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Student perceptions of partial charges and nucleophilicity/electrophilicity when provided either a bond-line, ball-and-stick, or electrostatic potential map for a molecular representation

Abstract

Education in organic chemistry is highly reliant on molecular representations. Students' abstract information from representations to make sense of submicroscopic interactions. This study investigates relationships between differing representations: bond-line structures, ball-and-stick, or electrostatic potential maps (EPMs), and predicting partial charges, nucleophiles, and electrophiles. The study makes use of students' answers on hot-spot question format, where they select partially charged atoms on the image of molecule and explanations. Analysis showed no significant difference among students when predicting partially positive atom with each representation; however, more students with EPMs were able to correctly predict the partially negative atom. No difference was observed across representations in students predicting electrophilic character; while representations did influence students identifying nucleophilic character. The affordance of EPMs was that they cued more students to cite relative electronegativity indicating that such students were able to recognize the cause for electron rich/poor areas. This recognition is central to rationalizing mechanisms in organic chemistry. This study offers implications on incorporating EPMs during instruction and provides an evidence-based support in how EPMs could be useful in promoting learning on topics that relate to an uneven charge distribution.

Introduction

Organic chemistry is a visual science where a variety of molecular representations are used to communicate chemical concepts (Davidowitz & Rollnick, 2011; Zhou et al., 2023). Representations in organic chemistry can be of many types from skeletal structures to NMR spectrums. For the purposes of this study, representations are operationalized as drawings or images that depict the molecule at the submicroscopic level, for example, the molecule of chloromethane can be depicted using a bond-line, ball-and-stick, or electrostatic potential map. An organic chemistry instructor may choose to depict 3D molecules using bond-line structures where students can denote the hybridizations of atoms, dashed-wedge diagrams where students learn the meaning behind a solid versus a dashed line, or an image of the ball-and-stick such that students can rotate on the screen to understand dimensionality. Organic chemistry instructors therefore have a choice in how much they want their students to abstract information from the given representation (Davidowitz & Rollnick, 2011; Jones et al., 2022; Popova & Jones, 2021; Smith, 2023). It therefore becomes essential that students in organic chemistry develop skills to work with the given representations, which leads to the importance of representational competency skills (Dood & Watts, 2023; Kozma & Russell, 2005; Offerdahl et al., 2017; Prain & Tytler, 2012; Talanquer, 2022; Watts et al., 2022).

A historical review of ACS exams showed that since 1982, 90% of the exam items contain at least one representation (Raker & Holme, 2013) directing to the importance of improving representational competency skills among organic chemistry students. Kozma and Russell (1997) presented representational competency skills and this study investigates one of the skills wherein students are able to identify and analyze features of a representation and use them to carry out the task-at-hand, for example, explanation of chemical concepts. Several studies have investigated the role of representations in students' understanding of a variety of chemical concepts. Past studies conducted semi-structured interviews with undergraduate organic chemistry students using chemical formula, Lewis dot diagrams, or bond-lines to investigate topics including applications of hydrogen bonding (Henderleiter et al., 2001), acid-base mental models (Cooper et al., 2016; McClary & Talanquer, 2011), completing reaction mechanisms (Crandell et al., 2020; Galloway et al., 2019; Grove et al., 2012), nucleophiles/electrophiles (Anzovino & Bretz, 2015; Eckhard et al., 2022), and explaining electron pushing formalism (Bhattacharyya & Harris, 2018; Watts et al., 2020; Webber & Flynn, 2018). These studies showed that students either rely on rote memorization for concepts or are unable to explain the *why* behind mechanisms. Beyond bond-line structures, studies have explored other visual representations such as dashed-wedge diagrams to explain enantiomers (Domin et al., 2008), translation between dashed-wedge, Newman, and Fisher (Olimpo et al., 2015; Ward et al., 2022, p. 39), chair conformations (Decocq & Bhattacharyya, 2019; Head et al., 2005), and reaction coordinate diagrams (Popova & Bretz, 2018a, 2018b; Watts et al., 2022). These studies that went beyond the popular bond-line structures showed that students might be focused on the surface features more than the molecule's functionality, and that they need more support understanding in-depth cues in representations. Two studies looked into organic chemistry students' use with visual representations including color shown in ball-and-stick (Ealy & Hermanson, 2006; Stull et al., 2012); the latter study made use of the tactile ball-and-stick model of molecules to investigate mental rotation. They concluded that organic chemistry students need more practice in working with such representations and this could be demonstrated by instructors during instruction. The role of representations was also investigated with chemistry graduate students (Bhattacharyya & Bodner, 2005; Kraft et al., 2010; Strickland et al., 2010). These studies made use of bond-line structures with curved arrows showing the electron pushing formalism. Similar to the undergraduate students, graduate students struggled in explaining the *why* behind curved arrow notations relying on memorization rather than process-oriented thinking. Combined, these studies call for helping students develop the skill of using the given representation to argue for how chemical species interact by promoting focus beyond the surface-level or structural features of the representations (Eckhard et al., 2022; Hand & Choi, 2010; Watts et al., 2022; Watts et al., 2021). Since movement of electrons or attraction between areas of high and low electron densities are necessary to rationalize why chemical species interact, this study therefore investigates how students explain using features of a representation that makes electronic distribution explicit.

<u>Studies investigating students' understanding of nucleophiles and electrophiles</u>

For this study, the chemical concepts chosen to investigate the role of representations are partial charges and nucleophiles/electrophiles. The reason behind choosing these topics is owing to their importance in organic chemistry and their reliance on electronic distribution. A national survey of organic chemistry instructors rated determining high/low electron density and recognition of nucleophiles/electrophiles higher than having knowledge of reaction mechanisms in organic chemistry (Bhattacharyya, 2013). Owing to this importance, this study investigated how students might use representations to aid in the process of assigning partial charges on atoms on molecules that are interacting and identify nucleophiles and electrophiles. In addition, students struggle to connect uneven charge distribution (partial charges) to its effect on reactions, which are central to organic chemistry education. Studies show that partial charges are typically drawn on representations, but in the absence of these drawings, students struggle in connecting implicit charge distribution to its effect on reaction mechanisms (Smith, 2023), activation energy (Caspari et al., 2018) or nucleophilicity/electrophilicity (Frost et al., 2023). Thus, continuous incorporation of representations that make electron distributions explicit may help students understand the effects of implicit charge distribution (Taagepera & Noori, 2000). This study therefore investigates the impact of a representation that makes charge distribution explicit to investigate how well it supports students identifying nucleophilicity/electrophilicity, which is impacted by the charge distribution.

