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Students' Sensemaking of Electrostatic Potential Maps within Substitution and Elimination Reactions

Isaiah Nelsen, Melissa Weinrich, and Scott E. Lewis*

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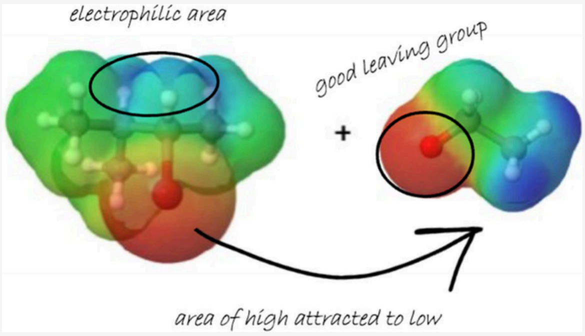

ABSTRACT: Reaction mechanisms are a difficult and foundational topic students encounter in organic chemistry. Consequently, students often memorize when attempting to learn the array of organic reactions. While interventions have been offered to encourage mechanistic reasoning as an alternative approach, a deeper struggle pertaining to students' comprehension of the underlying chemical principles driving reaction mechanisms is still prevalent. In this study, electrostatic potential maps (EPMs) were explored as a tool students could use to reason with some of these principles to predict and explain the outcomes of a reaction. Through semistructured interviews, 19 students' sense-making strategies were recorded and analyzed to uncover how they used the features of EPMs with concealed atomic identities and how they reconciled their answers once the identities were made explicit. Analysis revealed that the absence of atomic identities generated approaches centered around electron densities and their utility in predicting reaction mechanisms and outcomes. As the atomic identities were revealed, the majority of participants reverted to memorized mechanisms, while six participants attempted to relate the atomic identities to the interactions of the electron densities. These findings suggest utility in implementing EPMs in the organic chemistry curriculum and offer a feasible intervention to promote sense-making when students reason with organic reactions.

KEYWORDS: *Second-Year Undergraduate, Organic Chemistry, Testing/Assessment, Reactions, Chemical Education Research*

■ INTRODUCTION

Mechanistic reasoning is one of the core principles in understanding the underlying concepts of organic chemistry and is considered fairly difficult in the eyes of students.[1] The number of reactions that students are expected to learn over the course of organic chemistry can be perceived as overwhelming.[2] Knowing the reaction mechanism for each one of these unique reactions adds another layer of complexity that can propagate misconceptions in students' mechanistic reasoning and their understanding of the electron-pushing formalism.[3−10] Consequently, students may see little value in learning how to reason mechanistically and turn to rote memorization of reactants and products.[2,5,8,11] For students who memorize and reiterate reaction mechanisms, few have been properly instructed on how to explain the chemical reasoning behind the steps in a reaction mechanism.[3,12] As a result, students may not associate any physical meaning to the electron-pushing formalism, resulting in a product-oriented view of reactions.[3,5,12]

To address this disparity, researchers have attempted to implement curricular reforms to encourage mechanistic reasoning with a purpose. Flynn and Ogilvie have proposed a redesign of the organic chemistry curriculum where the electron-pushing formalism and reaction mechanisms are taught prior to organic reactions to mitigate reaction memorization.[13] Writing-to-learn assessments have also been presented as an option to elicit detailed mechanistic reasoning from students when working with reaction tasks.[14] While these approaches provide potential solutions to the rote memorization of reactions, students may not understand the determining factors behind electron flow in reactions and incorrectly use mechanistic reasoning.[15] In a study implementing Flynn and Ogilvie's approach, groups of students were found transplanting electrons from one atom to the next without chemical reasoning to support their decision.[15] Studies surveying students' conceptions of nucleophiles and electrophiles in reaction mechanisms uncovered a similar surface level understanding of organic reactions, where students categorized reagents as either a nucleophile or electrophile only after they had drawn out the mechanism.[8] This retrospective method of categorization was unsurprising considering the textbook used in the course did not draw connections between the determining factors of nucleophilicity and instead provided a

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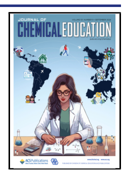

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checklist of features for students to follow.[7] Students' ability to identify nucleophiles and electrophiles and their relationship to electron density has been identified by instructors as pertinent to proficiency in organic reaction mechanisms.[7,16] However, a lack of clear instruction on the driving forces of nucleophilicity and overall reaction mechanisms have pushed students toward drawing electron pushing without a rationale.[5] Therefore, there is a need for instruction that promotes a deeper understanding regarding the rationale behind electron movement in reactions.

