engage with the language of organic chemistry, even if their understanding is not yet at the desired level. The shift in explanations from the *Absent* to *Descriptive* level reflects learners' growing familiarity with vocabulary for discussing reaction mechanisms, though the usage of these words remains scattered and largely surface-level. This becomes more organized and more coherent in explanations categorized at the *Foundational* and *Complex* levels as learners pare down their explanations more effectively by correctness and relevancy, and such explanations focus more on the underlying, implicit features rather than the typical "buzz" words observed in the lower levels. This shift in explanations also illustrates the principles of methodological interactionism; as learners refine their language, explanations, and vocabulary through discussions with instructors and peers, they should be able to connect concepts in a more cohesive manner.

■ LIMITATIONS

There are three key limitations to be considered in light of our findings.

First, our data were collected at one institution with a relatively standardized curriculum. This means that our data may not reflect all students learning with all curricula. We hypothesize, for example, that students engaged in learning environments that employ the POGIL[107] pedagogy or that specifically target science practice skills such as the OCLUE[108] curriculum, may have differing distributions of explanations at the different levels of sophistication. This, however, does not invalidate the results presented, as we have noted how our results corroborate those of others' work; additionally, we do not expect the patterns of word use or co-occurring word pairs to differ by learning environment context; we only expect differences to emerge as to how many explanations are categorized at each explanation sophistication level.

Second, per a restriction on how the data were collected within the scope of our IRB approval, we are unable to link data by learner; this includes linking two or more explanations collected at the same time or linking two or more explanations collected across a term or the year-long course sequence. Thus, we are unable to follow an individual learner and their progression; however, we acknowledge that such a study would be important to confirm our hypotheses about the availability of words to use in explanations and the development of explanation sophistication across a course. Such a study would be interesting in both "measuring" the level of explanation of sophistication for the same (or highly similar) reaction mechanism across multiple time points as well as "measuring" the level of explanation sophistication for multiple reaction mechanisms across multiple time points.

Last, the length of any given reaction mechanism explanation was insufficient to fully embrace the use of network analysis metrics (e.g., degree,[109] betweenness,[110] and eigenvector centrality measures[111]) based on linked word pairs. Our data reflect the co-occurrence of word pairs within an explanation; however, words did not have to appear after each other and could occur anywhere within an explanation. In a lengthier writing sample, such pairs could be observed, and thus network analysis metrics could be applied; however, such metrics would be applied for each explanation. Thus, a more meta-analysis of network metrics would need to be employed

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for such a study, i.e. an analysis of many analyses. Furthermore, our analyses were limited, by choice, to the 16 keywords and fixed positions within the network graphs for ease of visualization. While restricting the keywords to the most frequently occurring and related words present in learner explanations aided in the visualizations of the network graphs and allowed for a more focused discussion, this choice excluded less frequent but still relevant words (e.g., polarity or polarizability); the inclusion of these words could offer deeper insights into the learning patterns of the smaller subsets of learners who used them in their explanations. Additionally, the fixed positions of words within our network graphs limited our ability to explore the spatial relationships of the keywords; using a different layout algorithm (e.g., Fruchterman–Reingold) could better illustrate the underlying structure of the network. That being said, the results of our study illuminate our expected results while providing key implications for instruction and research; thus, we question whether longer explanations and the use of more advanced metrics are necessary to inform our teaching practices and understanding of student learning of reaction mechanisms.

■ IMPLICATIONS FOR INSTRUCTION

A question that has garnered little attention in the research on the teaching and learning of organic chemistry reaction mechanisms is whether expert-level reasoning is the goal or realistic expectation at the end of the first postsecondary organic chemistry course. We have been purposeful in our study to not make a value judgment as to what level of explanation sophistication is desired; in our learning context, we understand that our learning goals are to help learners to engage, at least, with descriptive reasoning and then to progress to higher levels of reasoning, if possible, but those may not be the same for all course contexts. It could be the case that a general-organic-biochemistry (GOB) course may set a goal for learners to be able to identify the nucleophile and electrophile in a particular reaction mechanism and denote which bonds are being formed or broken; this could be done by having a learner circle or square the nucleophile, for example. However, asking learners to use words in the form of a sentence could provide an additional piece of confirming evidence of learning. At the other end of the spectrum, an honors-level course designed for learners engaged in synthetic organic chemistry research may desire those learners to be able to explain in detail all aspects of a reaction mechanism, both explicit and implicit features, invoking causal-mechanistic reasoning. Learning outcomes should be context dependent; that being said, we advocate that evidence of learning reaction mechanisms, at whatever level, should extend beyond solely drawing the reaction mechanism.

