

Affordances of Electrostatic Potential Maps in Promoting Use of Electronic Features and Causal Reasoning in Organic Chemistry

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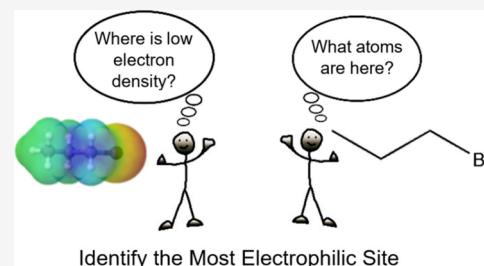
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ABSTRACT: Instructional materials in organic chemistry include a wide variety of representations, such as chemical formulas, line-angle diagrams, ball-and-stick diagrams, and electrostatic potential maps (EPMs). Students tend to focus on explicit features of a representation while they are reasoning about chemical concepts. This study examined the affordances of electrostatic potential maps in students' approaches when the maps were integrated into four foundational organic chemistry problems using an experimental design approach. First-semester organic chemistry students were surveyed from two different institutions, where they made predictions and explained their reasoning behind identifying an electrophilic site, predicting the product, selecting the faster reaction, and classifying a mechanism. Students were randomly assigned to one of four surveys that differed by the representation they were given for the prompts: chemical formula, line-angle diagram, ball-and-stick diagram, and EPM. Responses from students with EPMs were analyzed and compared to responses from students with the non-EPM representations. Results indicated that students with EPMs had higher performance depending on the problem. They were also more likely to cite electronic features such as electron density, nucleophilicity, etc., and were more likely to use causal reasoning in their explanations. This study offers evidence in support of affordances of EPMs in promoting students' use of electronic features and causal reasoning. This evidence adds to the chemistry education literature by offering a potential means for promoting students' use of electronic features and causal reasoning by incorporating EPMs into assessment items. Implications for instruction include using EPMs in both instruction and assessment as a tool to help students build skills around invoking electrostatics and causal reasoning to solve problems in organic chemistry.

KEYWORDS: Chemical Education Research, Organic Chemistry



INTRODUCTION

Due to the abstract nature of organic chemistry, representations depicting molecules at the submicroscopic level are prevalent.^{1–3} Instructional materials include a wide variety of representations, such as chemical formulas, line-angle diagrams, ball-and-stick diagrams, and electrostatic potential maps (EPMs). Students thus need to become adept at using representations and describing phenomena at the submicroscopic level.^{4,5} However, students might not have interacted with some of these representations (e.g., line-angle and EPMs) in courses prior to organic chemistry.² Moreover, each representation comes with its affordances and limitations depending on the task at hand.⁶ This study examines the affordances of electrostatic potential maps in students' approaches when the maps are integrated into four foundational organic chemistry problems using an experimental design approach.

A chemical formula is easily generated and gives information (e.g., atom identity) about the molecule quickly. A line-angle diagram, which is a common way of depicting a molecule in organic chemistry, is easier than some other representations to generate and manipulate. Ball-and-stick images also depict the molecular geometry. However, these three representations

might limit students' interpretation of electronic activities that are important to explain chemical phenomena in organic chemistry, and students might over rely on surface features to make interpretations about electronic activities.^{1,7,8} Recognizing this limitation, EPMs have been promoted for describing and studying electronic activities.⁹ EPMs explicitly depict the electron density of a molecule using color, with red indicating a highly electron-dense area and blue indicating a low area. In contrast, line-angle diagrams implicitly depict electron density, requiring the student to use element symbols and electronegativity values to predict if an uneven charge distribution occurs between two bonded atoms within a molecule. Compared to other representations, EPMs offer a distinct view of electron density, influencing how students conceptualize and reason about chemical properties, interactions, and electronic features.³ When students were given both ball-and-stick and

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EPM representations,¹⁰ it was found that successful students spent more time looking at the EPM representations than less successful students while solving problems in organic chemistry. Additionally, instructing students in electron density via EPMs can improve their understanding of electronic features in organic chemistry.^{11–13} However, organic chemistry textbooks provide minimal conceptual support for EPMs, which also appear less in end-of-chapter problem sets.^{2,3} This lack of support restricts students' interpretation and use of EPMs when reasoning about a chemical phenomenon.² Thus, it is important to understand the role EPM representations play in influencing students' thought processes.

We hypothesize that EPMs, by making the abstract concept of electron density explicit, can help deepen students' understanding of molecular interactions and properties. Although researchers have investigated students' reasoning on a wide variety of topics in organic chemistry using line-angle representations,^{14–26} literature has lacked research voicing how students treat EPMs.^{3,9,10} Thus, this study examined the influence of EPM and non-EPM representations by investigating how these representations contributed to the types of features (e.g., structural and electronic) and reasoning students focused on while solving problems in first-semester organic chemistry. The ability to use representations (i.e., its features) to make predictions, draw inferences, and/or solve problems (i.e., reasoning) is one of the representational competence skills.⁴ Representational competence is an essential skill in organic chemistry,^{1,27} which is defined as interpreting chemical meaning through the use of representations and utilizing those interpretations to explain structure–property relationships.^{4,28} This study focused on examining features present when students reason about fundamental concepts in organic chemistry with EPM and non-EPM representations. The fundamental concepts were identifying the electrophilic site, predicting the product of a reaction, selecting a faster reaction, and categorizing a mechanism of a reaction. Those concepts are included in anchoring concepts within the content of organic chemistry.²⁹ Identifying the electrophilic site is defined under the anchoring concept of atom, while other concepts related to different aspects of reactions are emphasized in chemical reactions. Through identifying affordances of EPMs in terms of features present and reasoning enacted while students solve those fundamental concepts, we aim to aid instructional strategies in organic chemistry and contribute to the broader discussion in enhancing students' representational competence.