Past studies have investigated how students define and consider involvement of nucleophiles/electrophiles in reactions. Interviews with second-semester organic chemistry students showed that students used electronic features such as charges to define nucleophiles and electrophiles but were unable to use these definitions as explanatory for *why* reactions, such as, acid/base occur (Anzovino & Bretz, 2015; Cartrette & Mayo, 2011). Organic chemistry students' ideas about nucleophiles/electrophiles seem to be fragmented (Anzovino & Bretz, 2016). Interviews with pairs of organic chemistry students where they had to explain and draw electron-pushing formalism found students able to identify nucleophile and electrophile correctly but confusion with where electrons (nucleophile to electrophile) or protons (electrophile to nucleophile) transfer (Bhattacharyya & Harris, 2018). Thus, connecting implicit partial charges to their effect on reaction mechanisms cannot be presumed. Crandell and colleagues (2019) also make the argument that students have difficulty in understanding the "source-to-sink" in electron pushing formalism, that is, where electrons move from that might promote understanding of *why* nucleophiles and electrophiles interact. Studies that have characterized students' explanations of mechanisms involving nucleophiles and electrophiles also show students' understanding as surface-level (Dood et al., 2020a; Frost et al., 2023; Yik et al., 2023). These studies pointed to the notion that even though students might know the definition of nucleophiles/electrophiles, they struggle in making sense of their role in reaction mechanisms, that is, relating the effect of uneven charge distribution within chemical species to determining which species will interact. A similar struggle was also observed with graduate chemistry students in explaining the *why* behind the role of nucleophiles and electrophiles (Strickland et al., 2010). However, in recent studies, we do see students trying to make those connections. Two studies that investigated organic chemistry lab students' explanations on comparing two mechanisms involving nucleophiles and electrophiles coded for features, wherein charge, induction, electronegativity, and resonance were prominent (Watts et al., 2020; Watts et al., 2021). These studies pointed out that there is value in students bringing back concepts about electron distribution they learned in general chemistry and apply it to reaction mechanisms in organic chemistry. To promote this application of connecting implicit properties of electron distribution to nucleophiles/electrophiles, representations can assist (Crandell et al., 2019; Dood & Watts, 2023; Ealy & Hermanson, 2006; Graulich, 2015), which this study will investigate.

Rationale

It is well established in the organic chemistry education literature students need to explain the *why* behind reaction mechanisms (Anzovino & Bretz, 2015; Caspari et al., 2018; Crandell et al., 2019; Dood & Watts, 2022; Graulich, 2015; Stowe & Cooper, 2017; Talanquer, 2018, p. 48). For this reason, in this study we ask students to explain how they identified partial charged atoms and then explain the first step of a nucleophilic aryl substitution reaction. The foundation of this study is the relationship between partially charged atoms within a molecule with predicting and explaining nucleophilic substitution. The focus is on electron density because excess or deficient electron density in molecular regions is essential to understand the functionality of nucleophiles and electrophiles (Anzovino & Bretz, 2015; Cartrette & Mayo, 2011).

Because representations are used in organic chemistry that depict the implicit properties of electron distributions' effect on nucleophilicity/electrophilicity, this study investigates the role of three representations in students' predicting and explaining partially charged atoms (electron density), recognizing nucleophiles and electrophiles, and explaining the first step in the mechanism of a nucleophilic aryl substitution reaction. By explaining the first step in this mechanism, there is an assumption that students are relating presence of partially charged atoms to recognizing the functionality of nucleophiles and electrophiles in this reaction. Past studies, that have used representations and investigated what students mention when they explain reaction mechanisms have predominantly used bond-line structures or dashed-wedge diagrams (Eckhard et al., 2022; Rodemer et al., 2021; Watts et al., 2020; Webber & Flynn, 2018), while a study also used electrostatic potential maps (Dood et al., 2020b). To date, no studies have compared representations to determine the impact of representations on explanations of reaction mechanisms. Conducting the study comparing representations on explanations adds to the literature to promote students in explaining the *why* using representations. Thus, the novelty of this study comes in two aspects: 1) investigating two chemical concepts that are needed to explain why chemical species interact, that is, partial charges, and nucleophilicity/electrophilicity and 2) comparing common representations that make charge implicit (bond-line structures and ball-and-stick) and explicit (electrostatic potential maps). Those three representations were chosen owing to how they depict uneven charge distribution. Bond-line structures are ubiquitous in instruction and assessments in organic chemistry owing to their easy construction. Electrostatic potential maps (EPM) show electron density as color variation. In contrast, ball-and-stick images also use varying color to demonstrate atomic identity but not relative electron density. These three representations fit the inquiry. With bond-line structures, students will need to abstract relative electronegativity from atom identity and infer molecular geometry. With ball-and-stick, students are presented molecular geometry but still need to abstract relative electronegativity from atom identity. With EPM, students are provided all the information of ball-and-stick (which is embedded within the representation) and a color map modeling electronic distribution. Thus, comparisons of EPM with bond-line demonstrate the impact of providing students with molecular geometry and electronic distribution versus students implicitly determining molecular geometry and electronic distribution. Comparisons of EPM with ball-and-stick demonstrate the impact of providing only the electronic distribution color map since all other features are identical. Comparisons of ball-and-stick with line-angle structures demonstrate the impact of providing molecular geometry.

Theoretical Framework

The study design was informed by the C-R-M model of the visual literacy framework by Schönborn and Anderson (Anderson et al., 2013; Schönborn & Anderson, 2009, 2010). The C in the model refers to students' prior conceptual knowledge, R is the cognitive abilities or students' reasoning, while M is the external features of the mode of the representation. R-M is the ability to reason using external features of a representation and in this study, the evaluation of students' responses across different representations was indicative of how students R-M is cued by differing representations. The application of this framework is also seen in other studies that use a variety of representations to decode students' understanding (Coleman et al., 2023; Sunyono et al., 2015; Ward et al., 2022, p. 38; Wright et al., 2017). This assumption is also supported by cognitive theories on learning with representations summarized by Rau (2017). Several theories were mentioned in the summary including cognitive theory of multimedia learning (Mayer, 2005), integrated model by text and comprehension (Schnotz, 2005), and structure mapping theory (Gentner, 1983). These describe how students gain representational competency skills, that is, how students map features of a given visual representation to a referent to build internal processes, which they then use to problem-solve. Referent is operationalized as what comes to mind when someone is given a visual representation, for example, when given a bond-line structure of alcohol, the referent could be the molecule of alcohol (a concrete object) or strength of nucleophilicity of the molecule (an abstract concept). Rau (2017) summarizes that these theories describe that students struggle in determining features of a visual representation that are relevant and irrelevant to the referent. Features in this context are similar to the external features of the representation (M) (Schönborn & Anderson, 2009). Once students focus on the feature, they access their prior knowledge from the long-term memory and insert it into the internal process they develop. Students then use this internal process for the task at hand using the representation which is the intersection of C-R-M (Schönborn & Anderson, 2009).

In organic chemistry, there are a variety of visual representations that show symbols of atoms connected with lines or circles (bond-line, Newman projections, Fischer projections, chair etc.) or colored entities (ball-and-stick, space filling, electrostatic potential maps, isosurface structures etc.). Across representations, a feature might differ in the way it is represented even if it means the same thing. For example, the feature of connectivity or two atoms bonded to each other is represented with a straight line in bond-line structures but a straight line and overlapping colorful spheres in EPM. Therefore, each way the feature is represented (M) requires a different level of abstraction to understand that it means two atoms are bonded to each other (R-M). Since feature across visual representations is presented differently but indicates the same concept – mapping a feature to the referent is likely to differ from one visual representation to the other. This leads to retrieval of different prior knowledge from the student's long-term memory and a different process for the task-at-hand using that representation (C-R-M). For example, while seeing a bond-line structure to understand that a straight line represents a bond, students would need to extract from their prior knowledge that the straight line depicts two electrons being shared between two atoms, whereas to understand that overlapping of spheres resulting in different colors students would extract knowledge of electrons cloud of atoms being shared with each other. Thus, the C-R-M model pairs with cognitive theories in learning with representations to offer an explanation that different visual representations can bring forth different processes in students since they have features that map onto similar concepts. Past work has evidenced this possibility by exploring the effect of representations in determining the polarity of a single molecule where polarity was implicit in each molecule (Farheen & Lewis, 2021; Rau, 2017). This study focused on the C-R-M that is what conceptual knowledge (C) do students bring forth while they are explaining (R) the given task at hand using the representation (M).

Research Questions

This study is guided by the following research questions to investigate the C-R-M of students, that is, what concepts students bring forth by relating features of the representation to justify of charges and nucleophilicity/electrophilicity.

