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ARTICLE

Analysis of Organic Chemistry Students' *Developing* Reasoning Elicited by a Scaffolded Case Comparison Activity

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Recent efforts in organic chemistry education research focus on investigating activities and strategies designed to elicit students' mechanistic reasoning. This study investigates how a scaffolded case comparison activity implemented in an introductory organic chemistry course elicits and supports students' mechanistic reasoning in an authentic classroom setting. The activity included an adaptation of a previously reported reasoning scaffold to support small-group student discussions comparing organic reactions. We analyzed students' written responses to the in-class activity using Hammer's resources framework and Toulmin's argumentation model, interwoven to create an anti-deficit approach to exploring students' developing reasoning. The analysis of students' written artifacts sought to identify ways in which a scaffolded case comparison implemented in a collaborative class setting may support students' engagement in complex reasoning and argumentation development. We found that the in-class activity elicited students' writing about various aspects of mechanistic reasoning, including identifying explicit and implicit properties, dynamic reasoning, and multivariate reasoning. These findings indicate that the activity can engage students in complex mechanistic reasoning aspects in the classroom setting. Furthermore, this study extends the literature by detailing the nuances of students' developing causal reasoning with energetic and electrostatic accounts as shown in their writing. The results highlight students' emerging causal reasoning with varying levels of complexity and conceptual integration. This study provides direct implications for instructors seeking to implement similar classroom activities. The findings indicate directions for future research on the development of instructional activities and tools that further support students' developing causal reasoning, such as adapting existing scaffolding structures to support argumentation development and the integration of challenging concepts such as energetics.

Introduction

Organic chemistry courses aim to support students' reasoning and problem-solving with reaction mechanisms, reflecting a central practice of organic chemists (Dood and Watts, 2022, 2023). Mechanisms are a central part of chemists' work, as they provide structural information necessary for understanding the relative energies of entities or for analyzing multiple reaction pathways (Goodwin, 2003). Organic chemistry curricula challenge students to develop all of the necessary content knowledge to engage with mechanisms as well as the reasoning patterns to integrate multiple concepts into the analysis of a given mechanism (Flynn and Ogilvie, 2015; Galloway and Bretz, 2015; Cooper *et al.*, 2019). However, research regarding the reasoning behind problem-solving indicates that students may produce correct answers to mechanisms but may need additional support to understand the underlying concepts or properties (Bhattacharyya and Bodner, 2005; Graulich, 2015). Existing research investigates approaches to support students' translation of conceptual understanding of salient properties, such as underlying electronics, into deeper-level reasoning during problem-solving (Caspari, Kranz and Graulich, 2018; Caspari and Graulich, 2019; Graulich, Hedtrich and Harzenetter, 2019; Graulich and Caspari, 2021; Dood and Watts, 2023). Yet, there exists a need for further research that translates these activities into the authentic classroom setting. Therefore, this research aims to analyze students' mechanistic and causal reasoning as elicited by a classroom activity intended to scaffold students' thinking about underlying properties.

Scaffolded Case Comparisons

One research-based approach that can support complex reasoning is scaffolding students' problem-solving. Scaffolds are temporary support tools or structures which help students reason through problems while lessening the cognitive load (Graulich and Caspari 2021). Scaffolded problem-solving can involve a variety of different techniques such as sentence starters, prompts, or guiding questions that facilitate the identification and connection-making parts of constructing an explanation (Kang, Thompson and Windschitl, 2014). In the context of organic chemistry, a primary goal of scaffolding is to support students' ability to identify and integrate implicit properties into their explanations of reaction mechanisms (Graulich and Caspari 2021). Implicit properties are underlying concepts or variables, such as resonance or induction, that are foundational for analyzing reaction mechanisms. Prior research indicates that students' reasoning highly depends on their

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ability to correctly identify and use implicit properties (Graulich, Hedtrich and Harzenetter, 2019). Scaffolding activities in organic chemistry can support students' ability to identify and integrate multiple implicit properties into the development of sophisticated, complex explanations (Caspari and Graulich, 2019; Graulich and Caspari, 2021).

In order to elicit student reasoning about implicit properties, scaffolds can be used in combination with case comparison activities in which students compare two different reaction mechanisms (Caspari and Graulich, 2019; Watts *et al.*, 2021). Reasoning in organic chemistry is often a comparative process, as organic chemists reason through similarities and differences in reactivity between different reaction environments. As such, contrasting two reactions against one another may elicit student thinking about additional implicit variables compared to considering an individual reaction, thus engaging students in more complex reasoning (Bodé, Deng and Flynn, 2019; Caspari and Graulich, 2019). Furthermore, case comparisons are designed to challenge students to consider and develop causal arguments through the identification of variables that might influence the mechanism and relative rate of the two reactions. By combining case comparison problems with scaffolds, students may work through reaction mechanisms using a stepwise reasoning structure (guided by the scaffold) (Caspari and Graulich, 2019; Watts *et al.*, 2021).

This project builds on existing research focused on promoting students' mechanistic and causal reasoning using a specific scaffolded case comparison activity (Watts *et al.*, 2020, 2021; Graulich and Caspari, 2021). In a study of this activity, Caspari and Graulich (2019) found that students who used the scaffolded case comparison described more variables in their reasoning than those who did not use the scaffold. Furthermore, they found that the scaffolded structure builds on the existing structure of students' comparative mechanistic reasoning (Caspari and Graulich, 2019). In another study using a scaffolded case comparison activity informed by the Graulich and Caspari (2021) structure, Watts et al. (2021) implemented the same activity in the classroom setting and investigated organic chemistry students' written responses. This study found the importance of supportive activities designed to elicit student reasoning and encouraged further exploration of in-class activities to support student reasoning, providing initial insight into how instructors can implement similar in-class activities on a larger scale (Watts *et al.*, 2021).

We aim to further explore how the scaffolded case comparison activities elicit students' mechanistic reasoning in a larger-scale, authentic classroom setting (Figure 1). This study therefore utilizes the structure of the scaffolded case comparison in a collaborative environment, in which students worked through the activity in two parts: a group-work portion followed by an individually written portion. Studies have shown that collaborative work environments encourage more hypotheses, alternative explanations, and entertainment of more explanations (Okada and Simon, 1997; Kaartinen and Kumpulainen, 2002). Given this, we designed this activity to combine the scaffolded case comparison activity with group participation to elicit mechanistic reasoning in student written responses.

Conceptual Framework: Mechanistic Reasoning

Several different reasoning frameworks exist for capturing different aspects of student reasoning in organic chemistry (Machamer, Darden and Craver, 2000; Kraft, Strickland and Bhattacharyya, 2010; Sevian and Talanquer, 2014; Cooper, Kouyoumdjian and Underwood, 2016; Caspari, Kranz and Graulich, 2018; Graulich, Hedtrich and Harzenetter, 2019; Dood *et al.*, 2020; J. Dood *et al.*, 2020; Yik *et al.*, 2023). These frameworks articulate the reasoning patterns, such as teleological reasoning, anthropomorphic reasoning, mechanistic reasoning, and causal reasoning (in order of increasing sophistication and depth) that students may employ (Dood and Watts, 2022). Although these frameworks seek to categorize student reasoning into different themes, modes, or levels, there are many existing definitions for mechanistic and causal reasoning across the different reasoning frameworks. For this study, we follow the synthesized definitions articulated by Dood and Watts (2022, p. 2869):

> "In a broad sense, mechanistic reasoning encompasses students' descriptions of *how* a reaction occurs, typically at a level lower than the observed phenomena; that is, descriptions of how reactions between molecules proceed through electron movements and changes in bonding. Causal reasoning encompasses students' explanations of *why* a reaction occurs, typically using the chemical or physical properties of reacting materials to provide an explanation that links causes to effects."

Following from these definitions, we conceptualize *causal reasoning* as one aspect of mechanistic reasoning.

Aspects of Mechanistic Reasoning

To explain *how* and *why* mechanisms occur, students may need to consider a variety of different aspects of mechanistic

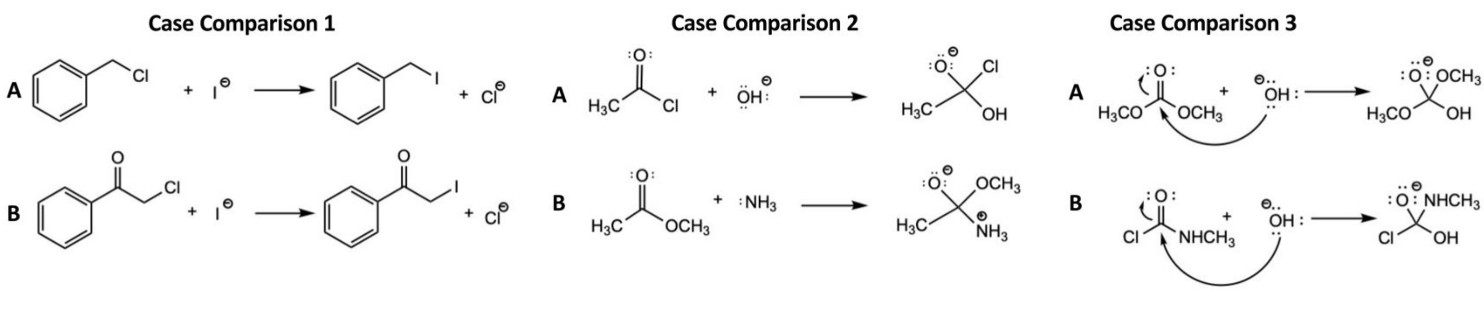


Figure 1. Three case comparison activities. Students were prompted to develop an argument about whether reaction A or B occurs faster. Students proposed curved arrows for Case Comparison 1 and 2, but curved arrows were provided for Case Comparison 3 to clarify the mechanistic pathway to focus on.

reasoning including the identification of explicit and implicit properties, dynamic reasoning, multivariate reasoning, and causal reasoning. The integration of several of these reasoning patterns together generally represents a more sophisticated and higher-order explanation of chemical mechanisms. However, students need support in navigating and developing different reasoning patterns through evidence-based instructional practices employed by instructors (Sevian and Talanquer, 2014; Weinrich and Talanquer, 2016; Caspari and Graulich, 2019; Watts *et al.*, 2020, 2022).