THEORETICAL FRAMEWORK

This work was built upon a model of how students interpret representations, which is representational competence.^{28,30,31} The model describes three major intersecting factors: the features of the representations, students' prior conceptual knowledge relevant to the representation, and students' cognitive processes and skills required to make sense of the representation. Features of the representation are defined as visually explicit characteristics of the representation. Each of these factors would be influenced by the task students engage in when using the representation. Based on this model, we expect the features of the representation to influence both the concepts that students use and cognitive processes while solving problems.

Students' prior conceptual knowledge relevant to the representation was defined using the granularity framework.^{16,18,27} When students construct explanations, they do so

at varying levels, including structural, electronic, energetic, or phenomenological levels. The structural level consists of structural features of atoms and molecules.¹⁶ For instance, the number of α -carbon substituents and atom size might be relevant structural features when students compare the plausibility of alternative mechanisms for given reactants and the rates for presented reactions.¹⁶ The electronic level refers to descriptions of electronic features of molecules and atoms such as electronegativity or partial charge.¹⁶ The energetic level focuses on thermodynamic and kinetic considerations. The relative stability of carbocations in a transition state and the calculation of transition state energies for a specific mechanism are examples of energetic considerations. Chemical phenomena depend on interactions among the structural, electronic, and energetic properties of atoms and molecules. Therefore, the phenomenological level captures descriptions of the chemical phenomena. For instance, within the acid–base context, structural, electronic, and energetic features can be used to explain acid and base strength. Students may focus on some of these features over other features; thus, students may productively answer a question without using all levels of granularity.

Students' cognitive processes to make sense of the representation can be inferred from students' explanations of chemical phenomena. Students' cognitive processes were defined using the modes of reasoning framework.^{16,23,32} Though there are varying terms and definitions in the literature for modes of reasoning, a consensus in the literature argues for promoting students' causal reasoning,^{33,34} and thus, this study distinguishes causal versus noncausal reasoning. Causal reasoning is evident when a student evokes a cause-effect connection between an underlying chemistry property and the effect of this property, that is, the “why” behind a chemical phenomenon. For example, a student can generate a causal explanation for the mechanism of a condensation reaction of a carboxylic acid and an alcohol by describing the attraction of the partially negative oxygen in the acid to the partially positive hydrogen in the alcohol. In contrast, noncausal reasoning may include students redescribing the problem (e.g., propene reacts with bromine to produce a halohydrin) or using memorized rules (e.g., since acetic acid can perform resonance, it is more acidic than ethyl alcohol). Noncausal reasoning includes both descriptive reasoning (where students redescribe the problem without referring to causes) and relational reasoning (where students use rules to arrive at an answer without referring to causes). Noncausal reasoning can be productive since these are quick reasoning processes,³⁵ but it is also important for students to use causal reasoning.

This study seeks to examine whether the use of EPMs, which make electronic density explicit, influences the granularity and modes of reasoning in students' explanations compared to other molecular representations. More specifically, this study pursues the following research questions.

RESEARCH QUESTIONS

RQ1: How do EPMs influence students' success when solving the following organic chemistry problems: identifying an electrophilic site, predicting a product, selecting a faster reaction, and classifying a mechanism?

RQ2: What is the granularity of features cued for students when given EPMs compared to other representations with these organic chemistry problems?

Table 1. Example of Representations and Questions Given to Students in the Survey^a

Identify electrophilic site	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$	
Predict the product	
$\text{CH}_3\text{CHCH}_2 + \text{Br}_2 + \text{H}_2\text{O} \rightarrow$	
Select the faster reaction (see Supporting Information for all representations)	
Case 1 $\text{CH}_3\text{CH}_2\text{O}^- + \text{CH}_3\text{CH}_2\text{CH}_2\text{Cl} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{Cl}^-$ Case 2 $(\text{CH}_3)_2\text{CHS}^- + \text{CH}_3\text{CH}_2\text{CH}_2\text{Cl} \rightarrow (\text{CH}_3)_2\text{CHSCH}_2\text{CH}_2\text{CH}_3 + \text{Cl}^-$	
Classify the mechanism	
$(\text{CH}_3)_2\text{CHCHBrCH}_3 + ^-\text{OCH}_2\text{CH}_3$	

^aStudents saw the chemical formula and the representation they were assigned, but not all representations.

RQ3: What are students' reasoning processes with these problems when given EPMs compared to other representations?

METHODS

Participants and Context

First-semester organic chemistry students at two doctoral granting universities in the southeast (University A) and midwest (University B) regions of the U.S. participated in this study. The textbooks (Klein fourth edition and Carey 11th edition) for these courses presented all four representations used in this study: chemical formula (CF), line-angle diagram (LA), ball-and-stick images (BS), and EPMs. One instructor said that they did not use BS or EPM representations in his lecture. The other instructor used BS early in the semester but did not use them throughout. Although this instructor did have EPM representations present throughout the semester, both institutions relied heavily on the CF and LA representations for instruction and assessments. Data were collected via surveys which were offered to all students as an extra credit opportunity and occurred after their in-term exam on the topics investigated. We analyzed 158 student responses (80 from University A and 78 from University B). The Institutional Review Board of University B approved this research. Both institutions signed an agreement, placing University B as the designated IRB responsible for overseeing the project. Response rate and more information about the institutions can be found in the [Supporting Information, section SI.A](#).