1. What is the relationship between representation and correct prediction of the location for the partial positive negative regions of a molecule?
2. What concepts do students cite while predicting the location of partial charges and how do representations relate to such features?
3. What is the relationship between representation and students' explanation for the first step of a nucleophilic aryl substitution reaction?

Methods

Participants, Research Setting and Ethical Considerations

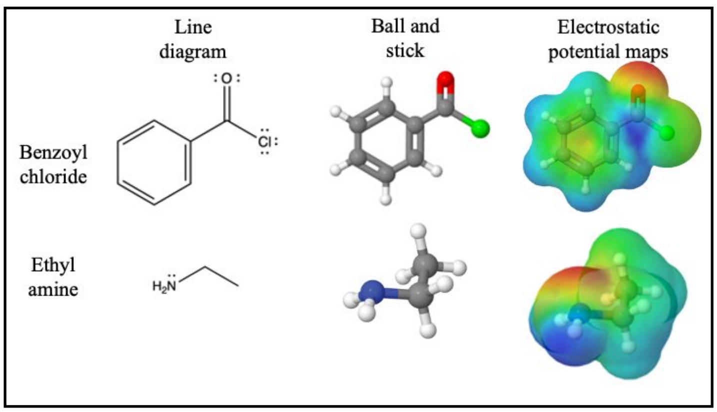
The participants for this study were second-semester organic chemistry course at a research-intensive university in the southeast United States. Students from second-semester organic chemistry were chosen for two reasons: 1) this cohort has gone through the first-semester organic chemistry training where they learn nucleophilic reaction mechanisms 2) this study makes use of students creating mechanisms using the software *Marvin JS* and this cohort has had experience working with this software in first-semester organic chemistry. Three classes of second-semester organic chemistry course were coordinated with the same instructor, syllabus, common class material, and exams. Students were recruited from all three courses and consented to participate on a voluntary basis. Out of 428 students, 81.1% (390) consented to participate in the research study. The institution's IRB approved this study as Study002446.

Study Design

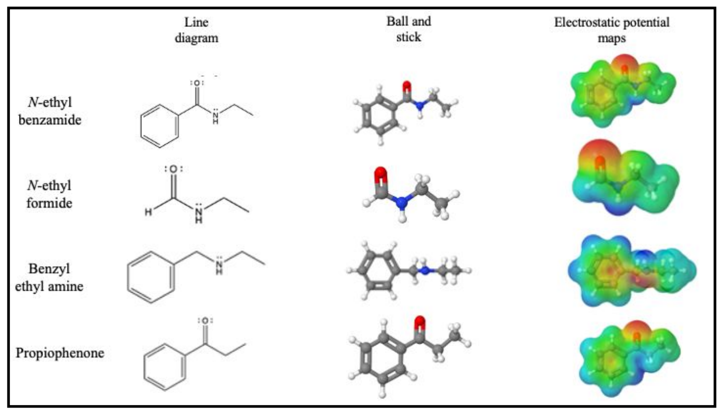
Three surveys were created and students from the second-semester organic chemistry were randomly assigned to one survey. Random assignment was conducted to mitigate the potential for inherent differences among the groups. Students were given five days after their third in-term exam to complete their assigned survey. Upon completion students received a small portion as an extra credit opportunity. Responses from students who consented were analyzed.

Each survey differed with the accompanying representation between bond-line, ball-and-stick, and electrostatic potential maps as shown in box 1 and 2. It is essential to point out that this student population has more experience working with bond-line structures as this is the most common representation used in assessments at the research setting. Thus, the results will describe students' interpretations of ball-and-stick and EPMs without formal training on either. Further, the ball-and-stick and EPM were implemented without a legend or direct instruction on how to interpret the representations, so the results herein may be most applicable to describe students initial encounter with these representations. The bond-line structures were created using *ChemDraw* and the ball-and-stick and electrostatic potential maps using *Jmol*.

For each survey, the same representation type was used throughout the series of prompts. That is, if a student was assigned to bond-line survey, they were provided only bond-line structures throughout the survey. Instructions that included the electronegativity values and difference in values to indicate a polar bond were given at the top of the survey. Students could use these instructions anytime during the survey. For prompts 1 and 2, students selected the atom with partial positive charge in benzoyl chloride molecule in the hot-spot and explained their prediction in essay. Hot-spot is when students are given an image and they are asked to click on the part of the image that they think is the correct answer. For example, a student clicked on the image of a ball-and-stick molecule of benzoyl chloride to indicate the partially positive atom in the molecule. For prompts 3 and 4, students selected the atom with the partial negative charge in ethyl amine and explained their prediction. Prompts 1 and 3 were designed to have quantitative data for the selection of the atoms with partial charges and prompts 2 and 4 for qualitative data to act as support for their selection. Prompts 1 and 3 were designed to answer the first research question about the impact of representations on students' prediction of charges, and prompts 2 and 4 the second research question on features cited. Hot-spot style was used instead of the traditional multiple-choice as it offered evidence of students clicking on the location in the image as their selection compared to them selecting a textual option from the multiple choices. For prompt 5, students were asked to use *MarvinJS* to construct a mechanism for the reaction between benzoyl chloride and ethyl amine and upload the mechanism; prompt 6 asked students to explain the first step in the mechanism. Note that students were not informed that the interaction between the two molecules was a nucleophile interacting with electrophile. Finally, prompt 7 asked students to predict the product. Table A1 in the appendix shows the instructions and survey prompts students received.



Box 1. Images of representations in each survey



Box 2. Images of products in each survey

<u>Data Analysis</u>

To answer the first research question about the relationship between representations and students' correct prediction of partially charged atoms, the proportion of correct responses were compared between the representations. Chi square analyses were run to test whether the type of representation had a significant influence on students' correct prediction; effect sizes are reported using Cohen's *w* where 0.1 is a small effect and 0.3 is a medium effect size (Cohen, 2013).

To understand the relationship between representations and students using certain features while predicting partially charged atoms or describing the first step in the mechanism, students' responses to open-ended prompts were open-coded (Given, 2008, p. 5 of 9). Codebooks for predicting partial charges (Table A2) and explanations of nucleophilic attack (Table A3) are presented in the appendix. Each codebook development took place in the following steps. Two researchers took a subset of responses different from each other and inductively coded to generate two separate codebooks. They came together to merge these codebooks to create a single codebook. This codebook was deductively applied to another subset of responses independently and the researchers came together to discuss disagreements and modified the codebook. This deductive application of the codebook occurred until no changes to the codebook seemed necessary. Once that was achieved, two researchers independently applied the codebook to the entire sample and came together to conduct consensus coding until all disagreements were resolved (O'Connor & Joffe, 2020). One coder was a graduate student and another an undergraduate student who did academically well in organic chemistry. Due to their familiarity with partial charges and nucleophilic aryl substitution reactions, there is trustworthiness in their interpretation of these data (Shenton, 2004). Consensus coding was carried out between the two researchers to further establish trustworthiness that these data were being interpreted appropriately to answer the research question by more than one researcher. By conducting coding with another researcher, this helps to mitigate any biases.

Results

RQ1: What is the relationship between representation and correct prediction of partially positive atom and partially negative atom?