Students often need to identify and reason through multiple properties to understand a given reaction mechanism, including explicit properties (e.g., charges) and implicit properties (e.g., nucleophilicity) (Weinrich and Talanquer, 2016; Caspari, Kranz, and Graulich, 2018). For example, students may justify a particular mechanistic step occurring by focusing on the explicit properties of reaction species (e.g., identifying that a positively charged carbon will react with a negatively charged oxygen) or they may justify mechanistic steps by considering the underlying, implicit properties (e.g., identifying that a carbon is electrophilic and therefore susceptible to react with nucleophilic species in the reaction mixture) (Anzovino and Bretz, 2015). The consideration of implicit properties is typically associated with more sophisticated reasoning (Graulich, Hedtrich and Harzenetter, 2019). However, students often need more support to engage in reasoning with implicit properties, as it can be more challenging to identify the salient implicit properties relative to explicit properties.

Furthermore, many problems in organic chemistry require focusing on more than one specific (implicit or explicit) property to construct an explanation. Multivariate reasoning, another aspect of mechanistic reasoning, entails the identification and thoughtful integration of multiple causal variables into explanations. Goodwin (2003) describes that beyond the identification of these properties and the dynamic interactions between them, students may need to integrate multiple variables into their analysis of a mechanism to construct a coherent explanation (Goodwin, 2003; Caspari and Graulich, 2019; Graulich and Caspari, 2021). Studies suggest that while students can engage in mechanistic reasoning to describe reactions, they may need further support to engage in multivariate reasoning (Sevian and Talanquer, 2014). As students integrate multiple causal variables into discussion, they must also weigh the impact of important chemical and physical properties on the overall reasoning about a mechanism.

Mechanistic reasoning also necessitates understanding that many physical and chemical properties emerge from dynamic movement and interactions within and between molecules (Caspari, Kranz and Graulich, 2018). As such, one aspect of mechanistic reasoning is dynamic reasoning, which entails providing dynamic explanation of *how* observed phenomena occur. Caspari et al. (2018) defines mechanistic reasoning as necessitating a static or dynamic approach to change and that constructing more complex explanations requires dynamic reasoning. For example, students may reason statically about explicit charges impacting potential energies, but in order to make a claim about activation energy, students must approach reactions dynamically (I. Caspari, Kranz, and Graulich 2018). Furthermore, to engage in causal reasoning, students may need support to identify the results of dynamic interactions between multiple components rather than relying on anthropomorphic or teleological reasoning. Supporting students' dynamic explanation of *how* mechanisms occur is integral in supporting higher-order causal reasoning about *why* mechanisms occur.

Research has conceptualized causal arguments to include chaining evidence to claims, including the development of structural evidence (i.e., the cause) to provide the basis for an energetic or electrostatic claim (i.e., the effect) (Dood and Watts, 2022). When prompting students' causal reasoning, students may integrate aspects of mechanistic reasoning. For example, students may begin with the identification of a structural feature (e.g., carbonyl group) that has salient implicit properties (e.g., resonance) and connect to the effect (e.g., lowered activation energy) on a particular mechanism (Dood and Watts, 2022). Students can engage in deeper-level causal reasoning when activities scaffold students' construction of arguments that connect structural evidence to developed claims (Caspari, Kranz and Graulich, 2018). The goal of this study is to investigate how an evidence-based activity in an authentic classroom setting elicits organic chemistry students' developing causal and mechanistic reasoning.

Theoretical Framework

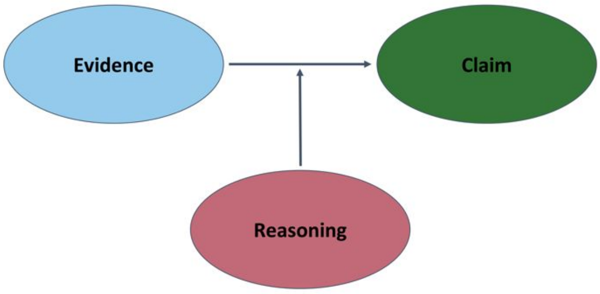


Figure 2. Toulmin Argumentation model.

This study utilizes two frameworks, which are interwoven to create an anti-deficit approach (Davis, 2019) to capturing students' engagement in reasoning as elicited by the activity. Anti-deficit approaches to student learning and interactions are a response to the conceptions of a *deficit* approach to students' capacity or capability of learning (Adiredja et al. 2020). The anti-deficit approach views students as capable, frames their attempts as assets, and acknowledges that students hold unique experiences and perspectives (Adiredja et al. 2020). This study aims to combine two frameworks to take this perspective on undergraduate student learning. To support students' high-level problem-solving and mechanistic reasoning in the classroom, we used Toulmin's model of argumentation to guide the development and analysis of the activity. In general, an argument requires building support for a claim and involves discussion between individuals who hold different perspectives and make different claims (Akbaş, 2021). Therefore, a central component of argumentation is its collaborative nature, which prompted us to include collaborative group discussion of the students' claims during the activity. Collaborative group discussion through argumentation can also be a useful tool in scientific education and classroom learning to connect students to the sociocultural practices of scientific communities (Kelly and Chen, 1999). Research on the integration of argumentation in science education through the lens of sociocultural perspectives on cognition indicates that students require time and opportunities to practice understanding the uses of data as evidence for developing claims in the science setting (Kelly and Chen, 1999). Thus, the activity central to this study gave students the opportunity to collaboratively and individually develop arguments in the classroom setting.

Toulmin's Model of Argumentation

The Toulmin model of argumentation structures the different aspects of building an argument to support a conclusion (i.e., the *claim*) (Toulmin, 2003). In the context of scientific discourse, the Toulmin model highlights the structure of an argument in terms of interconnected components of a claim, data to support the claim (i.e., *evidence)*, and warrants to connect a link between the data and claim (i.e., *reasoning*) (Erduran, Simon and Osborne, 2004). While the full Toulmin model contains additional components, claim, evidence, and reasoning are considered the essential components of an argument. Hence, the activity in this study utilized the essential components of the Toulmin model (Figure 2) for introductory engagement in argumentation in the science setting (Toulmin, 2003; Erduran, Simon and Osborne, 2004) by prompting students to discuss these aspects of the Toulmin model both directly and indirectly (see Appendix 1).

Evidence and Reasoning as Resources

Given that the identification of evidence serves as a foundational component of argumentation, we sought to investigate how students identify and weigh different pieces of evidence to support their claims. In Hammer's (2000, 2003, and 2005) resources framework, resources are fine-grained cognitive elements of knowledge. Evidence and reasoning that students utilize to support their claims can be considered conceptual resources (Hammer and Elby 2002, Hammer 2005). According to the framework, resources are *activated* in response to a given problem. Resources-based perspectives describe students' thinking about resources as productive or unproductive depending on how the student *frames* (i.e., interprets based on prior knowledge, experiences, and expectations) the activation of the resource based on the context (Hammer *et al.*, 2005). By viewing knowledge as emergent, the resources framework provides a contrast to more rigid frameworks that may evaluate cognitive elements as misconceptions; a resources-framed view of student learning promotes instruction to support students in activating resources productive for learning (Hammer and Elby, 2003; Hammer *et al.*, 2005). As students develop arguments, resources are both activated and reconciled, which refers to weighing the importance of various activated resources (Hammer and Elby, 2003). Students may encounter inconsistencies in the resources that are activated, and students can identify and weigh these inconsistencies to allow them to consider which activated resources best support their claims (Hammer et al. 2005; Hammer and Elby 2003).

The activity central to this study prompted student argumentation in response to the guiding question about the case comparison: "Which reaction occurs faster, A or B?" When students engaged in argumentation and identification of evidence to support their claim, they activated different *resources* (explicit and implicit variables) depending on the specific context of the activity. This study aims to analyze student engagement in mechanistic reasoning through an anti-deficit lens, by focusing on identifying the resources students activated. By capturing the resources activated within students' individual written arguments, we can better understand how students engaged in mechanistic reasoning. This analysis allows for an anti-deficit approach to capturing students' reasoning by identifying which productive resources they integrated into their argument as evidence and reasoning to support their claim. Since students activate resources to support a claim, both Toulmin's argumentation model and Hammer's resources framework are useful for describing students' written responses to the prompt. Furthermore, these frameworks guided our analysis and development of implications for supporting students' construction of arguments as they reason through reaction mechanisms.

Research Questions

This project translates research into practice by implementing a scaffolded case comparison activity in the classroom setting to elicit organic chemistry students' mechanistic reasoning. Furthermore, Toulmin's argumentation model and Hammer's resources framework are used to capture and identify students' developing causal reasoning, which may include developing connection-making between structural evidence to claims rooted in energetics or electrostatics. We aim to explore how the evidence-based activity prompts mechanistic reasoning as evidenced by students' written responses by asking three research questions:

1. How do students develop arguments using activated explicit and implicit resources as evidence for their claims?
2. How does the activity elicit organic chemistry students' resources related to dynamic and multivariate mechanistic reasoning in students' written responses?
3. How does the activity elicit organic chemistry students' causal and developing causal reasoning in students' written responses?