Constructing explanations (i.e., a process) is critical to developing the desired reasoning skills;[21,112] the process explaining *what* is happening in a reaction mechanism and *why* the reaction is occurring is not a one-time activity. As observed in our study, learners' growing familiarity with the language of organic chemistry was reflected in the shift from the *Descriptive* level to more complex levels of sophistication; learner explanations evolved from more scattered and surface-level to more organized and precise, attention shifting toward the importance of implicit features. However, our results, and those of prior work,[15,19,23,51,105] also suggest that learners need opportunities to construct explanations; learners need scaffolded or structured *experiences* to facilitate their construction processes. Within our study, generally, learners were able to use surface-level features in their explanations; however, learners struggled to consistently use certain key surface-level words like "electrophile" and "carbocation" and rarely incorporated implicit features into their explanations. This suggests that learners need more instructional scaffolding to help them become familiar with these terms and determine their relevancy to promote fluency.[31] Learners should not be expected to construct explanations of reaction mechanisms without opportunities to observe others (i.e., instructors, teaching assistants, and peers) construct explanations; if we adhere to the principles of methodological interactionism,[69,92,93] these social experiences are how students learn the language of organic chemistry, refining what word(s) or language is important until they are (near) fluent. This process comprises more than just having learners regurgitate explanations; true understanding of reaction mechanism concepts is demonstrated when explaining reaction mechanisms not yet seen by the learner. Learners need guidance on how to connect all the pieces into a coherent explanation; instructional scaffolding needs to include how to translate explicit features (e.g., lone pairs) into more implicit ideas (e.g., electron density). As corroborated by prior studies,[12,32,113−116] instructional staff should be purposeful and explicit in demonstrating the desired level of explanation sophistication, noting the process of constructing an appropriate explanation, and pointing out anticipated difficulties learners may encounter when constructing explanations on their own. Additionally, the peer-review process—where learners give and receive feedback from one another—can be highly insightful; observing how peers approach their explanations of reaction mechanisms in both similar and different ways may encourage deeper reflection and revision in their work.[117−121] Thus, we need to do more than tell; we need to model the desired skills; and we need to support learners as they work through and succeed at explanation construction.

■ IMPLICATIONS FOR FUTURE RESEARCH

Our results point toward two key opportunities for further research.

First, how does a learner's ability to construct an explanation vary across an organic chemistry course or across the yearlong organic chemistry course sequence? As we have noted in the *Limitations* section, we are unable to link our data by learner. While our data may appear to be set in a cross-sectional longitudinal way (e.g., carbocation reactions are a large focus of the first-semester organic chemistry course and aromatic reactions are a large focus of the second-semester organic chemistry course), data were collected in such a way that once a reaction mechanism had been taught in the course sequence, it could (and did) appear on any subsequent assessment. This means that explanations of reactions typically taught in the first-semester course were elicited not only from students in the first-semester course but also from students in the second-semester course. A more purposeful study would be illuminating the collected data across the yearlong course sequence that sampled explanations of reaction mechanisms as those reaction mechanisms were taught. Such a study would address whether explanation sophistication is developed across the course or whether explanation sophistication is reaction mechanism dependent. Furthermore, a study of this sort could point toward interventions (e.g., implementation of particular

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pedagogical techniques or curricula) that best promote the construction of explanations at higher levels of sophistication.