When aiming to emphasize the electronic components of reaction mechanisms, the chemical representations that instructors choose to communicate chemical concepts are vital to student learning.[17] Representations play a critical role in student understanding of chemistry topics and have the potential to directly or indirectly propagate misconceptions regarding chemical phenomena.[18] Therefore, instructors are encouraged to be intentional about the representations they introduce in the classroom.[17] Kozma and Russell argue that representations should be used as a means for explaining and defending claims about chemical phenomena.[19] Findings in the literature suggest, however, that there is a lack of focus on developing these meta-representational skills in the organic chemistry classroom.[20] Representations that reduce visual complexity by directly portraying molecular relationships can make these representational skills more accessible and have been shown to aid in students' interpretation of chemical properties.[21,22] Electrostatic Potential Maps (EPMs) are one type of representation within chemistry that carry the potential to provide students with a rich source of information to explain molecular characteristics and relationships. EPMs are graphical models that display the electron density distribution of a molecule through colors. While these representations can often be found in chemistry textbooks, direct instruction on how to interpret EPMs is not always included and their integration in end of chapter problem sets is sparse.[23] Their use within the chemistry classroom, however, has been linked to a deeper conceptual understanding of topics like polarity, intermolecular forces and chemical bonding.[21,24,25] In terms of reactionary constructs, EPMs have been found to positively influence students' predictions of molecular partial charges and nucleophilic character.[26] With these findings in mind, it is of interest to explore the utility of EPMs in promoting students' understanding of electron movement in organic reactions. The following study ventures into this interest and reports findings that offer insight into how students interact with EPMs in the context of organic reaction tasks. These findings speak to the potential utility of EPMs in organic chemistry instruction and the influence representations can have on students' explanations of chemical phenomena.

THEORETICAL FRAMEWORK

The sensemaking process can be described as the iterative construction of an explanation to address a gap in one's understanding.[17] The sensemaking process begins when discrepancies arise in a set of ideas an individual is attempting to relate.[27] To address these discrepancies, the individual must generate potential explanations using the resources they have at their disposal.[27] Sensemaking is an inherent aspect of the practice of chemistry where chemists delineate the cause of phenomena through trial and error. While representations in chemistry are often strictly used to depict chemical systems, they can act as tools to aid in this process by offering students features that can be reasoned with to develop an explanation for a phenomenon.[17] Encouraging students to utilize these tools as they embark on the sensemaking process begins with instructors reevaluating the representations used in the course and identifying the purpose they serve.[28] In organic chemistry, representations offer features that cater to certain aspects of the sensemaking process. For instance, in explaining the mechanism behind a reaction, line angle structures operate as tools that can depict the reaction step by step. However, it may be difficult for students to assess the origin of the reaction or the path of the electrons when only provided line angle structures.[15] To understand the driving forces behind these mechanisms, students may require additional representations offering features that they can make-sense of conceptually. Therefore, we aim to assess how students' sense-make about organic reactions when provided EPMs with and without atom identities. While it is not conventional to keep atomic identities concealed when presenting students with reactions tasks, doing so generates a task with an undefined answer that affords the opportunity to understand how students' sense-make with the features of the EPM. A prior study found that chemistry problems with undefined answers prompted chemistry experts to search for insight or information to deduce a solution rather than rely on pure chemical knowledge.[29] This study follows a similar direction to understand how students draw connections to their chemical knowledge to find a solution to a reaction task that only provides the EPMs of the reactants and products. Once the atomic identities are disclosed, it is of interest how students rectify the differences in their answers and make connections between their reaction mechanisms and the explicit features of the EPMs. Currently the literature base on the utility of EPMs in chemistry curriculum is limited and mainly concerned with how they can help students reach a correct answer. While the nature of this study is task specific, it goes beyond rate of correctness and explores how students sense-make with EPMs to generate chemical explanations for their predictions. The findings from this study can build a foundation for exploring students' sense-making of EPMs in a variety of chemical tasks, providing clarity on the affordances and limitations that need to be considered if the representation is implemented into chemistry curriculum.

RESEARCH QUESTIONS

The following questions were used to guide the path of this study:

- How do students sense-make with the features of electrostatic potential maps in an organic chemistry reaction task with atomic identities concealed?
- What impact does the disclosure of atomic identities have on students' sense-making with the electrostatic potential maps?

METHODS

Positionality

IN, a graduate student studying chemical education, recognizes the impact his training in chemistry and experience as an organic chemistry teaching assistant can have on his approach to this study. IN's experiences in the classroom as well as his prior research involving students' conceptions of chemical representations have informed his assumption that the resources students are provided play a pivotal role in their learning and comprehension of concepts. Additionally, he