Data Collection

Survey prompts were designed by researchers with expertise in chemistry education research and organic chemistry instruction and piloted in interviews with first-semester organic chemistry students from the semester prior to data collection to ensure that questions were being interpreted by students as intended by the

researchers. Modifications were made to the questions to prompt students to explain why they answered the way they did and what about the representation made them predict their answer. Instructors of each course reviewed the survey to ensure that the content and difficulty of each item aligned with course expectations.

Four surveys were used to collect data, and students were randomly assigned to one survey type following an experimental design. All four surveys included CFs, but they varied by adding a different representation type alongside it (LA, BS, EPM, or just CF). Each of these were static representations and could not be rotated. Each survey used the same set of questions, which were to identify the electrophilic site, predict the product, select the faster reaction, and classify a mechanism (Table 1). After each question, students were also asked to explain why they selected their answer and what about the representation made them select their answer. The survey was administered using learning management software, and students at University A were given a week to submit the survey, while at University B the survey was done in class. A full version of the survey can be found in the [Supporting Information, section SI.B](#). An example of an expert response to these problems can be found in the [Supporting Information, section SI.C](#).

Data Analysis

Data analysis focused on students' performance, granularity of features cited, and the type of reasoning used. When analyzing performance (RQ1), we identified the accuracy of the response dichotomously. The percent correct for each question was compared based on survey type as using EPM or non-EPM (CF, BS, or LA). This comparison was done to compare representations with explicit versus implicit depictions of electronics.

During analysis of granularity (RQ2) and modes of reasoning (RQ3), we focused on responses to the prompts, including "why" and "what" questions. Each member of the research team

Table 2. Coding Scheme on the Granularity of Electronic Features Students Paid Attention to, Including a Description and Example of Each Code

Code	Description (Student Mentioned...)	Example
Electronic entity	An entity such as a lone pair, electrons, valence electrons, an octet	It can easily accept a pair of electrons
Electronegativity	electronegativity of an atom	Bromine is an extremely electronegative atom
Charge	Charge or partial charge	The oxygen has lone pairs due to its negative charge
Polarity	Polarity or dipole	When a molecule is higher polarity, it makes the reaction quicker
Electron density	Electron density, more electrons in an area, electron rich or deficient	Electrophilic means that the area enjoys having a high density of electrons
Electrophilicity	Electrophile or strength of electrophile *Not applicable to q2–4	The electrophilic area is opposite the bromine at a secondary carbon
Nucleophilicity	Nucleophile or strength of nucleophile	I used the alkene in CHCH ₂ as the nucleophile to attack the Br ₂ and form a bromonium intermediate

Table 3. Coding Scheme on the Granularity of Structural Features Students Paid Attention to, Including a Description and Example of Each Code

Code	Description (Student Mentioned...)	Example
Size	Size of an atom or molecule; smaller/bigger	Br will attack the carbon double bond, and because it is so big, it will sit on both carbons
Bond type	Bond order, number or type of bonds (single, double, sigma), name (alkene), or hybridization	Bromine is added across the π -bond
Connectivity	How atoms are connected (next to each other), distance between atoms, branching, 1°, 2°, 3° carbon	O [−] is on a primary carbon
Orientation	Angle of bonds, shape of a molecule, stereoisomers, atom or bond pointing a specific way	The two Br would be added anti to each other on the opposite sides
Steric hindrance	Steric hindrance; sterically hindered	Case 1 has a primary structure, whereas Case 2 has a secondary; therefore, Case 1 has less steric hindrance

Table 4. Coding Scheme on Student Reasoning, Including a Description and Example of Each Code

Code	Description	Example
Type of Reasoning	The Student...	
Noncausal (descriptive)	Redescribed the phenomenon or problem. Tended to focus on surface features.	Because it is attached to 2 different carbons. From there, the carbon to the left is connected to 3 hydrogens, and the carbon on the right is connected to a Br and 2 hydrogens.
Noncausal (relational)	Used rules, correlations, or heuristics (e.g., more A = more B) to explain phenomenon.	I believe the area near or at bromine to be the most electrophilic, as it is the most electronegative atom on the molecule.
Causal	Used causal arguments to explain phenomenon or gave explanations of rules used.	Br is electron rich, resulting in the partial negative dipole, and pulls the electron density toward it, making the α -carbon electron deficient; electrophilic.

individually reviewed the survey data and developed an initial codebook for the features students used. The features were then used to identify the granularity within each response. A separate review of the data was conducted to develop a codebook on students' modes of reasoning. Based on the review, the team decided on two deductive coding schemes aligned with previous literature: the granularity of the features students focused on¹⁶ and the modes of reasoning.²³ Students mainly used features within electronic and structural levels of granularity, and the codebook was focused on those features (Tables 2 and 3). This decision was made because other types of granularity, such as energetic levels, appeared infrequently in the data. Of the 158 participants across the four representations, only 12 participants' writing could be coded as energetic. For example, participant 12 with EPMs wrote, "I think it makes sense that a smaller molecule would lead to a lower energy product, which creates a more stable molecule as well as more favorable because there's less energy being used." Previous studies have shown that students need more support to reason at the energetic level.^{19,36} Using the modes of reasoning framework, students' responses were coded for three types of reasoning: descriptive, relational, and causal (Table 4). Descriptive reasoning was infrequently used, so descriptive and relational were grouped together as noncausal reasoning. Additionally, this decision was made since causal

reasoning can be important for student understanding.²⁴ After completion of the coding scheme, at least two researchers independently coded data for reasoning and features. All discrepancies in coding were discussed, and we reached a consensus code assignment. Comparisons of the percentage of responses coded as electronic features, structural features, and causal reasoning for EPM participants versus non-EPM participants were conducted with a chi-square test. As an exploratory study, the differences will be characterized by effect sizes (Cohen's w) rather than statistical significance. Cohen's w values of 0.1 indicate a small effect and 0.3 a medium effect.³⁷ As a result, this work will generate hypotheses for further testing and will not make claims about the extent the results generalize to a broader population of students.