Table 1. Among the students given a particular representation, percentage of students who selected the correct partially positive atom in benzoyl chloride as the carbonyl carbon

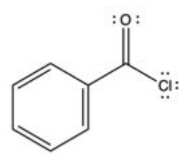
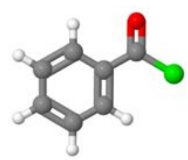
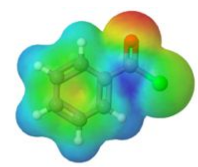
	Representations		
	 (*n* = 114)	 (*n* = 116)	 (*n* = 112)
Students who selected carbonyl carbon as partially positive	87.7%	83.6%	87.5%

Table 1 shows the percentage of students among a representation that correctly determined the carbonyl carbon as the partially positive atom in benzoyl chloride. The percentage of students who made correct predictions across the three representations are similar and range from 83.6% to 87.7%, with no statistically significant difference observed. There was thus no evidence to show a relationship between one representation over the other on students correctly predicting partially positive atom in benzoyl chloride. Students had a high success rate in predicting the partially positive atom in benzoyl chloride, independent of the representation used.

Table 2. Among the students given a particular representation, percentage of students who selected the correct partially negative atom in ethyl amine as nitrogen

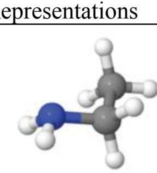
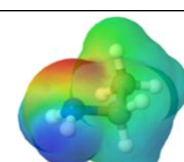
	Representations		
	(*n* =  114)	 (*n* = 116)	 (*n* = 112)
Students who selected nitrogen as partially negative	79.8%	87.1%	97.3%

Table 2 shows the percentage of students among a given representation who correctly predicted that nitrogen atom is the partially negative atom in ethyl amine. Differences among the representation groups was more pronounced when predicting the partial negative charge, with the percent correct ranging from 79.8% to 97.3%. Pair-wise chi-square analysis found no significant difference between students with bond-line and students with ball-and-stick. There was a statistically significant difference between bond-line and EPM ($X^2(1, N = 226) = 16.988$, $p < .001$, Cohen's $w = .274$, medium effect) and between ball-and-stick and EPM ($X^2(1, N = 228) = 8.237$, $p = .004$, Cohen's $w = .190$, small-medium effect). Students with EPM are more likely to correctly predict that nitrogen is the location of the partial negative charge in ethyl amine compared to the other student groups.

RQ2: What concepts do students cite while predicting partial charges and how do representations relate to such concepts?

As the rationale described, explaining how students predicted partial charges is important in organic chemistry. How students use the representations to map features of representation to predicting partial charges can help instructors learn more on the role of representations in predicting partial charges. Students' explanations when predicting partial charges were categorized as invoking one or two of the following concepts: relative electronegative, absolute electronegative, uneven charge distribution, resonance, color, connectivity, and electronic entities.

Students who use relative electronegativity made explicit comparisons of electronegativity values between bonded atoms. For example, in the case of benzoyl chloride, *"I believe that carbon will have a partial positive charge because it is bonded to two atoms* ***chlorine and oxygen that are both more electronegative than the carbon****, causing the shared electrons to be drawn closer to the chlorine and oxygen resulting in a partial positive carbon. [ball-and-stick]"* The same student with ethyl amine indicated *"The* ***nitrogen is more electronegative than hydrogen and carbon****, therefore, pulling the shared electrons closer resulting in a partial negative charge. [ball-and-stick]"* In both responses, the student describes the relative electronegativity between atoms that share a chemical bond.

In contrast, students who used absolute electronegativity did not make explicit comparisons. For example, "*The carbon has both* ***the electronegative oxygen and chloride*** *forcing the atom to be partial positive. [bond-line]"* Here a student does not mention whether carbon, oxygen, or chlorine, is more electronegative and does not enact comparisons based on bonded atoms. A similar example with the ethyl amine prompt was *"****the nitrogen will be the electronegative atom*** *in this situation and pulls the electrons in the dipole moments with the neighboring carbon and hydrogens towards itself becoming partially negative. [bond-line]"* There are two potential interpretations for why comparisons were not invoked. It is possible that students perceive the concept of electronegativity as an inherit characteristic of the atom. That is, certain atoms have high electronegativity and possess partial negative charges and atoms connected to them possess partial positive charges, without attending to the electronegativity value of the connected atoms. Alternatively, students may be omitting the electronegativity comparison as part of a colloquial phrase. In this interpretation, students may recognize that comparisons are needed but omit this detail in their explanation. Ultimately, absolute electronegativity is seen as ambiguous. Responses that invoked absolute electronegativity were demarcated from relative electronegativity to note the potential ambiguity in their processes.

Students also implicitly used the property of electronegativity, that is, they described the uneven distribution of charges by mentioning pull on the electrons or presence of electron withdrawing/donating groups. For example, "*Both the chlorine and the **oxygen pull electrons** more than the carbon so the carbon will experience a partial positive charge. [ball-and-stick]"* or *"The amino group is an **electron withdrawing group** in the molecule. The **nitrogen will draw electrons toward itself**. [EPM]"* Infrequently, an uneven distribution of charges was cited with relative electronegativity (3 students) or with absolute electronegativity (2 students). Overlaps of codes were infrequent and were not analyzed separately.

Some students also used the concept of resonance to justify the location of the partial charge. For example, a student wrote *"The carbonyl carbon has a partial positive charge **due to resonance** (the oxygen can take the pi bond as a lone pair). [bond-line]"*. This reasoning strategy was also observed with students with ethyl amine even though the molecule does not exhibit resonance properties. For example, *"**Due to resonance**, the Nitrogen will carry the negative charge. [ball-and-stick]"* Here a student describing ethyl amine used resonance to explain why nitrogen atom will be the partially negative atom in ethyl amine even though the lone pairs on the nitrogen are not delocalized.

There were also infrequent occurrences where students used the colors in the ball-and-stick or EPM to justify their selection. For example, *"You can see in the picture where the **red is negative** the will likely be a partial positive charge below it in the **dark blue area**. [EPM]"* or *"the atom with the partial positive charge is the **blue one**. [ball-and-stick, in ethyl amine]"* Using this concept showed that some students focused on surface feature of color to determine the location of partial charges.

Some students cited only connectivity to justify the location of partial charges, which were atoms connected to or bonded to each other. Example statements include *"because **it is a chlorine that's connected to a carbon** that is also **connected to an oxygen** with a double bond., [ball-and-stick]"* and *"the **Nitrogen is connected to 2 hydrogen atoms, a carbon atom**... making it have a partial negative charge. [bond-line]"*

In contrast, other students cited electronic entities such as charges, lone pairs, or number of valence electrons to justify their decision. For example, *"The **chloride and oxygen both have negative charges**, which means that the **carbon is the positive** that pulls down. [bond-line]"* and *"the nitrogen in NH2 would have the partial negative charge, particularly due to the **unshared electrons on the nitrogen**. [EPM]"* Responses coded for connectivity or electronic entities did not make explicit mention of electronegativity or uneven electron distributions in their justifications.