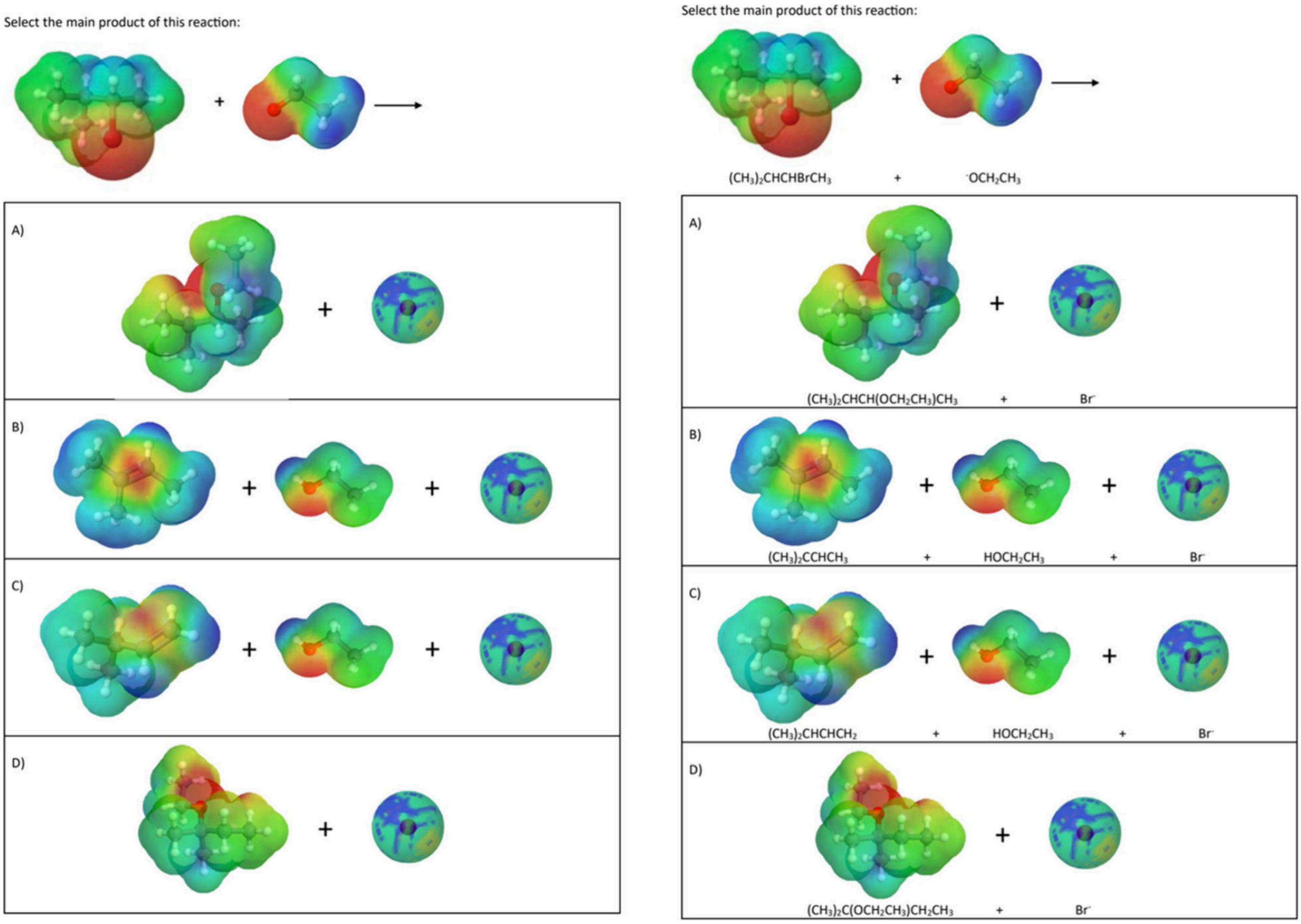

Figure 1. Left: In Part I of the task, students were given a set of EPMs without atomic identities and asked to predict the main product. Right: In Part II, the same task was presented with disclosed atomic identities.

holds to the view that student knowledge cannot be described in isolation and is instead founded on past experiences. As students encounter new pieces of information, they must assess its compatibility and form connections with their prior knowledge during the learning process. These perspectives have the potential to influence how IN approaches research.

MW's perspectives are informed by her background as a White cis-gendered female in academia. She is an associate professor and associate department chair at a Hispanic serving institution. MW teaches general chemistry, organic chemistry, conducts outreach, and mentors graduate students in chemistry education research. She assumes that student learning is influenced by a multitude of factors including the resources provided to them. Humans build new knowledge based on their prior experiences and grow when given the opportunity to express ideas in their own voice. These perspectives influence MW's approach to research.

SEL acknowledges experience as a chemistry instructor and education researcher that informed his approach to this study. These experiences have informed an assumption that people are rational actors and engage in sense making reliant on both their past and current experiences. Further, his socialization as a chemistry instructor has led to viewing science knowledge as both an evolving enterprise and dependent on near-universally acknowledged facts (e.g., scientific consensus). Although he recognizes that there is no objective knowledge, these perceptions likely influence his research.

Research Setting and Participants

Participants were recruited from first-semester organic chemistry courses at two doctoral granting universities in the southeast (University 1) and midwest regions (University 2) of the United States. Students were recruited to take part in a 60 min semistructured interview. A general announcement calling for participants for a chemical education study was posted on the students' course learning portal. Students that replied and indicated intent to participate were enrolled in the study. Ten students were recruited from University 1 while nine students were recruited from University 2. Each student was provided a description of the study procedures and their rights as a participant and signed an informed consent document granting permission for their responses to be used for research. Participants were compensated with a 25-dollar gift card for their participation in this study. During the interviews some participants acknowledged coming across EPMs in their classroom, adding that these encounters were brief. They also noted that, at points, the purpose of incorporating the EPM remained unknown, and they were unsure of its utility.