Methods

Research Context and Participants

This study was conducted at the University of Michigan. The activities were implemented in a second-semester introductory organic chemistry laboratory course during the Winter 2021 semester. As a result of the COVID-19 pandemic, this class was held in an online environment, which met synchronously via Zoom video-conferencing software. The organic chemistry laboratory course was offered separately from the lecture course and included an instructor-taught hour of lecture. Each laboratory section was 4 hours, had around 15 students enrolled, and was taught by graduate teaching assistants (see Appendix 2).

Students in the second-semester introductory organic chemistry laboratory course consisted mostly of first- and second-year students (Shultz, Gottfried, and Winshel 2015). Historically, the majority of students enrolled in the class have yet to declare their major, though most students enrolled in this course eventually declare majors including neuroscience, biopsychology, and biology. This course is often taken as a prerequisite for upper-level science courses such as biochemistry and biophysics. This is often the first course students take that includes learning objectives and content related to reaction mechanisms and mechanistic reasoning in chemistry. Students were recruited for participation via a Qualtrics form sent during class sessions in which students could agree to share their written responses for a research project. All participants voluntarily consented to participate in the study, and Institutional Review Board approval was obtained (IRB HUM00079234). Out of 802 students who received a final grade in the second-semester introductory

Table 1. Overview of the coding scheme.

Aspect of Toulmin's Argumentation Model	Code	Grain Size:	Student Example:
Claim	Claim	Sentence-level	"Reaction B will proceed faster than reaction A."
Evidence	Resonance[a]	Sentence-level	"They also donate or push electrons through resonance because of the delocalized lone electron pairs on the oxygen molecules"
Reasoning	Dynamic	Sentence-level	"The other starting material has a naturally electrophilic carbon in the carbonyl, given that carbonyls are electron-withdrawing groups that pull electron density out of the molecule and towards themselves, which leaves the carbon of the carbonyl with a partial positive charge."
	Multivariate	Sentence-level	"The chlorine group is electron withdrawing, as it creates a dipole with the carbon through induction, leaving a partial positive charge on the carbon."
	Causal	Argument-level	"Reaction B will proceed much faster than Reaction A because of its carbonyl group. Minus this carbonyl group, the molecules are structurally the same. This leads to the suspicion that the carbonyl group is what is influencing the speed of the reaction. The oxygen of the carbonyl is able to support more electrons than the single carbon in molecule A. This extra electrodensity supported by the carbonyl, and more specifically, the oxygen atom, allows for a faster SN2 reaction in Reaction B. While SN2 reactions do not form a carbocation like SN1 reactions, they are similar in the fact that a carbon with greater electrodensity near it will react more quickly. Therefore, Reaction B proceeds faster than Reaction A."

[a] The "Resonance" code is one example of an evidence codes; the full set of evidence codes are provided in Appendix 3, Table 2

organic chemistry laboratory course, 779 students consented to participate. All students enrolled in the class had to complete the activity for a grade; however, students provided consent to share their written responses with researchers to include in the study. Students' identities were anonymized by removing any identifying information from their submissions.

Classroom Implementation and Data Collection

The primary data for this study consisted of students' written responses to scaffolded case comparison activities. Three scaffolded case comparison activities were implemented throughout the 14-week semester, each with the same scaffolded prompts but differing case comparisons. The activities consisted of a worksheet that presented a case comparison of two reactions labeled A and B. Figure 1 shows the three case comparison reactions in the worksheet (See Appendix 2 for the full activity design). The activities included two written portions: a collaborative portion and an individual portion.

The collaborative portion utilized scaffolded questions to be worked through in a group environment within Zoom breakout rooms, each group consisting of 3-5 students. In alignment with the Graulich and Caspari (2021), these questions were scaffolded to prompt students' (1) identification of structural differences between the two reactions; (2) discussion of the chemical and physical properties of the reactions; (3) discussion of the changes that occur in Reactions A and B and description of why those reactions occurred. Finally, the last question utilized a sentence stem to prompt students to make a claim as a group using three pieces of evidence. After discussions in groups, students returned to a main breakout room where the whole class discussed ideas proposed in the group portion of the activity. The second part of the activities prompted students to individually *"Write a brief 2-3 paragraph argument describing which reaction you predict will proceed faster. Your argument should include a claim (i.e., Reaction A is faster than reaction B), evidence (i.e., description of the structural features and properties associated with molecules in each reaction), and warrant (i.e., a reasoning about why these structures/properties result in the changes that occur and lead to one reaction being faster than the other)."* Each student submitted a response which included both the collaborative portion and the individual portion for each activity. In contrast to the Graulich and Caspari (2021) scaffold, the prompts were presented to the students linearly to better facilitate students' discussion in a Zoom environment. A total of 3998 responses across the three activities were collected to comprise the dataset for this study. Discussion times were approximately 90 to 120 minutes for each case comparison activity.

Data Analysis

Data analysis focused on qualitatively analyzing the student written responses for each activity. The authors iteratively developed the coding scheme using constant comparative analysis. The coding scheme was developed both deductively and inductively through frequent meetings between researchers to clarify definitions and examples of codes (Saldaña, 2021). A set of deductive codes were developed in alignment with Toulmin's framework (codes for claim, evidence, and reasoning). Variations in students' use of evidence and reasoning were identified through inductive coding. Early in the coding process, we chose to focus the analysis using a sentence-level unit of analysis, meaning all applicable codes were applied at the sentence level.

The coding scheme aligns with the foundational parts of Toulmin's argumentation framework (i.e., claim, evidence, and reasoning) and with key aspects of comparative mechanistic reasoning (Table 1). The claim code was applied on the sentence level when students made a claim about reaction A or B occurring faster. Evidence codes were applied on the sentence level and included instances where students discussed activated resources such as explicit and implicit variables, including discussion of electronic properties, identification of nucleophilic and electrophilic groups, and description of events

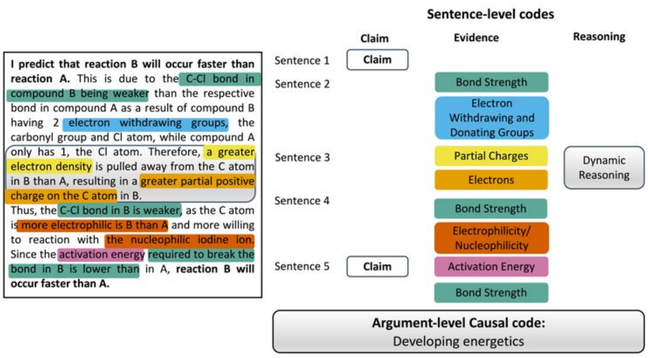


Figure 3. Visualization of coding scheme. Claim codes are bolded, evidence codes are highlighted in varied colors (green, blue, orange, yellow, red, dark pink), and reasoning codes are highlighted in gray. All codes were applied at the sentence level, except the causal code which was applied at the argument level. While the claim, evidence, and dynamic reasoning codes were applied to the sentence level, the highlighted text indicates the specific parts of each sentence that warranted the application of the codes. The boxed paragraph is one example of a student's entire written argument, which can vary from one paragraph to several paragraphs.

such as bond breaking and making (See Appendix 3). Reasoning codes (dynamic, multivariate, and causal) were initially all coded on the sentence level. While inductively coding for students' reasoning, we found that the sentence-level grain size for the analysis was not suited for capturing evidence of students' causal reasoning. However, causal reasoning was apparent when considering students' complete arguments. Because of this, we sought to identify students' causal reasoning at the argument level rather than the sentence level. Argument-level analysis required reading the entire individually-written argument section and assigning causal reasoning codes to the entire argument.

To begin inductively developing codes for students' attempts at causal reasoning, the first author memoed observations about the students' causal reasoning on the argument level. Then the research team met to read further samples of students' responses, memo observations of students' engagement in causal reasoning, and discuss varying interpretations. After the initial discussions, we individually analyzed 18 further samples of student writing at the argument level and inductively developed codes to identify the different ways in which students engaged in causal reasoning. Through the discussions with the research team, we identified three codes to identify students' causal reasoning: engaging with an electrostatics account, engaging with an energetics account, and developing causal reasoning (engagement in emerging causal reasoning with an electrostatics or energetics account). An example of the complete coding scheme applied to a single response is shown in Figure 3.

Reliability. Reliability was established separately for the sentence-level and argument-level coding. For the sentence-level coding, the first two authors separately and independently applied the sentence-level codes to 20 samples of student writing, followed by meetings in which we discussed the applied codes. In these meetings, inter-rater reliability (IRR) measures were determined by calculating fuzzy kappa (Watts and Finkenstaedt-Quinn, 2021). Fuzzy kappa is an agreement estimation for inter-rater reliability that is used for instances where multiple codes could be applied to one unit of analysis (Kirilenko and Stepchenkova, 2016). The coders achieved fuzzy kappa values that denoted strong agreement (>0.8) before any further analysis was done, and all samples included in the initial rounds of coding were re-coded with the finalized coding scheme. A subset of the participant data was randomly selected and 109 samples of student-written responses were analyzed at the sentence level.

For the application of the causal reasoning codes on the argument level, the first author randomly selected 50 responses and coded the data until reaching saturation (Saldaña, 2021). During weekly research meetings, the authors discussed the application of codes until reaching consensus for all responses, to establish dependability and confirmability of the findings (Lincoln and Guba, 1985). Together, the sentence-level and argument-level coding was used to identify trends with respect to how students engaged in identifying explicit and implicit variables, dynamic and multivariate reasoning, and causal reasoning.

Results and Discussion

This study sought to identify how mechanistic reasoning was present in the student writing samples produced from working through the scaffolded case comparison activity in the classroom. In the following sections, we address our research questions by describing how students engaged in reasoning as elicited through their individual written arguments. For research question 1, we provide an overview of the claims students made and the evidence students used to support their claims. For research question 2, we focus on key aspects of mechanistic reasoning which were evident on the sentence level (i.e., dynamic and multivariate reasoning). For research question 3, we highlight instances of student engagement in causal reasoning, which were evident on the complete argument level.