Table 3. Among the students given bond-line, ball-and-stick, or EPM, percentage of students who cited the following concepts while explaining partial positive in benzoyl chloride

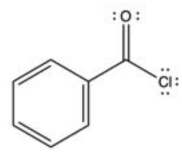
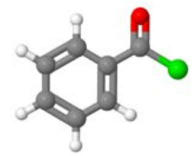
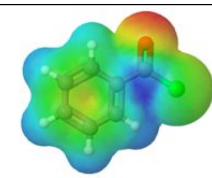
	Representations		
	 (*n* = 114)	 (*n* = 116)	 (*n* = 112)
Relative electronegativity	28.9%	31.0%	33.9%
Absolute electronegativity	21.1%	25.9%	23.2%
Uneven charge distribution	10.5%	12.9%	11.6%
Resonance	21.1%	12.1%	5.4%
Color	0.0%	1.7%	5.4%
Connectivity	8.8%	11.2%	11.6%
Electronic entities	12.3%	12.9%	19.6%

Table 3 shows the proportion of concepts cued in predicting the partial positive charge within benzoyl chloride, demarcated by representation provided. The percentages represent the proportion of those receiving a particular representation. For example, among students with bond-line, 28.9% of responses cited relative electronegativity. Electronegativity is the foundational concept that rationalizes presence of partial charges. Comparing relative electronegativity values between bonded atoms represents a required step in the process for determining partial charges. Absolute electronegativity carries ambiguity over whether the comparison of electronegativity values is conducted but may represent a similar process for some of the respondents. Even when students use uneven charge distribution in their response, it still shows that they are thinking about position of electrons without mentioning the term electronegativity. Combining the frequency of relative electronegativity, absolute electronegativity, and uneven charge distribution (for the occasional case of overlap, where a student's response received more than one code, those were counted only once when discussing trends among the combination of codes) and comparing across the representations showed a small effect that was not statistically significant (X^2 = 12.514, df=342,2 , p > .05, Cohen's *w*=.10, small effect). The uniform rate of invoking electronegativity or position of electrons across representations may explain why student success in predicting the location of the partially positive charge was independent of representation.

Concepts that showed a larger difference among the three representations were resonance (X^2= 12.514, df=342,2, p < .05, Cohen's w=.19, small-medium effect) and color (X^2= 7.388, df=342,2, p < .05 , Cohen's w=.15, small effect). The percentage of students with bond-line structures citing resonance was higher than the percentage of students with ball-and-stick or EPM. The presence of lone pairs being explicit within the bond-line structure may cue students to think about resonance since lone pairs are not explicitly visible in either ball-and-stick or EPM. Only two of the representations ball-and-stick and EPM explicitly show color. In ball-and-stick color of the balls was intended to identify atomic identity whereas in EPM color variation in the spheres was intended to signify electron rich/poor areas. Students with EPM infrequently relied exclusively on color as their sole reasoning, representing about one in twenty responses. The use of color in ball-and-stick was less frequent still and appear to note the atomic identity.

Table 4. Among the students given bond-line, ball-and-stick, or EPM, percentage of students who cited the following concepts while explaining prediction of partial negative in ethyl amine

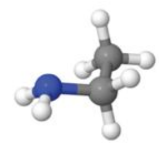
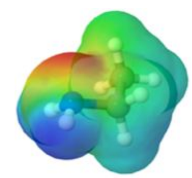
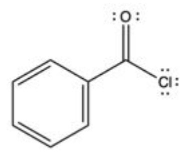
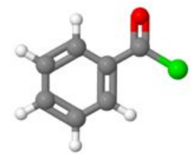
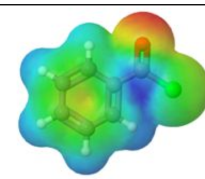
	Representations		
			
	(*n* = 114)	(*n* = 116)	(*n* = 112)
Relative electronegativity	39.5%	35.3%	50.0%
Absolute electronegativity	12.3%	19.0%	20.5%
Uneven charge distribution	7.9%	11.2%	9.8%
Resonance	7.0%	5.2%	0.0%
Color	0.0%	1.7%	5.4%
Connectivity	7.9%	4.3%	2.7%
Electronic entities	18.4%	15.5%	8.0%

Table 4 shows the percentage of students given a specific representation who cited a concept while explaining their prediction of the partial negative charge within ethyl amine. With partial negative, we see difference among the three representations in citing electronegativity or position of electrons (relative, absolute, and uneven charge distribution) (X^2 = 12.133, df=342,2, p < .05, Cohen's *w* = .19, small-medium effect). The percentage of students with EPM citing relative electronegativity, absolute electronegativity, and uneven charge distribution (80.3%) was higher than the percentage of students with bond-line (59.7%) or ball-and-stick (65.5%) (see table 4). This could explain why more students with EPM were successful at making the correct prediction about the partial negative charge than students with the other representations.

As with the partial positive charge, in the partial negative charge students use of resonance (X^2 = 7.067, df =342,2, p<.05, Cohen's w=.15, small effect) and color (X^2=7.388, df=342,2, p < .05, Cohen's w=.15, small effect) differed by representation. Students with bond-line were more likely to cite resonance, particularly compared to EPM where no students cited resonance. This trend matching the trend observed with partial positive. The reliance on color as an explanation remained constant from the partial positive prompt such that students with EPM cited this more than the other two representations.

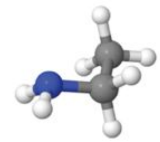
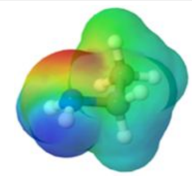
Table 5. Among the students given a particular representation and cited a particular concept, percent who predicted partial positive correctly

	Representations		
	 (*n* = 114)	 (*n* = 116)	 (*n* = 112)
Relative electronegativity	88% of n = 33	94% of n = 36	95% of n = 38
Absolute electronegativity	100% of n = 24	90% of n = 30	92% of n = 26
Uneven charge distribution	92% of n = 12	100% of n = 15	85% of n = 13
Resonance	96% of n = 24	86% of n = 14	100% of n = 6
Color	n = 0	0% of n = 2	83% of n = 6
Connectivity	90% of n = 10	62% of n = 13	92% of n = 13
Electronic entities	86% of n = 14	60% of n = 15	82% of n = 22

n refers to number of students within a representation who cited each concept

Table 5 shows the average proportion of the number of students who accurately predicted the partial positive charge, among those who cited each concept and with each representation. Students citing relative or absolute electronegativity, or uneven charge, identified the partial positive charge correct at a very high rate. Students with bond-line and ball-and-stick were more likely to cite resonance (Table 3), and citing resonance also corresponded to a high percent correct. Students with EPM who cited color also made correct predictions at a high rate.

Table 6. Among the students given a particular representation and cited a particular concept, percent who predicted partial negative correctly

	Representations		
	 (*n* = 114)	 (*n* = 116)	 (*n* = 112)
Relative electronegativity	98% of n = 45	93% of n = 41	98% of n = 56
Absolute electronegativity	93% of n = 14	96% of n = 22	96% of n = 23
Uneven charge distribution	22% of n = 9	85% of n = 13	100% of n = 11
Resonance	50% of n = 8	67% of n = 6	n = 0
Color	n = 0	50% of n = 2	100% of n = 6
Connectivity	56% of n = 9	60% of n = 5	100% of n = 3
Electronic entities	86% of n = 21	89% of n = 18	100% of n = 9

n refers to number of students within a representation who cited each concept

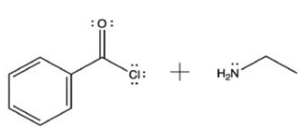
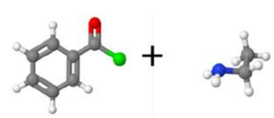
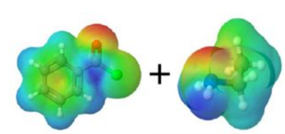
When predicting the partial negative charge, students who cited relative or absolute electronegativity, or uneven charge also had a high mean for correctly predicting partial charge across the three representations (Table 6), except for students with bond-line citing uneven charge. While no students cited resonance with EPM, the infrequent use of resonance with bond-line and ball-and-stick corresponded with a low percent correct; since ethyl amine does not exhibit resonance, this process was not expected to generate accurate predictions. As with the positive charge, color was seldom used as the sole reason for assigning a partial negative charge and when used was productive for EPM.

RQ3.What is the relationship between representation and students' classifying carbon as electrophilic and nitrogen as nucleophilic in nature?