Data Collection

The interviews were semistructured and conducted in person lasting approximately 60 min. Each interview was audio recorded as participants were presented with a set of tasks with static images of chemical representations. The interview protocol was divided into six tasks, the first three tasks

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involved card sorts, the fourth and the fifth tasks dealt with students' interpretation of representational features, and the final task consisted of a multiple-choice reaction question. This paper is centered around students' responses to the final task, consisting of two parts. In Part I, the students were presented with the electrostatic potential maps of two reagents (2-bromo-3-methylbutane and ethoxide) with atomic identities concealed (Figure 1 left). The participants were given four answer choices of EPMs with concealed atomic identities and asked to "Select the main product of this reaction." The reagents for this task were selected based on the target group's familiarity with the molecules' functionality in substitution and elimination reactions. Additionally, the EPMs for these reagents displayed distinguishable areas of high and low electron densities. In part II of the task, the same reaction was shown to students with the atomic identities disclosed, calling for a prediction of the product (Figure 1 right). Follow-up questions (i.e., *Why did you select that product?*) were asked to clarify students' reasoning for their answer choices.

Data Analysis

All 19 interviews were transcribed with the help of talk to text software. The transcriptions were reviewed manually for corrections. The final task of the interview transcripts was analyzed and open coded to synthesize one codebook that would help uncover themes on how the students utilized the EPMs' features when answering Parts I and II. (a detailed description outlining the development of the codebook is provided in the Supporting Information above Table S1). The first iteration of the codebook was applied to the transcripts, and a reassessment of the codes exhibited areas for improvement. A modified version of the codebook was generated and reapplied to the transcripts to verify functionality. Once the final codebook was established (Supporting Information Table S1), consensus coding was conducted on both parts of the final task in all 19 transcripts. The coded transcripts were analyzed to establish themes on how students were sensemaking with the EPMs. In association with RQ1, three themes involving students' sensemaking with EPMs when atomic identities were concealed were developed through analyzing the codes assigned to students' responses in Part I of the task. To answer RQ2, the impact of revealed atomic identities was identified by analyzing consistency and changes in assigned codes as students transitioned from Part I to Part II of the task. For example, if codes from the Attraction and Electron Distribution parent code (See Table S1) were assigned to a participant's response in Part I, but only codes from the Structural/Conceptual Reasoning parent code (See Table S1) were assigned to Part II, it was evident that atomic identity disclosure had an impact on the participant's sensemaking process with the EPMs. The themes were presented to the authors MW and SEL along with exemplary quotes from the transcripts to ensure coherence in the interpretations of the data.

RESULTS

The analysis of the transcripts produced three major themes that encapsulate how students go through the sensemaking process using EPMs on reaction tasks. When given the EPMs with concealed atomic identities in Part I of the task, participants called attention to electron densities' relation to molecular structure, charge and the interaction between reagents, and the prediction of reaction mechanisms. While some participants' sense-making strategies could be exclusively described by one theme, the majority of participants used several strategies that can be described by combinations of the three themes (Figure 2). Each of these themes are discussed in detail below. Upon unveiling the atom identities in Part II of the task, 13 of the participants reverted to memorized mechanisms while six students drew connections between the newfound identities and the features of the EPM to reason about their previous answers or to develop novel approaches to the task.

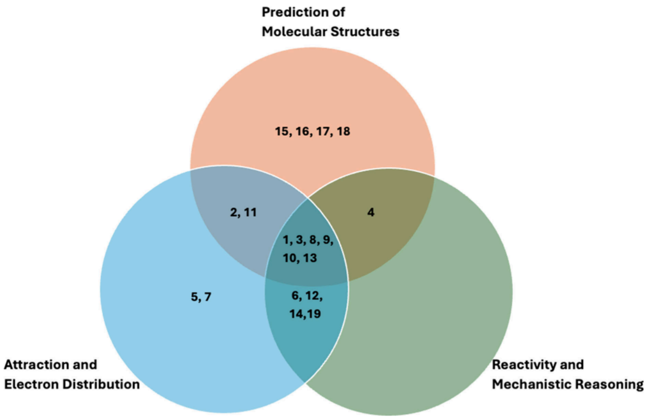

Figure 2. Participants organized by the themes that were observed in their approach to Part I of the reaction task.

Part I Theme I - Prediction of Molecular Structures

Participants' unfamiliarity with the features of the EPM representation and the absence of atomic identities instilled uncertainty and many participants were hesitant to begin working through the problem. Participant 15 expressed his discomfort with the task stating, "Oh. I think the EPMs hurt my brain with reactions. I think, oh, I haven't seen anything like this. I'm very used to the line structures, and names, so this really hurts my head." Several other participants echoed this discomfort, including Participants 9 and 11, as they attempted to interpret the meaning of the features of the unmarked representation. Participant 9 described the electron density plots as "little planets," and subsequently admitted, "I wish it would tell you what the atoms are." Participant 11 was more curious about the nature of the task itself, asking "Whoa. Do I have to know what the balls are?" Consequently, to remove some of the ambiguity from the first part of the task participants began by attempting to distinguish the atomic and structural components of each reactant using the electron densities (See Supporting Information Table S2 for detailed quotes from each participant that fell under this theme). Participant 1's approach exemplified this line of logic, as he explained "So my first thought is I don't use these that much and so I'm trying to like look inside the thing and kind of convert it." To accomplish this, several participants related the colors on the EPM to electronegativity to predict atomic identity, conveying that more electronegative atoms carry a higher electron density. Participant 11 used carbon as a benchmark when discussing the relative electronegativities of different elements stating, "I don't know what these ones are [referring to the red balls]. It has to be something more electronegative than carbon. They either go to nitrogen or oxygen. I would say oxygen..." The connection between color and atom identity was further utilized to determine the product