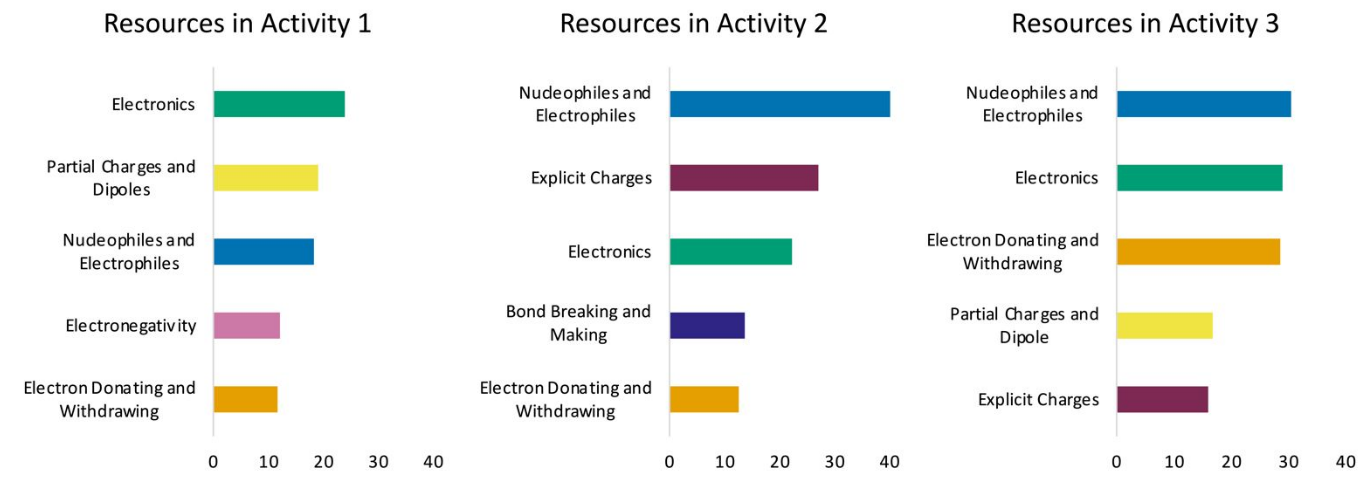


Figure 4. Top 5 explicit and implicit variables (activated resources) students used for each case comparison activity. Discussion of each variable, coded on the sentence level, were summed across each case comparison and divided by the total sentences coded for said case comparison. Across the case comparisons, students often discussed nucleophilic and electrophilic properties, electronics, explicit and implicit charges, and electron donating and withdrawing groups.

How do students develop arguments using activated explicit and implicit resources as evidence for their claims?

Student Claims. The activity prompted students to develop an argument about which reaction occurred faster. One scaffolding structure implemented to support students' development of their argument was a sentence starter outlining how students can (1) make a claim about which reaction occurred faster and (2) back their claim with evidence. Students responded directly to this sentence starter with claims such as:

> *"Reaction B occurs at a faster speed because the carbon of the carbonyl is more partially positive than that of reaction A, based on the fact that it has an electron withdrawing group, which makes it a better electrophile that reacts better with the nucleophilic alcohol."* [Case Comparison 3]

In this example, the student made the claim that Reaction B occurs faster and the student supported this claim using implicit properties including the presence of electron withdrawing functional groups and electrostatics as evidence. For each case comparison, all students made the same claim about which reaction occurred faster; we conjecture that this is likely due to the collaborative nature of the activity (i.e., students discussed their claims within small groups and with the full class before writing their individual argument). The goal of our analysis was not to identify correctness but rather to focus on the resources students activated to develop their reasoning through the activity. Despite the similarity in claims made, students' individually written arguments exhibited significant variation in the evidence leveraged to support their claim.

Evidence in Student Claims. The most common explicit and implicit variables students used in their arguments for each case comparison are shown in Figure 4. For example, the identification and discussion of nucleophiles and electrophiles was in the top 5 variables students discussed for each case comparison. One student included this variable by comparing nucleophilic and electrophilic properties:

> *"This decreased electron density and increased partially positive charge on the carbon center means that this electrophilic carbonyl is well positioned to react with the nucleophilic anionic alcohol. The strengthened electrostatic interactions of this reaction make it proceed faster than reaction A which has weaker electrostatic interactions"* [Case Comparison 3].

As in this example, students' analysis of the nucleophilic and electrophilic properties within the reaction often connected to their claims through direct comparison of the electrostatic interactions between the two reactions. This exemplifies how students used the identification and discussion of these implicit properties to construct their claim about which reaction occurs faster.

Furthermore, comparing across the case comparisons, we can identify how the design of the activity impacted students' writing about evidence (explicit and implicit properties) through the lens of Hammer's resources framework (Hammer, 2000; Hammer and Elby, 2003; Hammer *et al.*, 2005). The fluctuation in the use of explicit and implicit properties aligns with the specific structural differences between the two cases in each case comparison problem. These explicit and implicit properties represent activated resources, and the fluctuation in evidence across the three activities indicates that students activated different resources which correspond to the different phenomena and how students framed the activities. The evidence students activated to construct arguments in this activity align with the existing literature on the resources students activate when they are prompted to describe a mechanism using a scaffolded case-comparison activity (Caspari and Graulich, 2019; Watts *et al.*, 2021). For instance, in both prior research (Caspari and Graulich, 2019; Watts *et al.*, 2021) and the present study, students commonly activated resources about the charges of reacting molecules and the presence of electron donating and withdrawing groups. Identifying the resources students activate when considering case comparisons provides a starting point for identifying how students engage in mechanistic and causal reasoning within their written arguments.

How does the activity elicit organic chemistry students' resources related to dynamic and multivariate mechanistic reasoning in students' written responses?

Resources Activated in Students' Dynamic Reasoning. Dynamic reasoning included students' descriptions of mechanistic processes using active, rather than static, language. When students wrote about properties dynamically rather than statically, they tended to exhibit an increased depth of reasoning when connecting implicit properties to their claims. Many sentences that exhibited dynamic reasoning included discussion of electron movement, such as electron density being pulled by electronegative functional groups or providing active (rather than static) descriptions of the leaving group. For example, one student included dynamic electron movement by writing the following argument about case comparison 3:

"*The two methoxy side groups are electron donating, given that the delocalizable lone pair on the oxygens that can shift all the way to the carbonyl oxygen through resonance. The increased electron density pushed toward the carbon of the carbonyl decreases the electrophilicity of the molecule that is supposed to act as the electrophile in the reaction.*" [Case Comparison 3].

This case comparison differed by two different sets of functional groups (i.e., OCH_3 vs. Cl and OCH_3 vs. $NHCH_3$), which elicited student writing about how different electron donating and withdrawing groups impact electron density and therefore impact electrophilicity. In the example above, the student's identification of the electron-donating properties of the methoxy functional groups was further supported by their discussion of dynamic electronic movement. Rather than a more static approach to discussing electron-donating groups, the student utilized a dynamic description, suggesting that the student had a grasp of the concept of electron-donating groups that extends beyond classification and memorization-based naming into application and analysis. Caspari et al. (2018) found and asserted that supporting students' dynamic approach to change is highly important to building more complex causal reasoning arguments. Within our analysis, students' dynamic reasoning did not often directly relate to their claim, but instead was a resource activated to increase the depth of their evidence. While Caspari and Graulich's (2019) implementation of the scaffold primarily elicited students' multivariate reasoning, the scaffold implemented for the present study additionally elicited students' dynamic reasoning. This difference may relate to the different context between the studies (i.e., interviews *vs.* an in-class activity). In our context, students' dynamic reasoning often related to the process of change (e.g., electron movement, transition state, charge formation) rather than the change visible in the product (e.g., product formal charges, bond breaking and making).While students' engagement in dynamic reasoning did not change the claims they made, the elicited dynamic reasoning supported the depth of their evidence (e.g., the ability to activate resources related to activation energy) and supported the connection between evidence and claims.

Students Weighing Resources in Multivariate Reasoning. Students engaged in multivariate reasoning by weighing multiple explicit and implicit properties identified within each mechanism and integrating these variables into the construction of their arguments. Students' multivariate reasoning often utilized the case comparison to evaluate the similarities and differences between the reactions. Rather than discarding a property as unimportant because it was similar between the reactions, some students identified and considered the impact of that property as one of multiple properties that interact to influence reaction rates. In the following excerpts, students activated a variety of different explicit and implicit properties in the construction of their arguments.

In one example of a student engaging in multivariate reasoning, the student weighed the functional groups that differ between the cases in Case Comparison Activity 2:

> *"The electron withdrawing group in reaction A, chlorine, is electronegative and electron withdrawing through induction. The electronegative group in reaction B, the methoxy group, pulls electrons through induction but also donates electrons to the carbon through resonance."* [Case Comparison 2]

This student activated several resources for evidence in their argument: electron withdrawing and donating groups, electronegativity, induction, electronics, and resonance. They also identified that both functional groups are electronegative; however, they contextualized this variable by activating the properties of induction and resonance. Activating these related properties allowed the student to evaluate the carbon's electrophilic properties to make claims about the relative reaction rates. This sample response indicates how the identification of multiple implicit properties can strengthen students' arguments.

Students' activation and weighing of multiple resources is a part of mechanistic reasoning, leading to more complex meaning-making in argumentation. The in-class activity elicited students' thinking about a variety of implicit and explicit properties; however, not all of these properties were integral to the development of students' arguments. For example, in the following excerpt, the student activated a shared property between the two reactions in the case comparison:

> *"In both reactions there is the alkyl chloride group in which the chlorine is much more electronegative than the carbon it is bonded to: this means that the electrons are shared unevenly between the two and the carbon is partially positive, while the chlorine is partially negative"* [Case Comparison 1].