As mentioned in the rationale, when students describe the first step in the mechanism after predicting partially charged atoms within the molecules, it is assumed they are using this knowledge in determining nucleophilicity and electrophilicity. Analysis of prompts 1 and 3 where students identified partially charged atoms and prompt 6 where they explained the first step in the mechanism showed that the correct predictions for partial positive and negative charges corresponded to the correct identification of an electrophile and nucleophile respectively while students were describing the first step. Among those who said carbon is partial positive 55.9% identified carbon as electrophilic; among those who did not identify carbon as partial positive 19.1% identified carbon as electrophilic (X^2 = 21.9, df=342,1, p < .05, Cohen's *w* = .25, medium effect). Among those who said nitrogen is partial negative 55.5% identified nitrogen as nucleophilic; among those who did not identify nitrogen as partial negative 36.6% identified nitrogen as nucleophilic (X^2 = 5.2, df=342,1, p < .05, Cohen's *w* = .12, small effect).

Table 7 shows the percentage of students among each set of representations that mentioned whether carbon is electrophilic, and nitrogen is nucleophilic, when students explained the first step in the mechanism between benzoyl chloride and ethyl amine. As before, the percentages represent the proportion of students from each representation whose response matched the description; that is 50.9% of the students with bond-line structure mentioned carbon is electrophilic. The coding process included alternative phrasing that represented the same concept. Student responses that identified the carbon as the carbonyl carbon or the carbon double-bonded to oxygen were all assigned as "carbon is electrophilic"; also, students describing acyl chloride as electron poor, has a partial positive charge, has a positive charge, or is an electrophile were all assigned as "carbon is electrophilic". Similarly, "nitrogen is nucleophilic" was assigned when student responses described nitrogen, amine, or ethyl amine as electron rich, has a partial negative charge, has a negative charge, or is a nucleophile.

Table 7. Among a given set of representation, students mentioning carbon as electrophile and nitrogen as nucleophile

	Representations in each survey		
			
	(*n* = 114)	(*n* = 116)	(*n* = 112)
Carbon is electrophilic	50.9%	47.4%	54.5%
Nitrogen is nucleophilic	60.5%	43.1%	56.3%

Comparing the three representations, no difference was observed by representation in describing carbon as electrophilic (X^2 = 1.1, df=342,2, p > .05, Cohen's *w* = .06). Students with bond-line identified nitrogen as nucleophilic at a highest rate, followed by EPM, with ball-and-stick the lowest (X^2 = 7.6, df=342,2, p < .05, Cohen's *w* = .15, small effect). The 43.1% of students with ball-and stick that identified nitrogen as a nucleophile stands in contrast to the 87.1% of the ball-and-stick students who identified nitrogen as the location of the partially negative charge (Table 2). The difference in percentages may be a result of the explicit inclusion of electronegativity values in the survey while no explicit mention of nucleophilicity is included. Among students who predicted nitrogen as partial negative but did not identify nitrogen as nucleophilic their responses varied. Responses described the nitrogen will be attracted to carbon due to opposite charges, for example, "*the electronegative* ***nitrogen is attracted to the carbon,"*** wherein they do not mention that the nitrogen is nucleophilic. Students also mention that chlorine is a good leaving group, "*because* ***chlorine is a good leaving group****. Therefore, once chlorine leaves the carbo cation is formed which the* ***Nitrogen will then attack****."* Alternatively, they use the term "nucleophilic attack" without explicitly mentioning nitrogen as the nucleophile, "***nucleophilic attack*** *on the fairly positive carbon atom."* Thus responses were either vague in describing a nucleophile or mentioned alternative reaction pathways.

Discussion and Implications

Students with EPMs were more likely to predict the partial negative charge correctly, while success rate in predicting the partial positive charge was independent of representations. Students with EPMs were also more likely to cite electronegativity or uneven distribution of electrons in their explanation, particularly compared to students with bond-line. The concept of electronegativity offers explanatory rationale for partial positive and negative charges and may support students in identifying electrophilic and nucleophilic characteristics within a molecule (Frost et al., 2023; Yik et al., 2023). Partial charges are an implicit feature in bond-lines and ball-and-stick, and students need to access their prior knowledge in comparing electronegative values of atoms that share a bond and inferring molecular polarity from bond dipoles in exhibiting this concept. In contrast, EPMs use color variation among the spheres to make partial charges explicit. Using the cognitive theories in multimedia learning that posit students compare features of the representation to the referent and then access prior knowledge to fit into their internal process, EPMs use of color increases similarity to the referent and makes it easier to access electronegativity knowledge. Notably, only approximately 5% of students with EPM explained the location of partial charges based on color alone, suggesting that the strong majority of students mapped the representation (EPM) onto the referent (partial charges resulting from uneven electron distributions). This finding further supports that showing electron distribution explicitly can contribute to students' mental models [internal process] about this concept since students seem to be focusing on explicit features more than implicit properties (Graulich et al., 2019). The results of this study push the field of work with representations and students' learning mechanisms by offering evidence where students are supported to focus on the electron distributions. In the literature, students use of mechanistic reasoning and electron-pushing formalism are frequently studied and the take-away point is to allow students to understand that electron flow is from areas of high electron density to low electron density, which allows causal reasoning (Dood & Watts, 2023; Galloway et al., 2019; Kranz et al., 2023). Because EPMs make this implicit feature of electron distribution explicit, it can thus help students understanding electron-pushing formalism and making causal connection between electron density and *why* species interact.

More students with bond-line were cued to using resonance both with benzoyl chloride and ethylamine. Benzoyl chloride cueing resonance is also found in other studies where acyl chlorides or C=O are popular structures used to explain the concept of resonance (Brandfonbrener et al., 2021; Watts et al., 2020). In bond-line structures, lone pairs on oxygen in benzoyl chloride and nitrogen in ethyl amine were explicit, and the double bond in benzoyl chloride was explicit, which may have contributed to the higher citing of resonance. A review of the PowerPoint students were instructed on about resonance also showed predominant use of bond-line structures. While the tasks given within this study did not require resonance for tasks where resonance is needed, students may benefit from using representations where electrons are explicit. Additionally, for instruction that uses representations where electrons are implicit, students may benefit from modeling how to infer resonance from these representations, likely through translation to representations where the lone pairs are explicit. Finally, it is worth noting that a proportion of students may use resonance when it is not applicable, as was done here with ethyl amine. Building instruction and assessment where students determine whether resonance is applicable may help students distinguish when to use this concept.

There are instances in the literature that describe interventions that made use of representations to improve understanding of topics in organic chemistry, such as, using concept chemical formula, skeletal, and bond-line structures to create concept maps to solve reaction mechanisms (Hermanns, 2020), showing symbolic, microscopic, and macroscopic representations generated through software during instruction (Mekwong & Chamrat, 2021; Springer, 2014) and curriculums to address misconceptions such as the spiral curriculum (O' Dwyer & Childs, 2014). This work can support these effects by serving as a foundational evidence base for integrating representations within organic chemistry instruction. Owing to how EPMs cue an underlying concept in organic chemistry of electron rich/poor areas within a molecule (a concept that rationalizes why molecules interact), the implications for organic chemistry instructors is to incorporate EPMs when instructing about electron rich/poor areas. Based on the cognitive theory students could use features in EPM to better recall concepts related to charge distribution such as electronegativity. The results suggest that instruction that makes use of EPM may find learning gains with students invoking foundational concepts to explain mechanisms and reactivity; however, this hypothesized relationship was not tested herein and would require future evaluation. Students could be trained on software such as *Jmol* to construct EPMs and use them in explaining molecule interactions.