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based on where the electron densities resided in the answer choices. Students compared where they observed high electron density in the reactants to where the colors were pictured in the product. Participant 18 employed this method to determine if the electron densities rested in the correct location based on atomic electronegativity stating,

> *The red part is over the oxygen (referring to product options B and C), whereas in the equation given up top (referring to the reactants), the red part is over what I claimed as the oxygen molecule. So based on drawing in the lines and the structures. I'm thinking. I'm thinking it isn't options B or C.*

Several students elected to extend this approach to reason about the structural aspects of the product. Two (B and C) of the four answer choices contained a double bond, and participants inferred that if the double bond were to form from the reaction, the EPM would designate it as an area of high electron density with a red highlight. Participant 10 integrated this line of logic with what he knew about electronegativity, claiming that carbon−carbon double bonds are known to be electronegative.

Part I Theme II - Attraction and Electron Distribution

In determining the product of the reaction for the first part of the task, 14 of the participants (Figure 2) went beyond their initial structural analysis and employed the features of the EPM to reason about how the reactants would interact and the driving forces behind these interactions (See Supporting Information Table S3 for detailed quotes from each participant that fell under this theme). This process involved integrating their knowledge of electron densities' influence on charge, attraction, and stability. The concept of attraction was prevalent in participants' approaches as they reasoned with the colors of the electrostatic potential maps. Several participants correlated the colors of the EPM with partial charges, denoting blue as positive and red as negative. Upon deciphering these charges, Participant 1 reasoned, "So now my thought process is that the red would be attracted to the blue over here and the blue would be attracted to the red over here." Others applied their conceptual understanding of nucleophiles and electrophiles to the features highlighted in the EPM to determine where the two reactants would interact. In this process, the areas of highest and lowest electron densities were identified and denoted as the interaction points between the two reactants. Participant 14 followed this line of logic, reasoning "That low electron density area, I guess could be a spot where the higher electron density of the nucleophile on the larger molecule could come in and bond to it." For some participants, this method yielded deeper reasoning as to why electron density was a determining factor in reactions. Stability developed into an overarching theme in many of the participants' explanations as they tried to determine why the areas of highest and lowest electron densities would interact. Participant 10 concluded that the proximity of the high electron density areas produced instability and was the driving force for the reaction, stating "the product is going to be in an orientation so that the electronegative elements of the products are the farthest apart." Participants 2, 3, and 5 provided an alternative explanation founded in the partial charges that stemmed from high electron densities. These charges were equated with instability, and it was therefore determined that the electrons needed to be distributed to establish stability. Under this logic, students selected answer choices based on how the colors on the EPM were distributed throughout the product, acknowledging that the most stable product will also be the most neutral product. This phenomenon was observed in Participant 5′s approach as he reasoned "The more simple molecules combined, you can still see the redness, which is indicating that there may be two highly electronegative atoms together, but they're splitting those electrons with each other, so it's not as unstable as it was before."

Part I Theme III - Reactivity and Mechanistic Reasoning

As depicted in Figure 2, this theme was not observed in isolation but rather in combination with other themes. Once participants had predicted the provisional identities of components in the two reactants and postulated how they might interact, many began to use this foundation to reason mechanistically using the electron densities (See Supporting Information Table S4 for detailed quotes from each participant that fell under this theme). Participants 3, 4, and 9 began this process by integrating their chemical knowledge and using the electron densities to make predictions about the functionality of the molecular components. In these cases, leaving groups were identified through an association between high electron density (red color) and the group's probability of leaving. Participant 9 pin-pointed the role of stability in his explanation, clarifying "this one is like super red and so that probably, I'm guessing that that means it's a good leaving group because it's, it's probably like it can leave stable on its own." Through predicting the functionality of molecular components, participants were able to identify potential reaction steps and how they might influence electron densities in subsequent steps. Given the ambiguity of the task, answer choices and mechanistic explanations varied between groups of participants. The most common iteration of participants' mechanistic reasoning involved the notion that once the highly electronegative component departs, leaving behind an area of low electron density, another source of high electron density will come in as substitute. Participant 10 approached the task using this logic, stating "the element carrying the electron cloud would have left...but then that reasoning also goes both ways in the sense that there might be somebody coming in to fill that gap." Some students were more specific in their descriptions and assigned nucleophile and electrophile labels to each reactant. Identifying the nucleophiles and electrophiles appeared to be difficult for students, considering that both reactants had areas of high electron density (red color) and areas of low electron density (blue color). As a result, participants surveyed the products to delineate the reaction mechanism and identify the nucleophile and electrophile. Participant 14 offered one potential explanation, reasoning "But the smaller molecule is acting as a nucleophile...or acting as an electrophile, I guess, and taking a... Wait. No. A nucleophile and taking the hydrogen from the larger molecules." Through deductive reasoning, several participants were able to offer a prediction of the type of reaction occurring. Participant 4 postulated,

> *This guy (reactant on the right in the left image of Figure 1) is going to attack from the top... Because this guy (the red atom in the reactant on the left in the left image of Figure 1) is going to leave. So, this guy goes here kind of goes. It has negative part over here, so I believe it might be A and will be like an SN2 reaction.*

Participant 9 came to a different conclusion claiming that the reagents were undergoing an elimination reaction, citing the departure of a "big red group" and the addition of another molecule to promote stability.