As shown in this response, the student identified similar properties in both reactions: partial charges as a result of the same electronegative functional group. While the student activated this implicit property, they did not use this evidence in their comparison of the two reactions to evaluate the rate of reaction. Students often considered these properties as a way to describe other influential properties or functional groups.

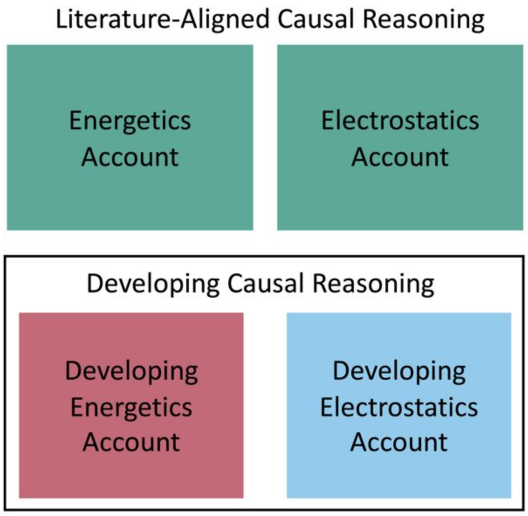


Figure 5. Students' written arguments are described as engagement in literature-aligned or developing causal reasoning. Within both full or developing causal reasoning, students may rely on an electrostatics account or an energetics account.

Aligning with previous research that has made connections between scaffolding and case comparisons to promote multivariate reasoning (Caspari and Graulich, 2019; Watts *et al.*, 2021), the responses to this activity show that students can successfully identify and weigh multiple properties within a reaction, even when these properties may not be useful to their argumentation. Building on the prior findings identifying students' individual responses to scaffold activities (Watts 2021, Caspri and Grauilch), our analysis suggests further insights regarding students' processes of engaging in multivariate reasoning. Specifically, during our analysis we identified that students considered these different resources within the written artifacts of the collaborative portion of the activity; however, in the individually written arguments, students focused on the resources that directly supported their claim (i.e. removing discussions about weighing similar properties between the two reactions). The activity may have expanded students' multivariate reasoning, as the collaborative nature may have influenced how students framed the case comparison problems, leading to discussions surrounding different students' ideas about the role of different properties for developing their arguments.

How does the activity elicit organic chemistry students' causal and developing causal reasoning in students' written responses?

To analyze students' causal reasoning, we expanded beyond the sentence-level analysis used to address the first two research questions by analyzing responses at the level of the entire individually written argument. Through this analysis, we observed multiple types of student engagement in cause-and-effect reasoning within students' responses to the individual portion of the activity after working collaboratively in their groups (summarized in Figure 5). As we discuss our analysis of students' individual arguments from the activity, we intend to provide a student-centered and non-deficit-framed discussion of student writing and reasoning (see Appendix 4 for excerpts of the students' written individual arguments). The resources framework provides an opportunity to recognize students' activated resources within their writing as evidence of developing reasoning, adopting an anti-deficit lens which has not been explored in previous literature on mechanistic or causal reasoning in chemistry. Therefore, our results and discussion about this broadest view of student argumentation in response to the collaborative scaffold activity explore areas for further supporting organic chemistry students as they engage in increasingly complex mechanistic reasoning.

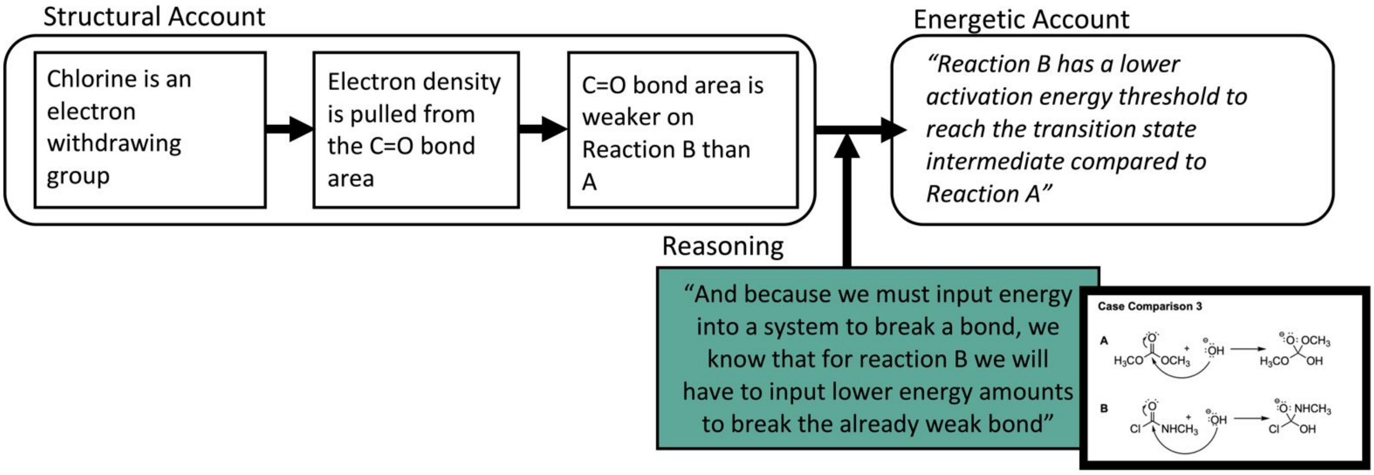


Figure 6. Energetic Account of Student Causal Reasoning. The construction of this causal reasoning argument chains the structural comparison between the two cases to the energetic change, which constitutes a fully connected argument. The turquoise reasoning box represents the literature-aligned causal reasoning between the structural and energetic account.

Literature-Aligned Causal Reasoning

Energetics Account. The first type of student engagement with causal reasoning aligns with a major definition of causal

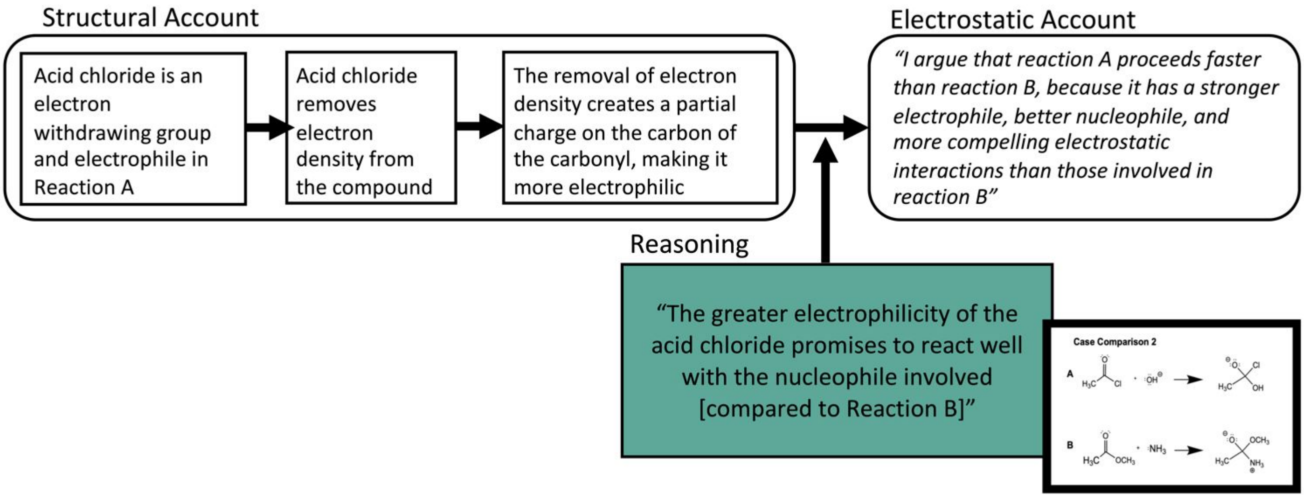


Figure 7. Causal reasoning using an electrostatics account. The construction of this causal argument chains the structural comparison between the two cases to the electrostatic interaction between the nucleophile and electrophile, which constitutes a fully connected argument. The turquoise reasoning box represents the literature-aligned causal reasoning between the structural and electrostatic accounts.

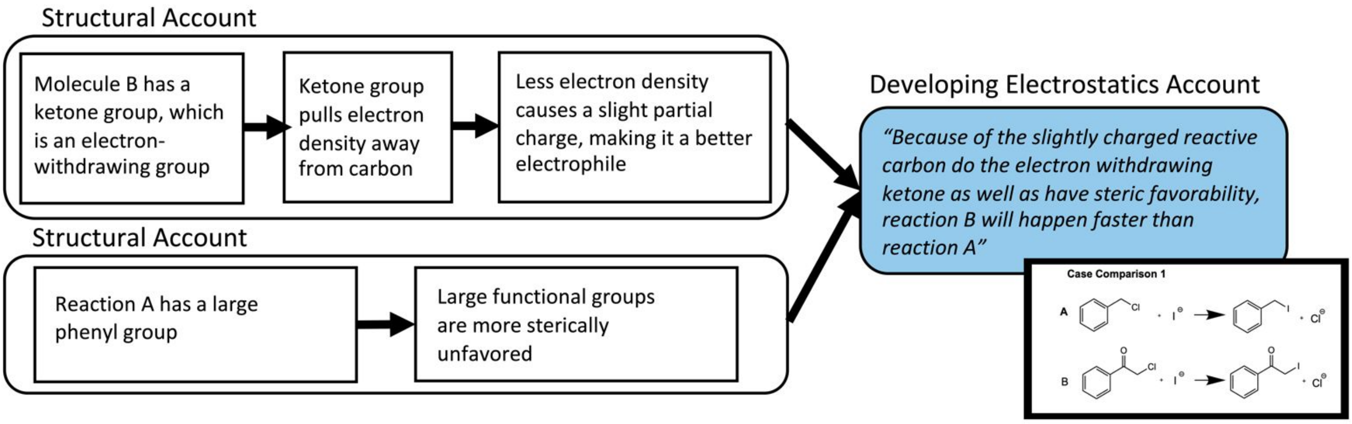


Figure 8. Developing causal reasoning with an electrostatics account. In this example, there were two separate structural accounts that were used to develop an electrostatics account as the claim. However, the student did not include reasoning to connect their activated resources chained together in the structural accounts to the claims made. Note that in contrast to the full causal reasoning figures, this student example has two structural accounts but does not connect to the electrostatic account using reasoning. There is no reasoning box, unlike Figures 6 and 7, and the electrostatic account is light blue, to denote the instance of developing causal reasoning with an electrostatics account.