RESULTS

RQ1: How Do EPMs Influence Students' Success When Solving the Following Organic Chemistry Problems: Identifying an Electrophilic Site, Predicting a Product, Selecting a Faster Reaction, and Classifying a Mechanism?

Students in this study who interacted with EPMs selected the correct answer more than students who were given different representations in all prompts except predicting the product

(Table 5). The most prominent difference, with a small effect size, appeared when selecting the faster reaction (16.2%), while

Table 5. Correct Prediction for Each Prompt Type of Students with EPM and Non-EPM

Prompt Type	Students with EPM (<i>n</i> = 40)	Students with Non-EPM (Chemical Formula, Line-Angle, or Ball-and-Stick) (<i>n</i> = 118)	Chi-Square and <i>p</i> Values	Effect Size (Cohen's <i>w</i>)
Identify electrophilic site	35.0%	33.1%	$X^2 = 0.051$ $p > 0.05$	$w = 0.018$
Predict product	15.0%	22.0%	$X^2 = 0.915$ $p > 0.05$	$w = 0.076$
Select the faster reaction	45.0%	28.8%	$X^2 = 3.545$ $p > 0.05$	$w = 0.150$
Classify mechanism	37.5%	29.7%	$X^2 = 0.849$ $p > 0.05$	$w = 0.073$

classifying the mechanism (7.8%) and predicting the product (7.0%) also approached a small effect size. The difference in identifying the electrophilic site (1.9%) was negligible.

RQ2: What Is the Granularity of Features Cued for Students When Given EPMs Compared to Other Representations with These Organic Chemistry Problems?

Students with all types of representations in this study used electronic (Table 2) and structural features (Table 3).

Electronic Features. For each of the four prompts, more students using EPMs wrote about electronic features while explaining their response than students with a non-EPM (Table 6). The trend was consistent with approximately a small effect

Table 6. Electronic Features Cued for Each Prompt Type for Students with EPM and Non-EPM

Prompt Type	Students with EPM (<i>n</i> = 40)	Students with Non-EPM (Chemical Formula, Line-Angle, or Ball-and-Stick) (<i>n</i> = 118)	Chi-Square and <i>p</i> Values	Effect Size (Cohen's <i>w</i>)
Identify electrophilic site	97.5%	88.1%	$X^2 = 3.049$ $p > 0.05$	$w = 0.139$
Predict product	59.0%	40.2%	$X^2 = 4.181$ $p < 0.05$	$w = 0.164^*$
Select faster reaction	72.5%	63.6%	$X^2 = 1.061$ $p > 0.05$	$w = 0.082$
Classify mechanism	87.5%	79.7%	$X^2 = 1.225$ $p > 0.05$	$w = 0.088$

size, and the largest difference (18.8%) was predicting the product, which was also statistically significant ($X^2 = 4.181$, $p < 0.05$, $w = 0.164$).

Students used electronic features such as areas of high and low electron density, properties of nucleophiles, electrophiles, and polarizability to build explanations while answering the prompts. Students with EPMs varied in how they used electronic features to explain their reasoning with exemplar quotes provided in Table 7. These quotes are meant to characterize how students with EPMs cited electronic features beyond the proportions in Table 6. A closer look at the student explanations offers support for the following: (1) these students related the color pattern in EPMs that depict high and low electron density areas to

Table 7. Explanations from Students Citing Electronic Features When Given EPM or Non-EPM Representations (Electronic Features Are Bolded)

Prompt Type	Electronic Features	
	Students Quotes with EPM	Students Quotes with Non-EPM
Identify electrophilic site	E1: Because the blue is red and means it has a higher electron density , which hence would make it more electrophilic than the other side or the middle would be. The electrons and everything are pulling and moving toward one side, which is the right side. E2: Electrophilic sites occur where there are areas of low electron density , and according to the key, blue is the area with the lowest electron density . E3: The red areas in CH_3CHCH_2 indicated that the π -bond would act as a nucleophile . E4: The bromine is already electron rich due to its polarizability . When one bromine attaches to the double bond, the other bromine becomes less electron rich . Then the water, which is now more electron rich , comes and replaces the second bromine. This makes sense due to the coloration on the molecules. E5: Case 2 had a larger red electron cloud on the sulfur than the oxygen in Case 1. E6: Negative regions will be attracted to the positive regions.	N1: The middle is the most electrophilic because it has the lowest electron density . N2: Since the Br is very electronegative , it will not want to form bonds with carbon, so H–O–H will instead bind to the carbocation , forming an alcohol at the secondary carbon. N3: It is an $\text{S}_\text{N}2$ reaction because Cl is a good leaving group on a primary α -carbon and ethoxide is a strong nucleophile and strong base, and Case 2 is almost the same but the S is larger than oxygen, so it is polarizable . It is also not a bulky base. N4: Ethoxide is a good nucleophile and strong base. Br leaving would also form a secondary carbocation which, in all, favors the E2 mechanism.
Predict product		
Select the faster reaction		
Classify mechanism	E7: The electrophilic area is opposite the bromine at a secondary carbon. The blue area is opposite the bromine, while the oxygen is red, so the areas should attract. E8: Oxygen is electronegative and polar with a negative sign , which shows to be strong nucleophilic that could form bonds.	