Part II - Atomic Identities Revealed

As atomic identities were revealed in the second part of the task, 13 participants resorted to translating the EPMs into line angle representations and reasoned mechanistically without reference to the features of the electrostatic potential maps. After detailing a mechanism for the reaction, Participant 17 explained her approach:

> *I was mostly thinking of what we just recently learned, so elimination substitution. I was mostly thinking of substitution with that one... I was more looking at the arrangement of the molecules itself. For me personally, the EPM just kind of gets in the way.*

Participant 15 expressed similar difficulties with the EPM representation, stating "I have trouble visualizing them when they're in big blobs" and explained the utility of using learned mechanisms as an alternative, reasoning "I was trying to think of the mechanism because that helps me with figuring out products." Nevertheless, six students were able to draw connections to their initial answers in the first part of the task, implementing the information they pulled from the features of the electrostatic potential maps (See Supporting Information Table S5 for detailed quotes demonstrating the patterns discussed in this section). The revelation of the bromine atom proved to be the most influential piece of information, causing two participants to change their answers. Drawing from their prior knowledge of organic chemistry, participants recognized bromine as a good leaving group and used this information to reconsider the steps of the reaction. In the first part of the task, Participant 3 had predicted the red component of ethoxide would be the leaving group. However, once the atomic identities had been revealed he emphasized the impact bromines' departure would have on subsequent steps of the reaction detailing,

> *...knowing that bromine left helps a lot. In the beginning because I think. I thought that the 2nd molecule (oxygen on the ethoxide) was the leaving group, so knowing the formula and now the Br is in the first molecule, I know that electronegative portion left which caused the partially positive charge in the middle where the negative was able to attack it so it would change my answer. I think.*

Participant 10 also revised his answer, establishing that bromine does not interact with an electron deficient species after it leaves as he had previously predicted. He was, however, able to confirm his prediction of the overall reaction mechanism from Part I, substantiating that the bromine would be the electron dense group leaving while the double bond would be the structural agent filling the leaving group's void. Two participants (Participants 7 and 18) elected a more direct approach requiring less mechanistic reasoning and selected their answers by verifying whether the electron densities resided over the correct atom or structural feature. For participant 7, the association of the red color and the electronegativity of atoms was the most important factor, claiming that A was the best answer choice because the red resided over oxygen. Participant 18 elected a parallel method, reiterating the erroneous portrayal of the double bonds on the EPMs in options B and C explaining, "I'm going to eliminate option B and also option C just with the double bond forming and seeing that the red is mostly over that."

■ DISCUSSION

In this study, the utility of EPMs was explored in reaction tasks as a potential bridge between the driving forces behind electron movement in reactions and reaction outcomes. Participants responses indicated several avenues that show promise in promoting sense-making when students reason with EPMs in organic reaction tasks. Additionally, several unconventional applications of EPMs were uncovered that must be considered when discussing the utility of EPMs in the organic reaction curriculum. The significance of these findings as well as their implications are discussed below.

Part I - Theme I

The literature reports that when presented with novel tasks without an explicit solution, students' recognition of their unknowing is followed by a search for insight to formulate an answer and an explanation.[29] In this study, Part I put forth a novel prompt that tasked students with utilizing the features of EPMs without their respective atomic identities to predict the major products of a reaction. Participants began the sense-making process by acknowledging the foreignness of the task as they expressed their discomfort with the unmarked EPMs. Participants' search for insight produced systematic approaches to remove some uncertainty and determine the atomic components of the EPMs. The EPMs encouraged these participants to consider electron density's relation to the properties of molecular components. Seeing that there was no conventional way to identify the atoms in Part I, the participants invoked chemical properties, like electronegativity, and related the colors of the EPM to explain the patterns in electron density distribution. Interestingly, rather than referring to electronegativity as an inherent feature of elements, a struggle established in the literature,[30] students described the concept using colors in a relativistic manner, dependent on the electronegativity of adjacent atoms. In prior work, students predicted the location of intermolecular forces based on the magnitude of each atom's electronegativity values, indicating that electronegativity values were perceived as the direct driving forces behind molecular attraction.[30] The current study's outcomes suggest that EPMs may be a candidate for addressing this concept by portraying the physical implications of electronegativity values in molecules with multiple atom types.