reasoning in the literature, in which students provide an energetic account of why the mechanism proceeds. Goodwin (2003) noticed that questions surrounding reaction rates are generally answered by appealing to facts about the energy of the reaction's transition state and through dynamically explaining relative energy differences between reactants and products. If claims for mechanism case comparison tasks focus on the relative energies of the products, the evidence should provide structural accounts that account for the energy differences of the products (Goodwin, 2003). Thus, students' individually written arguments engaged in causal reasoning with an energetic account when students connected structural accounts to energetics. For example, Figure 6 shows a student's individual argument which demonstrates cause-and-effect reasoning of the structural and energetic changes occurring for case comparison 3.

The excerpt highlights how a student engaged in cause-and-effect reasoning by analyzing the explicit structural differences to understand the structural and energetic changes occurring in the reactions. The student's structural account focused on a discussion of electron density and bond strength. To connect this structural account to their energetics account, the student activated reasoning about how energy is required to break a bond. As seen through this response, the student's discussion of energetics highlights how activated resources provide the necessary connections between evidence and claims through reasoning. The discussion of activation energy as a piece of evidence allowed the student to construct a causal claim that fully connected their evidence of electron withdrawing effects to the changes within the reaction that allowed bond breaking to occur at a faster rate. Without an instructor prompting explicitly about energetics, the student framed the question on reaction rate to construct an argument utilizing their knowledge about energy.

While some students exhibited causal reasoning with an energetics account for the activity (13/50 analyzed), some participants did not focus on activated resources aligned with energy concepts (12/50 analyzed). This aligns with the context of the activity's implementation, in which the introductory organic chemistry curriculum at this institution does not emphasize energetic accounts of reaction mechanisms (largely a pedagogical and instructional decision made about foundational conceptual topics). Therefore, students may not identify implicit cues to discuss energetic effects of physical and chemical properties, which would allow for more full description of differences in reaction rates. While some mechanistic reasoning studies prioritize mechanistic reasoning with an energetics account, Noyes et al. (2022) included appropriate electrostatics discussions as evidence of causal reasoning, which is the second type of literature-aligned causal reasoning we identified in our data.

Electrostatics Account. The second type of cause-and-effect argumentation involved students focusing on constructing causal arguments using electrostatics accounts. Within this activity, many students focused on nucleophilicity and electrophilicity to construct cause-and-effect relationships with an electrostatics account. This observed reasoning pattern (i.e., focusing on electrostatics) may be connected to a common heuristic in organic chemistry, in which students are prompted to identify a "strong" nucleophile and electrophile (Graulich, Hopf and Schreiner, 2011).

Figure 7 provides an example of a student's individual argument engaging with causal reasoning using an electrostatics account. The student's argument weighed the strength of the nucleophiles and electrophiles as the core piece of evidence to develop their claim that Reaction A is faster. Specifically, the student identified the nucleophilic and electrophilic strength of Reaction A as better than Reaction B without relating these properties to activation energy or energetics. However, the student utilized dynamic reasoning to explain electronic movement and the impact on electrophilic strength. Additionally, the student identified salient electrostatic interactions, such as the electron density drawn due to electronegative structural features, which impacts electrophilicity. The student's discussion of electrostatics connected to reactivity highlights the identification of salient implicit properties within a mechanism; however, this argument lacks the connection between reactivity and energetics, which does not allow for the argument to fully connect to reaction rate. This highlights an area to further support students' conceptual problem-solving and causal reasoning development toward including energetic accounts. Previous research suggests that discussions of stability and reactivity are important for supporting students' reasoning about structure and energy (Caspari, Kranz and Graulich, 2018).

Developing Causal Reasoning

As depicted in the previous examples, students are capable of engaging in cause-and-effect reasoning in constructing their arguments. There are two main ways that students attempted to construct their arguments, connecting activated resources of implicit properties to either an energetic or electrostatic account. Within the previous examples, the activated resources were connected to energetic or electrostatic accounts via deeper-level reasoning, resulting in fully developed cause-and-effect arguments. However, some students may activate similar resources regarding implicit properties, but with varying levels of development of a full causal argument, which we refer to as developing causal reasoning. Developing causal reasoning may look like students providing multiple activated resources (productive or unproductive), without reaching a full, cohesive description of how and why one reaction occurred faster than the other. The goal of identifying students' developing reasoning is to include an anti-deficit description of student learning to capture what resources students activate in the early stages of reasoning and to better highlight areas to support students.

Students who engaged in developing causal reasoning often began with similar activation of resources as those with full causal arguments, highlighting the ways the scaffolded case comparison elicited student writing about a variety of different implicit resources. Some previous studies have investigated partial causal reasoning or attempts at causal reasoning, including through an electrostatics account, which led to careful and intentional activity design to provide support and opportunities for students to make meaningful learning connections (Noyes *et al.*, 2022). One way that students may construct partial arguments is by explaining how a variety of different properties are present within a reaction, without explaining how those properties directly relate to *why* one reaction occurs faster than the other. In our analysis, we identified developing causal reasoning for both electrostatic and energetics accounts.

Developing Electrostatic Account. The students' response shown in Figure 8 demonstrates an example of a developing causal electrostatic account, which some students' written responses exhibited (9/50 analyzed). The cause-and-effect writing pattern started with a structural account, identifying that the ketone in Reaction B pulls electron density from the carbon, which causes a slight positive charge and thereby increases carbon's electrophilicity. Then, the student shifted their focus to a structural account of Reaction A to engage in comparative reasoning between the two reactions. However, their argument only contrasted evidence from Reaction B with evidence from Reaction A. In doing so, the student concluded with their claim that the electron withdrawing ketone and steric favorability make reaction B happen faster, without connecting their evidence to their claim via reasoning. This highlights the type of student argumentation in which the student engages with the case comparison by evaluating evidence between the two reactions rather than constructing a full argument that explores why particular evidence supports their claims (e.g.,"Because the carbon in the starting material of reaction B has two electron withdrawing groups on either side of it, it has more partial positive charge than the carbon in Reaction A. This means that the Sn2 reaction in reaction B is faster than in Reaction A."). This highlights an area of future support for student argumentation patterns and conceptual development in scaffolded activities. A variety of researchers categorize student argumentation which lacks robust reasoning (i.e., including justifications or warrants) as an example of relational reasoning, which is characterized as non-causal reasoning (Moon et al., 2017; Bodé, Deng and Flynn, 2019). Rather than categorize this type of reasoning as non-causal, we seek to identify these statements as developing causal reasoning to highlight where students may require more support; in this case, students may benefit from support in constructing robust, explicit reasoning statements between the resources they activate and the claim they make about reaction rate.

Developing Energetics Account. The students' response shown in Figure 9 demonstrates an example of a developing energetics account, which some students' written responses exhibited (16/50 analyzed). In this example, the student successfully identified a structural account of the electronegative functional groups and provided dynamic reasoning of electronic movement and bond breaking and making. This student attempted to reason at a deeper level by connecting this evidence to their claim about reaction rate utilizing an energetic account. While the students' idea that "more energy required to break a bond, the slower the reaction" is a broad

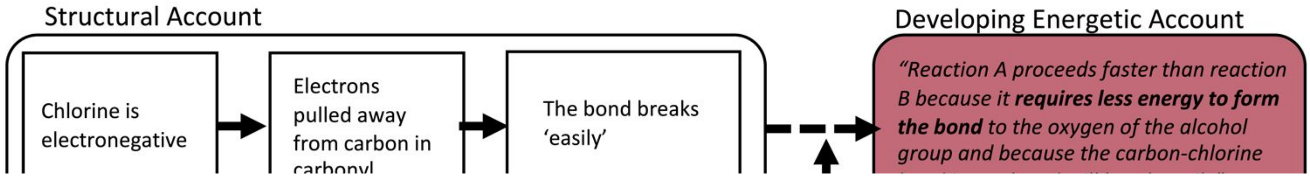
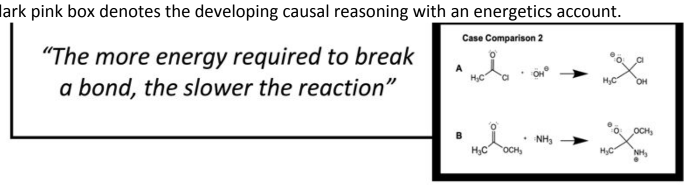


Figure 9. Developing causal reasoning with an energetic account. In this example, a structural account informed an energetic account through reasoning about bond energy. However, there were activated resources that were unproductive for the student's argumentation and did not align with the literature related to the concepts, such as common thinking about bond forming requiring energy input. The dashed line from structural account to energetic account denotes the disrupted connection between the structural evidence and the unproductive activated resource in the structural account. The dark pink box denotes the developing causal reasoning with an energetics account.



generalization that does not capture the nuance of many organic chemistry mechanisms, the student nevertheless made an attempt at deeper level reasoning. Furthermore, we identified that within the construction of this argument, the student activated resources that may be characterized as “alternative conceptions” or unproductive resources (e.g., the idea that reaction A proceeds faster “because it requires less energy to form the bond”), aligning with prior research on students’ conceptions on bond energetics (Hunter et al., 2022). While this statement does not capture the conceptual understanding that bond formation releases energy, the student does possess the content knowledge that bond breaking requires energy, as seen in their statement about how a methoxy leaving group “will require more energy to leave.” Identifying these nuances in students’ responses suggests the importance of Cooper et al.’s (2013) implication to identify areas of conceptual confusion about bond formation and energetics rather than broadly categorizing students’ alternative conceptions as misconceptions. Similarly, this research provided implications to implement consistent, socially mediated opportunities for organic chemistry students to construct understandings including writing (Cooper, Corley and Underwood, 2013); our findings demonstrate the use of collaborative scaffold activities to promote these types of socially mediated construction of ideas.