Second, the ability to incorporate assessment items (either on a homework assignment, quiz, examination, etc.) is dependent on the time and resources to provide meaningful feedback to learners. Such feedback cannot be simply limited to correct or incorrect; rather, feedback necessary for promoting reasoning skills must be targeted and purposeful. Even with a small class ($n \sim 20$ students), the inclusion of multiple reaction mechanism assessment items can quickly become cumbersome; for a large class ($n = 180$ students per section; there are six such first-semester organic chemistry course sections at our institution in a fall term), the inclusion of even one such assessment item may be impractical. Computer-based scoring models provide one avenue for not only handling a large number of responses but also providing near-instant feedback to learners. Martin and Graulich's scoping review[122] considered the variety of machine learning models developed to capture mechanistic reasoning within chemistry education research. Such scoring models have been developed and disseminated for use of the Lewis acid−base model in explanations of acid−base reactions or explanations of acidity/basicity/amphoteric properties;[24,34,37] these scoring models have been paired with adaptive tutorials to provide real-time learner-specific experiences[33,52] and real-time feedback.[38] Such a model that scores explanations of reaction mechanisms using the levels of explanation sophistication has the potential to extend current work in this area, providing a tool for educators and learners to further the development of the desired reasoning skills. Additional models have also been reported for scoring other types of organic chemistry learners' explanations: essay responses (e.g., writing-to-learn prompts),[123] argumentation skills related to reaction mechanisms,[124] and multilingual (German and English) written scientific arguments.[125]

The work herein, though, points to a potential challenge in developing such a predictive model: at each level of sophistication, the desired keywords for a given reaction mechanism are present and co-occurring with each other, albeit at differing levels of frequency. Imbalanced data, though common in educational contexts, can present challenges when training a generalizable predictive and may result in reduced scoring accuracy.[126−129] Thus, the presence or absence of keywords (as was the main basis for a previously reported Lewis acid−base model) is insufficient for the development of a predictive model, other factors will need to be taken into consideration to overcome these limitations. In alignment with results from Gombert et al.,[85] the structure, or the network of word use, will need to be considered during the feature engineering phase of model building. Other data augmentation methods and metrics for model performance (e.g., F_1 score, Matthews Correlation Coefficient, ROC-AUC) previously reported in the literature[37,54,130] may also need to be considered for a more robust model. While a single model would be ideal, the differences we observed by reaction type may necessitate further feature engineering or predictive scoring models for each reaction type.

CONCLUSIONS

The results of our study extend the growing body of research on how learners reason about reaction mechanisms. Generally, learners use a wide variety of surface-level features in their explanations, they consistently omit words explicitly relating to the electrophile (e.g., "electrophile" and "carbocation"), corroborating findings from prior work.[12,15,55,56] Using network analysis, we investigated patterns in the keywords used within learner explanations and visualized the co-occurrence of these keywords via network graphs. Our findings suggest that learners consistently use explicit surface-level features (e.g., "nucleophile" and "attack") in their explanations, with some features used more frequently than others based on reaction context (e.g., "double" and "bond" in the aromatic reaction type). These trends also hold for each level of sophistication; though, with a progression of words used and coherency as explanation sophistication increases, shifting in focus from mainly surface-level toward implicit features, until explanations are near "expert-like". These results provide opportunities for instructors to reflect upon their teaching practices to better support students as they construct these connections between surface-level and implicit features with suggested steps for providing the space and structure to aid learners in making these connections. These results also offer researchers opportunities to better understand if and how learner reasoning changes over time and considerations for the development of predictive-scoring models for quick snapshots of understanding for large sets of learner explanations as well as to provide adaptive tutorials and feedback to learners.

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Author Contributions

C.J.C. and J.R.R. conceptualized the project. Data were collected and analyzed in prior reported studies. C.J.C. conducted analyses. C.J.C. and J.R.R. discussed and interpreted study results. C.J.C. authored the paper. Both authors read, edited, and approved the final manuscript.

Notes

Any opinions, findings, and conclusion or recommendations expressed in this material are those of the authors and do not necessarily reflect the view of the National Science Foundation. The authors declare no competing financial interest.

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