attraction, polarizability, nucleophilic/electrophilic properties, and leaving group, and (2) students introduced electronic behavior in their responses using electronic features, despite this behavior being an implicit property in the representation. Two students, when given EPMs, made a connection between color and electron density, but the student in E1 (the E prefix denotes a student who received an EPM) mentioned pulling of electrons, while the student in E2 mentioned a relationship between electrophilicity and electron density without offering information on the movement of electrons. Furthermore, students in E3, E5, and E7 mentioned color without relating it to electron density. These students mentioned the color and related it to the “ π -bond” (E3), the size of the “red electron cloud” (E5), or how the “areas should attract” (E7). This supports that students tend to cite explicit features, and since EPMs show color explicitly, instances of citing color without relating it to electron density were observed.

Overall, students with non-EPMs used electronic features in a similar way to students with EPMs. They also discussed areas of high and low electron density (N1), electrophiles and nucleophiles (N4), and polarizability (N3). The N prefix denotes a student who received a non-EPM representation. One main difference in how non-EPM students were cued to electronic features was that they could not use color since electron density is not depicted using color in the non-EPM representations, and thus, electron density had to be inferred by the students. To do this, they often used electronegativity or charge (N2 and N4). These are properties also used by students with EPMs (E6 and E8). Even though electronic features were manifested in a similar fashion with students with non-EPMs, it occurred less often than did students with EPM.

Structural Features. For each prompt, more students with non-EPMs cited structural features (Table 8), with a medium

Table 8. Structural Features Cued for Each Prompt Type for Students with EPM and Non-EPM

Prompt Type	Students with EPM ($n = 40$)	Students with Non-EPM (Chemical Formula, Line-Angle, or Ball-and-Stick) ($n = 118$)	Chi-Square and p Values	Effect Size (Cohen's w)
Identify electrophilic site	20.0%	61.9%	$X^2 = 20.956$ $p < 0.05$	$w = 0.364^*$
Predict product	62.5%	71.2%	$X^2 = 1.054$ $p > 0.05$	$w = 0.082$
Select the faster reaction	62.5%	77.1%	$X^2 = 3.271$ $p > 0.05$	$w = 0.144$
Classify mechanism	62.5%	70.3%	$X^2 = 0.849$ $p > 0.05$	$w = 0.073$

effect for identifying electrophilic site, 61.9% with non-EPMs versus 20.0% with EPM ($X^2 = 20.956$, $p < 0.05$, $w = 0.364$), and approximately small effect sizes on the remaining three. Thus, the influence of non-EPM representations on citing structural features was observed here when compared to EPM.

When not using electronic features, students with non-EPM representations used structural features with exemplar quotes shown in Table 9. Structural features described bonding properties, such as the number of bonded carbons or type of carbon (N6, N8, N10, N11, and N12) and type of bond (N7). Other features included the identity of the atom (N5) and the size of the atom (N9). These students offer support to the claim that non-EPM representations cued structural features that

Table 9. Explanations from Students Citing Structural Features When Given EPM or Non-EPM (Structural Features Are Bolded)

Prompt Type	Students Quotes with EPM	Structural Features	Students Quotes with Non-EPM
Identify electrophilic site	E9: As the end is all by itself, and it [Br] was given no other carbons or hydrogens to be able to have on itself.		N5: The line-angle formula helped predict my answer because there is only one C bonded to something else besides a C or H atom. N6: I believe that electrophilic means that it is the area that is most readily bonded to. Therefore, I chose the area with [the] highest amount of carbon bonded to it.
Predict product	E10: Why I predicted this product is because I recall when there are multiple substance for one thing, in this case bromide , it takes “over” in a sense where the double bond is.		N7: The double bond between the second and third carbon was an indication that the reaction was going from an alkene to an alkane, and following Markovnikov's rules, this is where I came to my conclusion. N8: This model demonstrates that the middle carbon (Carbon 2) is the more substituted carbon and that is why the OH gets attached to it. The model also shows that Carbon 3 is the less substituted carbon , and that is why the Br gets attached to it.
Select faster reaction	E11: I predicted that this reaction would proceed faster than the other because the smaller oxygen atom has less steric hindrance.		N9: The second reaction is faster because of the larger sulfur atom that can bond easier to the chlorine atom. N10: Although a bigger atom is more stable, I chose Case 1 because of steric hindrance. The less carbons around, the quicker the reaction will happen.
Classify mechanism	E12: The molecule is a secondary structure , which eliminates the possibility of S_N2 , so it must be E2.		N11: It is secondary , which is hard to determine S_N1 versus S_N2 , but the second molecule does not have a protonated molecule (if it did it would be OH, H attached to it), meaning S_N2 . N12: At first, I thought it was S_N2 , but then after looking for a while, I believe the carbon is either tertiary or secondary, so the E2 reaction would be the major.