The results also indicate that students may benefit in using representations such as ball-and-stick and EPMs in making predictions. Practicing chemists generate EPMs from experimental data and use the resulting model to detect high reactivity within a molecule. Examples of this are included in the popular journal *Nature* where several articles are published using EPMs during the year this paper was written (Jain et al., 2023; Kang et al., 2023; Shalaby et al., 2023). Being able to interpret and utilize EPMs is becoming an essential skill of a practicing chemist and should be considered as part of student training. A review of chemistry textbooks found that EPMs were frequently included but lacked conceptual support for students' use of EPMs (Hinze et al., 2013). Beyond observing models during lectures or in textbooks, students should be given opportunities to interact with them (Kumi et al., 2013). This study calls for instructors to incorporate EPMs during instruction and demonstrate how to translate between EPMs and line diagrams. Students can be guided and tasked with generating EPMs and explaining the charge distribution within a molecule or rationalizing reaction mechanisms.

Conclusion

There is a call to use more computer-generated EPMs as they have the ability to explicitly show uneven charge distribution that can be used to rationalize mechanisms (Fleming et al., 2000; Hinze et al., 2013; Sanderson, 1959; Sanger & Badger, 2001; Shusterman & Shusterman, 1997). This study offered evidence in support of that notion. It was found that more students with EPM correctly predicted partially negative atom than students with the other representations. It was also found that more students with EPM cited electronegativity, a concept central to predicting charges. No difference was observed across representations in students predicting electrophilic character; while representations did influence students identifying nucleophilic character. Results of this study informed that EPMs have affordances in cueing electron rich/poor areas within molecules that could promote students identifying electrophilic and nucleophilic characteristics and also understand the *why* behind mechanisms, especially nucleophilic substitution on aromatic compounds. Abstractness of organic chemistry should not be an obstacle in understanding chemical reactivity (Friesen, 2008). As EPMs make the implicit property of uneven charge distribution explicit, they are likely to offer support to students in seeing attraction between oppositely charged parts of molecules leading to leaving groups leaving, substitution occurring, or acid/base reactions.

Limitations

This study took place within one semester at one setting and cannot speak to generalizability but offers evidence of transferability by specifying what representations organic chemistry students work with at the research setting. Since students' explanations were involved and interpreted to answer the research questions, hermeneutic considerations play a role as another researcher could have interpreted these data differently. Further, as the study relied on single survey prompts for students to explain their processes, there was no opportunity to seek clarification. Thus, the results presented represent students' initial explanation when receiving the prompt. To address this limitation, the potential for ambiguity in interpreting student responses was acknowledged in the results presented. The authors also acknowledge that students at the research setting were not assessed with ball-and-stick or EPM, thus interpretations of their explanations using these representations is how students are likely to perform without formal instruction and that future studies need to be conducted on how students with formal training perform. Also, the survey provided the students with electronegativity values which was likely to prime students to use the concept in explanations. Future work that explores the impact of providing differing information to students (e.g. omitting electronegativity values, adding a legend for EPMs) would be helpful in providing more insight into the role these factors play in student reasoning.

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Appendix

Table A1. Survey prompts: The survey was single page and students could go back and forth between the prompts.

Instructions as seen by students; present at the top of each survey	Electronegativity values for atoms: Hydrogen 2.1 Carbon 2.5 Oxygen 3.5 Nitrogen 3.0 Chlorine 3.0 Differences in electronegativity values: Polar bond: Equal to or above 0.5 Nonpolar bond: Below 0.5
Informed Consent	○ Yes, I consent to participate in the research study. ○ No, I DO NOT consent to participate in the research study.

Type	Prompt Number	Survey Question
Hotspot	Prompt 1	Click on the atom that will experience a partial positive charge in the image below for benzoyl chloride (C_6H_5COCl). [Insert Representation for specific survey* from Box 1]
Essay	Prompt 2	Please explain your prediction for the atom with the partial positive charge.
Hotspot	Prompt 3	Click on the atom that will experience a partial negative charge in the image below for ethylamine ($NH_2CH_2CH_3$). [Insert Representation for specific survey* from Box 1]
Essay	Prompt 4	Please explain your prediction for the atom with the partial negative charge.
File-upload	Prompt 5	Draw the mechanism using MARVIN JS. Once in the Marvin JS tab, go to gear symbol on the top horizontal toolbar and make sure "show lone pairs" is checked. Save as MRV file and upload. Keep the tab open to be used for the next question. benzoyl chloride (C_6H_5COCl) and ethylamine ($NH_2CH_2CH_3$). [Insert Representations for specific survey* from Box 1]
Essay	Prompt 6	Please explain why the reactants benzoyl chloride (C_6H_5COCl) and ethylamine ($NH_2CH_2CH_3$) interact the way they do in the first step of the mechanism you proposed. [Insert Representations for specific survey* from Box 1]
Multiple-choice	Prompt 7	Predict the product for the reaction between benzoyl chloride (C_6H_5COCl) and ethylamine ($NH_2CH_2CH_3$). [Insert Representations for specific survey* from Box 1] ○ *N*-ethyl benzamide ($C_6H_5CONHCH_2CH_3$) [Insert Representation for specific survey* from Box 2] ○ *N*-ethyl formide ($HCONHCH_2CH_3$) [Insert Representation for specific survey* from Box 2] ○ Benzyl ethyl amine ($C_6H_5CH_2NHCH_2CH_3$) [Insert Representation for specific survey* from Box 2] ○ Propriophenone ($C_6H_5COCH_2CH_3$) [Insert Representation for specific survey* from Box 2]

*Specific survey indicates the representation the student was assigned to, for example, bond-line, ball-and-stick, or EPM

Table A2. Codebook for partial positive and partial negative explanations. See Appendix for exclusivity among codes

Code	Definition	Example Quote (Complete responses by students)
Pull on electrons without mentioning any feature[a]	An atom is pulling on electrons or electrons are moving between atoms without mentioning or explaining any features such as electronegativity, resonance, dipole, induction or polarity	*Nitrogen will **pull electron density from** the hydrogens and carbon that it's bonded to.*
Feature without mentioning pull on electrons[b]	Features other than electronegativity or resonance are mentioned but response is missing electrons are being pulled.	*Nitrogen has the stronger **dipole moment** so it holds the negative charge.*

Absolute electronegativity and pull on electrons	Electronegativity is mentioned using words such as electronegative, high, very, more without comparing to another atom, most and electrons are being pulled	*The Nitrogen atom is **an electronegative atom** meaning it will **pull the electrons** in the C-N bond towards itself resulting in a partial negative charge.*
Absolute electronegativity without pull on electrons	Electronegativity is mentioned using words such as electronegative, high, very, more without comparing to another atom, most but response is missing electrons are being pulled	*It is next to **an electronegative oxygen** and chlorine*
Relative electronegativity and pull on electrons	Electronegativity is compared using words such as more than, higher, lower, or values are subtracted and electrons are being pulled. For this to code to be applied, the student needs to mention another atom or within the molecule	*The nitrogen is **more electronegative than** hydrogen and carbon, therefore, **pulling the shared electrons** closer resulting in a partial negative charge.*
Relative electronegativity without pull on electrons	Electronegativity is compared using words such as more than, higher, lower, or values are subtracted but response is missing electrons are being pulled. For this to code to be applied, the student needs to mention another atom or within the molecule	*Oxygen and Chlorine are both **more electronegative than** the carbon atom*
Resonance and pull on electrons	Resonance is mentioned and electrons or lone pairs are being pulled	*This carbon will experience a partial positive charge **during resonance** after **2 electrons from the double bond are moved onto the oxygen**. the oxygen atom will then experience a partial negative charge.*
Resonance without pull on electrons	Resonance is mentioned but response is missing electrons or lone pairs are being pulled	*If the compound undergoes **resonance**, the Oxygen will be negatively charged, allowing the carbon to be partially positive*
Electron withdrawing group and pull on electrons	Electron withdrawing groups are mentioned and electrons are being pulled	*The oxygen is an **EWG**, so **it pulls electron density from** the Cl.*
Electron withdrawing groups without pull on electrons	Electron withdrawing groups are mentioned but response is missing electrons are being pulled	*NH2 is an **EWG***
Electron donating groups without pull on electrons	Electron donating groups are mentioned but response is missing electrons are being pulled	*NH2 is **electron-donating** and thus the C bonded to the N will experience a partial negative.*

a: lower priority than other codes, but higher than "feature without pull on electrons"; exclusive, cannot occur with other codes.
b: lower priority than all codes; exclusive, cannot occur with other codes