For several participants, engagement with the task and their search for insight resulted in novel ideas that proved to be unproductive. Their approach to the task incorporated their conceptions of atomic and structural properties as they attempted to identify the answer choices that they felt contained an error in the location of electron densities on the EPM. This appeared to hinder students' progression in the sense-making process about reaction mechanisms as they ruled out potentially correct answer choices solely on the pattern of the EPM and not on the type of reaction occurring. Participant 18's response to Part 1 evidenced this phenomenon where his main reason for eliminating options B and C was the depiction of high electron density around the double bond. Rather than assessing the feasibility of the product options when considering the electron densities Participant 18 focused on whether the colors in the EPM accurately portrayed the electron densities of the molecule's structural components. That is, students saw this task as evaluating which product showed an accurate EPM instead of using the reactants to determine which product would result. Predictions of this

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nature, contingent on a cursory explanation of the EPM's explicit features, likely stem from participant's unfamiliarity with the representation. Throughout the study, students either expressed unfamiliarity or discomfort when addressing the EPMs. According to Talanquer,[31] when approaching novel tasks, students may rely on information that is readily accessible and familiar to decrease the difficulty of the task. In the case of this study, several participants followed this line of logic preventing the development of more comprehensive explanations for the formation of the product.

Part I - Themes II and III

As students continued in the sensemaking process, the EPMs appeared to promote connections between reactionary components and electron densities. Participants utilized the electron densities to predict the probability that an atom would depart from the molecule and be stable on its own. While electron density is not the sole predictor of leaving groups in organic reactions, students were forgoing memorized constructs and utilized chemical concepts to make assertions about the functionality of molecular components. The potential utility of EPMs in sensemaking about reaction mechanisms was further evidenced by students' predictions of nucleophiles and electrophiles and the driving forces behind their interaction. As discussed previously, nucleophiles and electrophiles are typically identified by students only after a mechanism has been assigned to a reaction.[8] While a set of participants still employed this retrospective method, several students utilized the electron densities of the EPMs to predict nucleophilic character and interaction sites between the reactants prior to determining the mechanism. As students continued in the sensemaking process, it appeared that rather than describing the reaction, they began to form arguments to support their assertions by utilizing the features of the EPMs. The EPMs elicited further explanation as students described the potential driving forces of the electron movement, associating the red color (high electron density) with instability and the reactants' tendency towards neutrality. Kozma and Russell[19] describe this phenomenon as an essential skill in representational competence, where representational features are levied to defend claims about chemical phenomena. Another skill outlined in the representational competence construct is the ability to explain chemical phenomena using representations.[19] When presented with the product choices, many participants attempted to think retrospectively about the electron densities to ascertain the reaction mechanism of the reactants that would produce each product. Rather than focusing on memorized reaction mechanisms, students used intuitive reasoning to predict how the electron densities would interact to produce the final product. Therefore, in contrast to the current literature on students' explanations of reaction mechanism,[3,5,12] participants were attributing a physical meaning to electron movement in reactions. This finding suggests that the integration of EPMs can potentially provide students with information that encourages them to think about the chemical principles governing electron movement to make informed predictions about the steps in a mechanism.

Part II

The disclosure of the atomic identities prompted participants to translate the EPM to line-angle representations to establish familiarity. Once participants had constructed the line-angles from their respective EPM, a clear divide arose, where a large proportion of students utilized a product-oriented approach, and neglected the features of the EPMs, while a small group of students employed a more process-oriented approach, relating the features of the EPM to the newfound atomic identities. Students utilizing a product-oriented approach focused on determining the correct product and were less concerned with the causal reasoning for the reaction.[32] Consequently, these participants did not attempt to reconcile their answers from Part I to the newfound atomic identities and reverted to memorized elimination and substitution mechanisms. This was evident in Participants 15's explanation, where he emphasized the advantages of using mechanisms to determine products. Conversely, the group of students that used process-oriented approaches were more concerned about the properties and reactivity of the reactants and how they relate to the overall reaction mechanism.[33] These participants related the properties of the atoms relayed in the EPM to the mechanistic steps of the reaction.[34] Two participants in this group even revised their previous answers through connections they made between the atomic identities and the electron densities shown in the EPMs.

These findings suggest that while EPMs can encourage students to critically think about the reactions they have memorized and articulate the chemical principles contributing to the pattern of their mechanisms, students tend to default to the method they are most comfortable with when given the opportunity.[31] In Part I of the task, students were only given the features of the EPM to construct an answer and could not rely on their previously memorized mechanisms. Despite expressing discomfort, participants implemented varying sense-making strategies that resulted in predictions founded on their conceptions of different chemical principles. The majority of these sense-making strategies, however, were absent when transitioning to Part II of the task, as students used atom identities to establish an answer, following reaction mechanisms that were explicitly modeled during instruction. This change in approach from Part I to Part II speaks to the utility of tasks that provide students with the freedom to explore the conceptions they hold without the constraints of an explicit solution. As evidenced in previous studies and Part I of this study, uncertainty can be a motivator for students to engage in the sense-making process about chemical phenomena.[29] Uncertainty is a cornerstone in scientific practice and is a driving force for inquiry within the classroom.[35,36] Nevertheless, as depicted in participants' avoidance of the EPMs in Part II, students may refrain from uncertainty when another path to the solution is available, in fear of producing an incorrect answer.[29] Familiarizing students with EPMs may lessen some of this uncertainty and encourage students to use the electrostatic features in tandem with their existing mechanistic knowledge when solving reaction tasks. Methods to introduce EPMs in organic reaction curriculum are discussed below.