Table 10. Causal Reasoning Used for Each Prompt Type for Students with EPM and Non-EPM

Prompt Type	Students with EPM	Students with Non-EPM (Chemical Formula, Line-Angle, or Ball-and-Stick)	Chi-Square and <i>p</i> Values	Effect Size (Cohen's <i>w</i>)
Identify electrophilic site	62.5% (<i>n</i> = 40)	37.9% (<i>n</i> = 116)	$\chi^2 = 7.279$ $p < 0.05$	$w = 0.216^*$
Predict product	38.5% (<i>n</i> = 39)	24.5% (<i>n</i> = 110)	$\chi^2 = 2.755$ $p > 0.05$	$w = 0.136$
Select faster reaction	62.5% (<i>n</i> = 40)	54.9% (<i>n</i> = 113)	$\chi^2 = 0.702$ $p > 0.402$	$w = 0.068$
Classify mechanism	46.2% (<i>n</i> = 39)	22.5% (<i>n</i> = 111)	$\chi^2 = 7.891$ $p < 0.05$	$w = 0.229^*$

centered around bonding properties and describing the characteristics of the atom.

To show how bonding properties were used in the explanations, students in N6, N8, N11, and N12 focused on the “amount of carbon” or the number of substituents describing “more or less substituted carbon” or “secondary or tertiary carbon.” These terms signify students’ justifications based on the α -carbon’s bonding properties. For example, the student in N8 described their reason for the OH and Br bonding to particular carbons because of the substitution at those carbon sites. Another student used the same strategy in N11 to describe where the OH would attach. The student in N10 stated that fewer carbon atoms around will help in the reaction proceeding quicker. In N7, the student concentrated on identifying the type of bond present in the molecules, specifically recognizing a double bond helped them determine the reaction pathway that the molecules would follow, aiding in their conclusions.

Another structural feature involved characteristics of the atoms. The student in N5 prioritized identifying atoms, while students in N9 and N10 emphasized atomic size. The student in N5 explained that they identified the electrophilic site by noting the connected atom, specifically finding a carbon atom that was “bonded to something else besides a C or H atom.” Here, the student related the identity of the atom as the pattern to focus on while describing the electrophilic site. In N9, the student described how a larger atom causes a faster reaction, and in N10, the student described how the bigger atom would be more stable.

Structural features were also manifested in similar ways for students with EPMs, including using the number of atoms or substituents (E12), atom identities (E9), atom size (E11), and bond types (E10).

RQ3: What Are Students Reasoning Processes with These Problems When Given EPMs Compared to Other Representations?

Students’ reasoning patterns were categorized as causal or noncausal (descriptive and relational) reasoning following the coding described in Table 4. Students with EPMs were more likely to provide explanations using causal reasoning than students with non-EPMs across every prompt, with the percents tallied in Table 10. The influence of students with EPMs using causal reasoning more than students with non-EPMs was seen with identifying an electrophilic site and classifying a mechanism, both with small to medium effect sizes, and a small effect size was observed for predicting the product.

Exemplar responses of students using noncausal or causal reasoning are presented in Table 11.

Noncausal Reasoning. This type of reasoning occurred with all types of representations but occurred more often with non-EPM representations. These students described their

reasoning using surface features that directly cited the information given in the prompt or described a relationship between the presence of a chemical species and a phenomenon to justify the reactivity. These students focused more on the what or how in their explanations instead of incorporating the why.

While using noncausal reasoning, these students described the what by mentioning the surface features of the identity of atoms (N13), type of bonds (N14), or chemical formulas given (N15 and N16). In N14 the student described the double bond as where groups would attach with no description of what would cause this attachment. The student in N16 identified a good nucleophile and a good leaving group to justify their selection of an S_N1 reaction mechanism for this problem, without a description on why these constituents can serve as a nucleophile or leaving group. Another noncausal method these students used involved highlighting relationships by explaining the how without delving into the why. For example, the student in N13 explained that bromine acts as a leaving group, and the connected atom was the electrophilic site. They, along with others, cited the presence of a chemical species to justify their responses to the prompt. However, they did not clarify why an electrophilic site would be connected to a leaving group. The student in N15 identified relationships between structural properties and reactivity, noting that a lower substitution of the carbon would lead to faster reactivity. Here, the type of carbon mattered, but an explanation for its influence on reactivity was not provided.

Noncausal reasoning also manifested in very similar ways for students with EPM representations. Example quotations of noncausal reasoning from students with EPMs can be found in the Supporting Information, section SI.D. Although the nature of the noncausal reasoning was similar for EPM and non-EPM students, the main difference was the frequency of occurrence of noncausal reasoning between these groups.

Causal Reasoning. This type of reasoning occurred with all types of representations but occurred more often with EPM representations. While using causal reasoning, students rationalized their answers by describing the effect of certain chemical properties on causing interactions or reactivity. In addition to describing what they saw in the given prompt, these students also described why it happened, that is, the underlying factors they considered while building their reasoning.

For example, the student in E13 discussed the effect of high electron density causing uneven movement of the electrons. In this case the student identified the electrophilic site as the region next to an electron rich area because this area would pull electrons toward it, creating an electron deficient region, which they identified as the electrophilic site. This student described what an electrophilic site was and how and why the electrons

Table 11. Explanations from Students Using Noncausal and Causal Reasoning When Given Non-EPM and EPM representations