Pull is operationalized as an atom or element causing an action on electrons such that they are moving to one side. For example, pull on electrons, shift in electron density, or lone pairs moving between atoms. Features are operationalized as characteristics within a representation that can be explicit such as lone pairs in line diagram, or implicit such as negative charge of an atom in line diagram due to connectivity. Features include dipole, induction, polarity, connectivity, lone pairs or valence electrons, positive or negative charge of an atom, nucleophile, electrophile, color, type of bond such as covalent or pi bond, bonds breaking or forming, hydrogen bond. Partial positive or partial negative are not features.

Table A3. Codebook for nucleophilic attack explanations. See Appendix for exclusivity among codes

Code	Definition (Student mentions…)	Example Quote (Complete responses by students)
Presence of element only	"Nitrogen" or "Carbon"	*The **nitrogen** acts as the nucleophile and attacks the partial positive **carbon** electrophile, pushing the electrons from the double bond onto the oxygen*
Presence of molecule only	"Amine", "ethylamine", "carbonyl", "C=O", "ketone", "acyl chloride", "acid chloride", or "benzoyl chloride"	*The reactants **benzoyl chloride** and **ethylamine** interact the way they do in the first step because there is a protonation step*
Presence of element and molecule	"Nitrogen" or "Carbon", and "amine", "ethylamine", "carbonyl", "C=O", "ketone", "acyl chloride", "acid chloride", or "benzoyl chloride"	*The **nitrogen** atom of **ethylamine** with its lone pair acts can act as a nucleophile, and the **carbonyl carbon** of benzoyl chloride is very electrophilic. The nitrogen nucleophile thus attacks the carbonyl carbon*

Presence of neither element nor molecule	Neither "nitrogen" or "carbon", nor "amine", "ethylamine", "carbonyl", "C=O", "ketone", "acyl chloride", "acid chloride", or "benzoyl chloride"	*The partial negative charge will nuc. attack the position of the partial positive charge*
Nitrogen has a partial negative charge[a]	Nitrogen, amine, or ethyl amine exhibit a partial or slightly negative charge	*The* ***partial negative nitrogen*** *atom is attracted to the partial positive carbon atom in the acyl chloride group causing the lone pairs in the nitrogen to form a double bond with the carbon. This reaction forces to C=O double bond to break apart and makes the oxygen a negative ion*
Nitrogen has a charge that is unclear[a]	Nitrogen, amine, or ethylamine has a charge without implying partial	***Net negative on Nitrogen*** *and Net positive on carbon react.*
Nitrogen is nucleophilic	Nitrogen, amine, or ethylamine is nucleophilic	*The* ***nitrogen is nucleophilic*** *in nature so it attacks the carbonyl carbon*
Nitrogen is electron rich	Nitrogen, amine, or ethylamine is electron rich	*Since the nitrogen is partially negative and* ***electron-rich****, it will act as the nucleophile and attack the partially positive carbon of the carbonyl/acid chloride*
Carbon has a partial positive charge[b]	Carbon, carbonyl, C=O, ketone, acyl chloride, acid chloride. or benzoyl chloride has a partial positive charge	*The nitrogen acts as a nucleophile, attacking the* ***partially positive carbon*** *in the carbonyl of the benzoyl chloride, punching the electrons in the double bond up to the oxygen giving the oxygen a negative charge*
Carbon has a charge that is unclear[b]	Carbon, carbonyl, C=O, ketone, acyl chloride, acid chloride. or benzoyl chloride has a charge without implying partial	*The Chloride is a good leaving group, so there is a* ***+ charge on the carbon****, especially since the double bond on the oxygen breaks*
Carbon is electrophilic	Carbon, carbonyl, C=O, ketone, acyl chloride, acid chloride. or benzoyl chloride is electrophilic	*The amine is nucleophilic and the* ***carbonyl carbon is electrophilic***
Carbon is electron poor	Carbon, carbonyl, C=O, ketone, acyl chloride, acid chloride. or benzoyl chloride is electron poor	*The electron dense nitrogen will act as a nucleophile and attack the* ***electron poor carbonyl carbon***
Attraction of opposite charges	Positive and negative charges attract	*The* ***partial negative charge*** *of the nitrogen is* ***attracted*** *to the* ***partial positive charge*** *of the carbon a part of the carbonyl, thus the nitrogen performs a nucleophilic attack on the carbon*
Attack that is unclear[c]	Attack but no mention of nucleophile, nitrogen, or lone pair i.e. no specification of the agent attacking	*The most electronegative atom of one molecule* ***attacked*** *the most positively charged atom of the other molecule*
Nucleophilic attack that is unclear[d]	Nucleophilic attack but no identification of the attacking agent or the receiving agent.	*Amines are very strong Lewis Bases (electron donors) which makes them nucleophilic. Thus, it will perform a* ***nucleophilic attack*** *as the first step in the mechanism*
Nucleophile attacks electrophile[d]	Nucleophile attack on electrophile OR attack and identification of nucleophile and electrophile	*the ethylamine would act* ***as a nucleophile and attack the electrophile****, which is the benzoyl chloride since it wishes to donate it's electrons (Electron donating group)*
Nitrogen attacks carbon	Nitrogen, amine, or ethylamine attacking carbon, carbonyl, C=O, ketone, acyl chloride, acid chloride, or benzoyl chloride	*The first step was a nucleophilic attack. The nitrogen has a partial negative and the carbon has a partial positive. This allows for the* ***nitrogen to attack the carbonyl group****.*
Lone pair attacks	Lone pair is making the attack	*The* ***lone pair*** *on the partial negative nitrogen* ***attacks*** *the partially positive carbon on the other molecule. The pi bond on the oxygen then moves up and makes the oxygen negative*
Chloride as leaving group	Chlorine leaves or gets kicked off	*The benzoyl chloride and ethylamine interact the way they do in the first step of the mechanism because the* ***chlorine serves as a leaving group*** *and is used to add the ethylamine to the central molecule*

Carbon has only four bonds	Carbon has only four bonds or cannot exceed four bonds	*The carbon in the carbonyl group is extremely electrophilic. With the nitrogen acting as a nucleophile, it would make sense that it would attack that carbon. Due to the fact that* ***carbon cannot have more than 4 bonds****, the 2 electrons of the double of the carbonyl would move up to oxygen*
Double bond to atom	Electrons of the double bond within carbonyl move onto the oxygen atom	*The nitrogen acts as a nucleophile, attacking the partially positive carbon in the carbonyl of the benzoyl chloride,* ***punching the electrons in the double bond up tot he oxygen*** *giving the oxygen a negative charge*

a. Exclusive with each other
b. Exclusive with each other
c. Exclusive with nucleophilic attack unclea, nucleophile attacks electrophile, nitrogen atatcks carbon, and lone pair attacks
d. Exclusive with each other