Overall, the student's response shown in Figure 9 highlights how a student may attempt to engage in the construction of an argument that connects a variety of activated resources within a structural account to an energetic account via cause-and-effect chaining of information. However, the student was limited by their content knowledge, which may entail the activation of unproductive resources or the misapplication of content knowledge within the multiple variables the student integrates into their argumentation. This student employed the resources of how bond breaking and making relates to energetics; however, the application of this resource was not productive for this argument. As students engage in higher-level argumentation and reasoning, it may be necessary to provide more instructor-led support or increased opportunities to practice integrating a variety of higher-order conceptual understandings. This recommendation echoes that of Bodé et al. (2019), who highlighted the importance of carefully designing such educational opportunities to elicit students’ causal mechanistic reasoning, especially in the context of argumentation to support cognitive, metacognitive, and social aspects of learning (Bodé, Deng and Flynn, 2019).

Through both of these examples of student’s developing causal reasoning, we can identify how the activity prompted students to construct an argument while activating a variety of resources that served to deepen their reasoning about the underlying properties in a mechanism. The students identified and integrated discussion of multiple implicit and explicit properties into the construction of their arguments. Furthermore, the students began to engage in chaining these ideas together to create some cause-and-effect arguments. However, we identified areas for further exploration or support in the construction of students’ higher-order reasoning and the construction of argumentation. The use of the resources framework to analyze these data elucidated that students activated conceptual resources, even when responses did not align with previously defined causal reasoning in the literature. This indicates an anti-deficit approach to identifying areas to support students in further developing their causal reasoning. Our findings regarding students’ developing causal reasoning corroborate prior research on how students construct scientific arguments. Specifically, supporting students may involve identifying beyond what students consider evidence or reasoning, and focusing on supporting students in utilizing reasoning to connect their evidence to their claim (Lieber *et al.*, 2022). From the examples above, students may have employed unproductive resources or partial discussion of connections between activated resources and claims due to several possible reasons such as a gap in curricular knowledge of energetics, unproductive conceptions about energetics or reaction rates, or different conceptions of argumentation, aligning with prior research on the challenges students face while engaging in argumentation (Lieber *et al.*, 2022). Each of these possibilities require further investigation to find ways to better support students’ development of reasoning. Specifically, causal reasoning is related to how students view the nature of argumentation, which can be influenced by their framing and the way prompts or scaffolds support the activation of resources. These challenges students may face while constructing arguments need to be further explored in order to continue to support student development of argumentation in conjunction with deeper reasoning patterns.

Limitations

The primary limitation of this study is due to the data collection methodology focusing on written documentation only. Written artifacts can illuminate important information about students’ reasoning; however, we are limited in the claims we can make about how the scaffolded case comparison activity influenced students’ learning development and experience because we did not conduct observations or interviews. Due to the nature of COVID and the remote learning experience, we are aware that some students were not fully engaging in the materials in the collaborative environment, which may have influenced students’ experiences and their exhibited reasoning. While we may consider the impacts that a collaborative environment may have had on students’ written argumentation, we cannot make sweeping claims about the utility or effectiveness of this activity on student learning experiences or outcomes. Furthermore, because we did not engage in methodologies like classroom observations, we cannot make claims regarding the specifics of student interactions. For our study, the resources students activated may have been a result of in-class group activity discussion or individual interpretation of the activity and framing of the activity. The collaborative nature of scaffolded activities has been demonstrated as important in previous research studies (Lieber and Graulich 2020), however more qualitative information is needed to describe how the collaborative discussions support students' learning. Thus, the discussion of students' reasoning as activated resources elicited from the activity are carefully considered as written artifacts of students' argumentation and mechanistic reasoning, rather than claims about their conceptual beliefs, knowledge, or ideas. The findings of this study are not meant to be generalizable to larger populations of students or students at different institutional settings with different contexts including background, identity, and experience.

Conclusion

This study investigated the implementation of a research-based activity (the scaffolded case comparison) into the larger-scale classroom setting, with the goal to support students' engagement in complex mechanistic reasoning by activating students' resources about organic chemistry concepts and underlying problem-solving structures. The larger, authentic classroom setting for this study builds on the existing research that describes the efficacy of this structure in eliciting students' mechanistic reasoning. Grounding our study on argumentation development and viewing the evidence elicited by the activity as resources, we aim to highlight ways to further support students' complex reasoning and argumentation development. This study highlighted that the students' discussion of implicit and explicit properties parallel the existing literature on how scaffolded case comparison activities elicit students' activated resources. Furthermore, we captured the ways this activity may elicit student engagement in more complex mechanistic reasoning aspects such as multivariate and dynamic reasoning. These findings indicate how engaging students in collaborative scaffolded activities can promote students' multivariate and dynamic reasoning as analyzed through student writing, extending previous research into the classroom setting. Furthermore, we observed a range of student engagement with causal reasoning. Through capturing different styles of engagement in causal reasoning, we describe how this activity elicited student thinking about causal reasoning in the argumentation setting, and how students in the early developmental stages of causal reasoning begin to employ reasoning patterns to construct emerging causal reasoning. The implications of this research may further support organic chemistry students' complex reasoning by encouraging instructors and researchers to develop tools or implementation strategies which might further support students working through conceptual, argumentative reasoning.

Implications

This research contributes to the broader field of investigating organic chemistry students' mechanistic reasoning through exploring developing reasoning skills, situating student writing as resources activated by the in-class activity. This study shows how an in-class activity can scaffold, support, and elicit students' mechanistic reasoning through writing. The study employed a resources lens to highlight students' developing engagement in complex reasoning to identify areas for support from instructors and faculty. Furthermore, the results of this study lead to more areas for research on the ways that students may reason through reaction mechanisms in classroom settings.

Implications for Teaching. Within this project, we aimed to capture areas where students demonstrated engagement in causal reasoning, including some early developmental examples of students' attempts at integrating causal reasoning into their writing. Through capturing these examples of developing causal reasoning through the lens of argumentation, this research suggests implications for instructors to create strategies to support students' further engagement in complex causal reasoning. Literature has highlighted that combining argumentation with causal reasoning can prove challenging for students (Lieber *et al.*, 2022), so relevant support strategies should be a focus when enacting activities that elicit students' reasoning. One implication for support is utilizing the existing attempts at the scaffold as an intervention strategy to identify challenges with argumentation or conceptual integration, and to target further instruction to support students through these strategies. Similar to diagnostic scaffolding (Lieber *et al.*, 2022), this will allow instructors to identify areas where explicit and additional scaffolding of questions may be useful.

Another implication of this study is that students may need additional, informal support tools to provide feedback on their argumentation. These support tools may include online resources, rubrics to evaluate peer arguments in class, explicit instruction or prompting about potentially productive resources, or explicit teaching strategies to elicit student thinking about how to connect their evidence to claims via reasoning. These support interventions may be a way to introduce students to more complex reasoning patterns.

Finally, this study identified students' conceptions of energetics and electrostatics in developing mechanistic reasoning, which may be valuable to explore further. This may highlight opportunities for energetics to be emphasized in introductory organic chemistry courses as a gateway concept which can also lead to more interdisciplinary thinking in chemistry. For example, a focus on energetics may highlight connections between organic chemistry concepts and biochemistry, engineering, and physical chemistry, leading to more rich and transferrable content acquisition.

Implications for Research. This project captures students' developing causal reasoning patterns which may indicate areas for future research. One way future research can identify areas to further support students who engage in developing causal reasoning in argumentation is creating a machine learning model which could detect areas for support, which students interact with to get explicit support strategies (Watts, Dood and Shultz, 2022, 2023; Martin and Graulich, 2023). Online support tools that informally provide feedback on student writing may help extend the reasoning patterns employed in the in-class activity toward new instructional experiences. As students begin to become more comfortable leveraging the benefits of machine learning and artificial intelligence, research must also investigate effective instructional strategies for how to effectively integrate feedback from external support tools. Furthermore, research must evaluate the usefulness of automated text analysis tools to support students' developing causal reasoning.

Another aspect of future research may include further development of the in-class activity to support increasing complexity and independent learning through metacognition (Tsaparlis, 2021). The scaffold may be added upon to introduce more complex questions to elicit activation of resources that may be more challenging conceptually, such as additional support for working through energetics. Scaffolding is designed to serve as a temporary support tool for students to utilize while learning complex reasoning and problem-solving skills. Future research should explore the impacts of slowly fading the scaffold and identify if the reasoning patterns can be transferred to new instructional contexts (McNeill *et al.*, 2006; Graulich and Caspari, 2021). Fading the scaffold has been shown to improve students' reasoning as it requires independent learning in the long term (Reiser, 2004; McNeill *et al.*, 2006). A combination of adding to the scaffold and then fading may provide insights into supporting not only conceptual knowledge and mechanistic reasoning development but also independent problem-solving and metacognitive skills for students.