Prompt Type	Causal Reasoning (with EPMs)	Noncausal Reasoning (with Non-EPMs)
Identify electrophilic site	E13: Br is electron rich, resulting in the partial negative dipole, and pulls the electron density toward it, making the α -carbon electron deficient; electrophilic.	N13: The Br is a leaving group, so the carbon connected to it must be an electrophilic center after the Br leaves.
Predict product	E14: In this scenario, the O in H_2O had the highest electron density, meaning it can donate electrons, which we saw when it reacted with the CH_3CHCH_2 molecule. Also knowing that Br_2 can be a nucleophile or electrophile led me to the decision it will accept electrons due to it being surrounded by electrons with high density.	N14: The angle line formula helped me predict my answer by showing where the double bond is and where the β -carbons are, which would show where the bromine and hydroxide attach.
Select faster reaction	E15: The S^- in the second atom acts as a better, faster leaving group. This also in turn stabilizes the carbocation. The S^- is also a darker red, making it more electron rich, which means a better leaving group.	N15: The O^- being on a primary carbon and rather than the S^- being on a secondary carbon leads me [to] believe that the reaction between $\text{CH}_3\text{CH}_2\text{O}^-$ would take place faster.
Classify mechanism	E16: EtO^- is a strong base, weak nucleophile, so either E2 or $\text{S}_{\text{N}}2$ will occur. Br in this case is connected to a secondary carbon, which means E2 will be favored. Br would be a leaving group because the electron density is high as shown in the diagram.	N16: I see a good nucleophile in the $^-\text{OCH}_2\text{CH}_3$ and a good leaving group (Br) in $(\text{CH}_3)_2\text{CHCHBrCH}_3$.

moved. They incorporated causal reasoning by describing the effect of a property (electron density) that causes an electrophilic site. Similarly, the student in E14 connected an area of high electron density to the action of donating electrons. They also connected the presence of areas of high electron density to causing the bromine to be able to accept electrons. Additionally, students mentioned how the electron density influenced other properties. For example, the student in E15 mentioned that high electron density made sulfur a better leaving group and connected this to causing a more stable carbocation. This example highlights that using causal reasoning does not mean that the student was correctly reasoning through the problem. We saw slightly more correct responses and more causal reasoning from students who interacted with EPM representations, but this does not mean that all students using causal reasoning gave the correct answers. Meanwhile, in E16 the student highlighted why they knew that Br would be a good leaving group. These students, after describing the effect of electron density on other properties, rationalize their reasoning about why they came to the conclusions they came to about the given prompt.

Causal reasoning also manifested in very similar ways for students with non-EPM representations. Example quotations of causal reasoning from students with non-EPMs can be found in the [Supporting Information, section SI.D](#). Although the nature of the causal reasoning was similar for EPM and non-EPM students, the main difference was the frequency of occurrence of causal reasoning between these groups. Additionally, students who used electron density to build their causal reasoning were able to use explicit features of the representation if they had EPMs but needed to use implicit features if they had non-EPMs.

DISCUSSION

This study investigated affordances of EPMs through identification of students' performances in solving problems, their reasoning, and electronic features present in students' reasoning about four phenomena in organic chemistry. While doing this, we utilized representational competence, which is the ability to use representations with its features (i.e., conceptual) to solve problems (i.e., reasoning)^{4,30,38} as a guiding framework. The results of this study revealed that EPMs might relate to higher performance depending on the problem type, more use of electronic features, and the enactment of causal reasoning in four fundamental problem types in organic chemistry. We found students using electronic and structural features and causal and noncausal reasoning in similar ways, but these were cued with different frequencies with EPM and non-EPM representations. The nature of chemistry shows that chemical phenomena (e.g., electrophilicity) are explained through electrostatics as producers of change and entities as recipients of this change (e.g., the more and less electronegative atoms and their connectivity). However, describing activities of entities based on electronic features has been shown to be more difficult for students since they tend to focus more on structural features such as atom identity and bond type. Contrary to those findings, a majority of students surveyed in this study used electronic features to describe electronic behavior in their explanations for these phenomena, despite this behavior being an implicit property in the non-EPM representations. Even so, students with EPM representations were more likely to invoke electronic features. A closer look at the descriptions of electronic behaviors indicated that students associated the color pattern in EPMs with electronic behaviors, which is in line with the fact that

surface features (i.e., color pattern) are accessed easily by novices. Therefore, EPMs offer a potential avenue for instruction to cue students to consider electrostatics (i.e., conceptual) when describing or predicting phenomena (i.e., reasoning) in organic chemistry, which has the potential to enhance representational competence.

A series of studies shows that students' use of causal reasoning to solve unfamiliar problems correlates with performance on organic chemistry tasks.^{24,32,39} In this study, students with EPMs had a higher performance and enacted causal reasoning more than the students with non-EPMs. Although this study is exploratory without demonstrating statistical significance, this observation is compatible with the hypothesis that features of representations influence students' ability to successfully interpret the representation.^{30,38} This can also be explained by the activation of relevant units of information that one can access during reasoning (i.e., cognitive resource)^{40–42} and enactment of more foundational perceptions about the entities including established properties and relationships (i.e., mental model).^{43,44} Thus, when reasoning with EPMs, mental models^{41,45} and resource activations⁴⁶ were triggered by the features of the task. Accordingly, while enacting causal reasoning students with EPMs justified their explanations by describing how chemical properties caused interactions or reactivity such as the effect of electron density causing leaving groups or nucleophilic areas.^{40,41,45–48} Therefore, EPMs have the potential to support students in developing expert-like reasoning where entities, activities, properties, and their relationships are encoded as single chunks, which stimulate cognitive resources and mental models.²⁷