■ IMPLICATIONS

The findings from this work uncover the utility for EPMs in evoking students to consider the electrostatic factors that play a role in deciding reaction mechanisms. Therefore, there may be benefits to be gained by including EPMs as a representation in instruction. As noted by Flynn and Ogilvie who advocate for a pattern-based understanding of reactions, visualizing reactivity as patterns of electron movement is an effective way of predicting and explaining new reaction mechanisms.[13] The introduction of EPMs early in the organic chemistry

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course can familiarize students with different patterns of electron movement that can be used to understand some of the key factors dictating unfamiliar reaction mechanisms. One potential path instructors could take when implementing EPMs is incorporating reaction problems similar to Part I of the task discussed in this study. If instructors wish to provide students the opportunity to make predictions and formulate explanations concerning reactivity prior to exploring a mechanism, they can present a task where EPMs are provided, and atomic identities are concealed. The nature of this intervention can focus students' attention on the electrostatics guiding the reaction and affords the instructor the opportunity to build on ideas that may arise. If an instructor chooses to subsequently reveal the atomic identities, as seen in this study, they need to also consider that this may work against the potential of the open-ended task and indirectly communicate to students that no matter the nature of the task, there is always one "correct" solution to a chemistry problem. This approach may be problematic as students may see little value in partaking in the sensemaking process. An alternative method for implementing EPMs involves presenting a reaction mechanism and, thereafter, providing the associated EPMs with atomic identities to emphasize the electrostatic principles responsible for the reaction. If instructors wish to further encourage students to consider electrostatics in cases where EPMs are not provided, they can incorporate instruction where students practice translating line angle structures to EPMs, either via creating an EPM by hand or via introduction to software that creates EPMs. This intervention could get students comfortable with visualizing electron densities and mapping them onto non-EPM representations to assess how electronics might play a role in dictating the course of a reaction.

While the results from this study highlight the utility of EPMs in sense-making about reaction mechanisms, it is equally important for instructors to disclose the limitations when implementing these representations. Throughout this study, students made assertions based on the EPMs that were inaccurate of the reaction occurring. Therefore, it should be established that the features of EPMs cannot be used in isolation to decide the overall course of reaction mechanisms, as noted by Participant 10 who realized his prediction of a later step in the mechanism was incorrect once the atomic identities were revealed. Most reactions are far more complicated and involve a variety of factors that are not directly observable in EPMs.[37] Consequently, students should receive instruction on how the features of EPMs can be used alongside other chemical principles to explain the course of a reaction mechanism. Additionally, students should be informed when the EPMs presented are meant to be accurate models of the relative electron density and students do not need to evaluate the accuracy of EPMs as part of the task.

LIMITATIONS

The research conducted in this study had several limitations that must be taken into consideration when assessing the outcomes. Due to the small sample size as well as the specific context in which the study took place, claims regarding the generalizability of the findings are limited. Nevertheless, the similar themes uncovered at both institutions included in this study further support the potential utility of EPMs within the organic chemistry curriculum. It is important to note, however, that the task where the data in this study originates was part of a broader interview exploring how students work with EPMs in different types of tasks. It is unknown if students' exposure to previous tasks in the interview involving EPMs had any impact on how they utilized the EPMs in the presented reaction task. Additionally, only one reaction type was explored in this work. Further research is needed to ascertain if students' sense-making strategies with EPMs differ when alternative reaction types are assessed. Lastly, the potential for positive selection must be acknowledged. Participant selection parameters were dependent on if a student replied to the initial announcement and showed interest in participating. Therefore, it is possible that the participants selected do not fully represent the student population of organic chemistry students.

CONCLUSION

Reaction mechanisms are a foundational topic in organic chemistry that has proven difficult for students. The current literature reports a trend in student use of memorization to circumnavigate this difficulty and determine the outcome of reactions. This study assessed the utility of EPMs in promoting sense-making in reaction tasks and uncovered several ways students' reason with the features of EPMs to ascertain and explain reaction outcomes. Students utilized the electron densities represented by colors in the EPM to predict the identity and functionality of molecular components. When predicting the products of the reaction, participants found further use in the electron densities, relating them to reactivity and locating reaction sites based on charge and stability. Participants were even found predicting reaction mechanisms based on the interactions between the electron densities. These findings suggest a potential utility for EPMs in communicating some of the chemical principles governing organic reactions and show promise for enhancing student usage of sense-making when approaching reaction tasks.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00696.

Codebook and detailed quotes from participants categorized by theme (PDF, DOCX)

AUTHOR INFORMATION

Corresponding Author

Scott E. Lewis – *Department of Chemistry, University of South Florida, Tampa, Florida 33620, United States;* orcid.org/0000-0002-6899-9450; Email: slewis@usf.edu

Authors

Isaiah Nelsen – *Department of Chemistry, University of South Florida, Tampa, Florida 33620, United States*

Melissa Weinrich – *Department of Chemistry and Biochemistry, University of Northern Colorado, Greeley, Colorado 80639, United States;* orcid.org/0000-0002-7370-3933

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.4c00696

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