Author Contributions

All authors contributed. The authors D.B.H., F.M.W., and A.J.D. contributed to the conceptualization, data analysis, visualization, and the editing of this study. G.V.S. contributed to the design, data collection, implementation of the assignment, and revision. The manuscript was written by D.B.H., with extensive, valuable feedback from F.M.W., A.J.D., and G.V.S. All authors read and approved the manuscript.

Conflicts of interest

There are no conflicts to declare.

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Appendices

Appendix 1. Activity Questions

Group Portion. This section is to be completed collaboratively with your small group, which will be assigned by your GSI during the lab session. You will carefully examine a pair of reactions (A and B) for differences and briefly describe them using the guiding questions below. Then discuss it with your group. You should come to a consensus about your responses. Be prepared to share out with the larger group. *NOTE: This is a two-step reaction. Your comparison should only focus on the first step of the reaction.*

1. What structures differ in both reactions A and B? Specify the functional groups or atoms in which the reactants differ.
2. What chemical and physical properties do the functional groups or atoms in (from question 1) have?
3. What changes occur from reactants to products in both reactions A and B? Note the changes, such as forming a charge, breaking a bond, or making a bond.
4. Why do the changes in question 3 occur?Describe as precisely as possible how the properties described in question 2 influence the property changes in question 3. Do the influences of the properties accelerate the reaction step or slow it down? Do they have no effect at all compared to the other reaction?
5. Provide a statement that answers the question: **does reaction A or B occur faster? If stuck, consider using this sentence stem: "Reaction _______ occurs at a faster speed because _______ , _______ , and _______ ."**

Individual Portion. This section is to be completed individually by you during your lab session. Please note that your GSI is available to help you during your lab session so be sure you don't have any questions before you leave.

6. Write a brief 2-3 paragraph argument describing which reaction you predict will proceed faster. Your argument should include a claim (i.e., Reaction A is faster than reaction B), evidence (i.e. description of the structural features and properties associated with molecules in each reaction), and warrant (a reasoning about why these structures/properties result in the changes that occur and lead to one reaction being faster than the other).

Appendix 2. Graduate Teaching Assistants' Role

The organic chemistry laboratory course was offered separately from the lecture course and included an instructor-taught hour of lecture followed by 4-hours of laboratory taught by graduate teaching assistants. The instructors held a weekly staff meeting for the GTAs. Case comparisons were discussed throughout the semester in both the lecture and laboratory. Six graduate teaching assistants (GTAs) were specifically trained in leading discussions about case comparisons, and they facilitated the scaffolded case comparison activities. GTA training involved graduate teaching assistants working through each of the three activities as students under the guidance of the instructor, noticing areas that may present conceptual challenges for students. The GTAs then discussed potential student challenges and how to address them. Afterwards, GTAs would lead each of the three activities to classes six times over a three-week period.

During the collaborative activity, the trained GTAs or lead instructor would check in on the breakout rooms to answer questions and ensure that the implementation of the activity was aligning with the design. Between class meetings, GTAs communicated about student behavior and interaction and discussed potential methods to encourage participation and engagement as a teaching team.

Student work was graded by the GTAs utilizing a rubric designed based on the scaffolded case comparison rubrics (Caspari and Graulich 2018). These were translated to U.S. student understanding, typically through terminology taught and used. The lead instructor made additional adjustments to the rubrics during staff meetings, following feedback from the trained GTAs. The group responses to the scaffolded questions as well as the individually written arguments were graded by the GTAs. The assessment was completed independently of the presented analysis.

Appendix 3. Coding Scheme Evidence Codes

The coding scheme evidence codes were briefly described in Table 1, but all of the codes evidence or activated resources are defined with an example from student responses in Table 2.

Table 2. Evidence code definitions applied on the sentence-level.

Evidence Codes	**Definitions**	**Examples**
Activation Energy	The students' writing included discussion of activation energy	"The Activation energy of reaction B is higher than Reaction A…"
Bond Breaking and Making	The students' writing included discussion of bonds are broken and formed	"[Bond] breaks and [bond] forms"
Bond Strength	The students' writing included defining the bond strength as weak or strong	"The bond is weak"
Charges	The students' writing included discussion of explicit charges	"The negatively charged functional group"
Electron Donating and Withdrawing Groups	The students' writing included identifying functional groups that are considered Electron Withdrawing groups or Electron Donating Groups	"The functional group is withdrawing/donating"
Electronegativity	The students' writing included discussion of electronegativity of functional groups	"The oxygen is more electronegative than…"
Electronics	The students' writing included discussion of electrons and electronics, Describing if something is "electron deficient/poor/rich", having "delocalized or localized electrons"	"[functional group] providing electron density", "accessible electrons"
Energy Changes	The students' writing included discussion of energy difference between the reactants and products of the same reaction or energy changes compared between reactions	"The energy of the reactant in B is higher than the energy of reactants in A", "The energy of the reactant is higher than the energy of the products…"
Leaving Group	The students' writing included identifying a functional group as a leaving group	"The chlorine is a good leaving group"
Nucleophiles and Electrophiles	The students' writing included discussion of a functional group/molecule as a nucleophile/electrophile or by its nucleophilic/electrophilic properties	"[functional group] is a nucleophile"
Partial Charges and Dipoles	The students' writing included discussion of the partial charges (partial positives and negatives) as well as discussing the polarity of bonds (bond dipoles)	"The partial positive charge on the [atom] in this functional group," "Dipole moment in the bond",
Properties	The students' writing included discussion of properties of the molecules/atom including discussion of pKa, acidity/basicity, size of atoms and steric hinderance	"I- is a weak base", "[atom] is larger, causing more steric hindrance"
Resonance and Induction	The students' writing included identifying when functional groups have inductive properties or draw electrons through induction and explicit description of resonance or resonance structures.	"[Functional group A] provides resonance" or "donating resonance structures", "inductively pulls electrons"
Stability	The students' writing included discussion of stability of the molecule and discussions of reactivity (evaluations of how reactive/unreactive a molecule is)	"The functional group makes the molecule more stable"
Strength of Bond in Bond Breaking and Making	The students' writing included discussion of how the bond strength relates to the ability for it to be broken / formed	"This bond is easier to break", "Less likely to form a new bond"
Transition State	The students' writing included discussion of the transition state	"The higher energy transition state"

Appendix 4. Students' Individually Written Paragraphs

For Figure 5, the following excerpt of a student's individually written argument was used to develop the figure outlining the engagement of causal reasoning using an energetics account.

> *"In terms of the C=O carbonyl double bonds in each reaction system, it is important to note that in reaction B, because of the strong electron withdrawing group of Cl, electrons are taken from the C=O bond area, making it weaker. Because the C=O center is weaker in reaction B than it is in Reaction A, then it is more easily broken. And because we* ***must input energy into a system to break a bond****, we know that for reaction B we will have* ***to input lower energy amounts to break the already weak bond****. The certainly affirms that reaction B has a* ***lower activation energy threshold to reach the transition state intermediate*** *(tetrahedral structure) compared to reaction A. It is for all of these reasons*

described above that reaction B inevitably proceeds at a faster rate than reaction A."

For Figure 6, the following excerpt of a student's individually written argument was used to develop the figure outlining the engagement of causal reasoning using an electrostatics account.

*"I argue that reaction A proceeds faster than reaction B, because it has a stronger electrophile, better nucleophile, and **more compelling electrostatic interactions** than those involved in reaction B. In terms of our electrophile, the acid chloride in reaction A has a stronger partial positive charge than that of the ester in reaction B. We know this because the chlorine in the acid chloride is an electron-withdrawing group, which removes electron density from the compound making it less nucleophilic and thus more electrophilic (which creates a partial positive charge on the carbon of the carbonyl)…The greater electrophilicity of the acid chloride promises to react well with the nucleophile involved. We also know that acid chlorides are more reactive than esters, which supports the theory that reaction A (containing an acid chloride) reacts at a faster speed than reaction B (which contains an ester)."*

For Figure 8, the following excerpt of a student's individually written argument was used to develop the figure outlining the developing causal reasoning with an electrostatics account.

*"Between the two of these reactions, the reaction that will likely occur at a faster rate is Reaction B for several reasons. The molecule in reaction B has a ketone group that is adjacent to the reactive carbon pulls electron density away from the carbon as ketones are electron withdrawing groups. With less electron density, the carbon has a slight positive charge that makes it function better as an electrophile. Meanwhile in reaction A, there is not as strong a shift of electron density meaning the reactive carbon is not as good an electrophile as the reactive carbon in reaction B. Along with this the reactive carbon in reaction A is attached to the phenyl group, a fairly large group that makes the reaction more sterically unfavored compared to the further out reactive carbon in reaction B. **Because of the slightly charged reactive carbon do to the electron withdrawing ketone as well as steric favorability, reaction B will happen faster than reaction A.**"*

For Figure 9. the following excerpt of a student's individually written argument was used to develop the figure outlining the developing causal reasoning with an energetics account:

*"Because the chlorine is highly electronegative and pulls electrons away from the carbon, the bond between the two atoms will break easily and require very little energy, making this part of the reaction very fast. Additionally, the nucleophile attack from the alcohol proceeds very quickly because the oxygen is so electron rich and wants to donate electrons to become neutral. Reaction B proceeds slower because the bond between the carbonyl carbon and the methoxy is stronger due to resonance and its double bond character. That means that the methoxy is a poor leaving group and require more energy to leave in the tetrahedral form. The **more energy required to break a bond, the slower the reaction…**Reaction A proceeds faster than reaction B because it requires **less energy to form the bond** to the oxygen of the alcohol group and because the carbon-chlorine bond is weak and will break easily."*

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