Students with EPMs did not perform better than students with non-EPMs in predicting the product. Students' performances in this prompt were evaluated based on the degree to which they correctly wrote the condensed chemical formulas of products of the halohydrin reaction between propene, bromine, and water. For correct predictions, students needed to identify the alkene functional group in propene (i.e., bonding property) and the identities of bromine and water (i.e., characteristics of atoms and molecules). Students receiving non-EPM representations were more often cued to structural features that centered on bonding properties and describing the characteristics of the atom. This may explain why students with non-EPMs outperformed students with EPMs on predicting the product prompt. Students are familiar with line-angle diagrams and therefore prefer to reason with those diagrams when predicting the products of a reaction⁴⁹ since line-angle diagrams can facilitate the access to relevant cognitive knowledge by decreasing cognitive load or the capacity to process units of information with the memory resources available when learning.⁵⁰ For problems in which students can effectively utilize heuristics on atomic identity and connectivity, EPMs may hinder students by requiring students to decode shapes and colors in the representation before accessing the heuristic. This is consistent with research indicating that problems with representations that do not include a supporting explicit property are more difficult for students than problems in which explicit properties support identifying the correct answer.²⁰

■ IMPLICATIONS FOR RESEARCH AND TEACHING

Improving students' ability to generate mechanistic explanations for phenomena has gained interest in organic chemistry education in recent years.¹⁹ Although teachers view developing

students' ability to use causal reasoning as important, their instructional practices often do not reflect this understanding.^{51,52} Mechanistic reasoning includes several key aspects, which are explicit and implicit properties, dynamics (i.e., how), causes and effects (i.e., why), and multiple variables.^{14,23} The results of this study indicated that EPMs have the potential to stimulate the use of implicit and explicit properties and support the enactment of causal reasoning, which form a baseline for mechanistic reasoning. This type of reasoning is also an indication of students' interpretation and utilization of representations to predict and solve problems—representational competence.⁴ Therefore, instruction and assessment should focus on the enactment of causal reasoning through invoking electronics.

To promote causal reasoning, EPMs may be used to cue students citing electronic behavior, although students need guidance when explaining phenomena using EPMs.^{30,38} As a first step in guidance, instructors should ensure that students can decode the color of EPMs by explaining how to use color codes for several molecules with different polarities to understand the electrostatics of the molecules. This can be done at the beginning of the semester, when organic chemistry students begin to learn different representations. Instructors should also provide information about the symbols and formulas of chemicals since EPMs limit identity information. Moreover, a description of implicit and explicit properties through several examples should be provided to students to increase the benefit gained from reasoning with EPMs. Gaining familiarity with the features of EPMs can form a baseline to enact causal reasoning.

Causal reasoning involves explanations about the activities that cause a change such as electronegativity causing a difference in electron density in a molecule.^{19,53,54} The results of this study revealed that EPMs are beneficial in cueing students to describe electronic activities, even if not always correctly. Therefore, depending on the problem, instructors can use EPMs when they want students to explain why a phenomenon happens. For instance, when asking students to identify an electrophilic site in a molecule such as $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$, instructors could include an EPM and prompt students to "explain in full detail why you determined that site is the most electrophilic one on this substance" and "what about the electrostatic potential map made you predict your answer?" Based on the results of this study, these types of activities have shown potential in leading students to use causal reasoning. Students can use causal reasoning incorrectly, but such responses are an asset, as they can help the instructor gain insights into students' thought processes and guide students toward productive reasoning to explain a phenomenon. Additionally, assessments can be used to communicate the importance of a topic or process to students,⁵⁵ and therefore, EPMs can also be incorporated into exam problems to emphasize the electronic activities that cause a phenomenon to occur. While the integration of EPMs into multiple choice assessment items can encourage students to consider electrostatic potentials when selecting an answer, open response items may be a better overall measure of students' understanding. Open response items can capture how students are using the features of an EPM to craft explanations for their predictions. Another avenue could involve items with structures parallel to those of the tasks in this study, where follow-up questions are embedded for students to expound on their initial answer choice. Nevertheless, it must be acknowledged that any further recommendation for assessment design exceeds the conclusions drawn from the data in this study. Therefore, further

research would be needed to establish the most effective method for integrating EPMs into assessment.

LIMITATIONS

The results of this study are limited to the students from two different institutions. However, institutions differ to a certain degree, which enhances the transferability of the results to other institutions. The sample size was not large enough to demonstrate statistical significance of small effect sizes, which prevents supporting generalizable claims; however, it does provide an evidence base for hypotheses to further test. As with any study in which participants are offered extra credit for participating, there may have been sampling bias for students who were interested in earning extra credit. Since all representations were static, not being able to rotate BS or EPM representations could have influenced student reasoning, but this was authentic to how chemists publish static electrostatic potential maps in journals. Students were allowed to draw while working through these problems, but these drawings were not collected. This data could have been informative had it been collected since drawing impacts student learning.⁵⁶ The results of this study may be limited to the problems asked in this survey and not to broader problem types since students only interacted with one problem of each of the four problem types. Additionally, these students were more familiar with line-angle diagrams and were not formally trained on EPMs at one institution, and they saw them occasionally at the other institution. The results of this study do not reflect students who have experience interacting with EPMs on assessments. Thus, a future area of research is to explore what students do with EPMs after formal training and assessment about the advantages and limitations of this representation.

CONCLUSIONS

When students were randomly assigned to one of four representations to explain fundamental phenomena in organic chemistry, students with EPMs outperformed students with non-EPM representations in all phenomena except in predicting the product. Students with EPMs cited electronic features more than students with non-EPMs, while there were differences among students with EPMs regarding how they used electronic features to explain their reasoning. More importantly, causal reasoning was enacted more by students with EPMs who rationalized their responses by describing the effects of certain chemical properties that cause interactions or reactivity. As an exploratory study, the results point to the potential of EPMs to support student learning in organic chemistry problem solving, which will require further testing.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00500>.

Institution information, survey questions, example answers, and additional participant quotes (PDF, DOCX)

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Notes

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