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Attention is currency: How surface features of Lewis structures influence organic chemistry student reasoning about stability

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Abstract

Despite representations' central role in conveying chemical phenomena, mastering them is not trivial, given the wide variety of different conventions to interpret and use them. Furthermore, instructional approaches and materials may overlook explicit discussion on how students should reason with representations. To gather evidence that could guide improvements in teaching strategies and the creation of more effective instructional materials, we explored how students use Lewis structures to make inferences about stability. Through interviews with twenty-eight organic chemistry students, we have captured a range of resources that they employed, including the features of Lewis structures they paid attention to, the conceptual resources they activated, and the sophistication of their explanations. We found that students referenced all the explicit features of the provided Lewis structures but primarily attributed stability to the unique eye-catching features of each representation. Importantly, the surface features to which students attended impacted the conceptual resources they activated and their reasoning. Specifically, some students misapplied chemical principles to make justifications that fit their correct or incorrect claims about stability. Moreover, students primarily relied on lower-level reasoning and heuristics when constructing explanations. These findings underscore the importance of probing student reasoning so that instruction and assessments can be tailored to enhance students' ability to effectively use representations to reason about chemical phenomena. By understanding the reasoning patterns students adopt, educators can develop targeted strategies that promote deeper understanding and productive use of chemical representations.

Introduction

Student learning about and with representations

Organic chemists formulate theories as to why molecules form, how they react, why they are stable, and why compounds have the observable properties they possess (Hoffmann, 1995). Since molecules are not typically visible but account for the observable properties of substances, chemists have designed representations—symbolic depictions with surface features that can be perceived and manipulated—and utilize them routinely to convey knowledge about imperceptible entities and processes (Kozma *et al.*, 2000; Olimpo *et al.*, 2015). In organic chemistry, multiple domain-specific representations such as chemical formulas, concrete models, and two-dimensional (2D) and three-dimensional (3D) molecular diagrams have been designed for a variety of purposes (Paulsen, 1982; Harrison and Treagust, 2000; Goodwin, 2008; Johnstone, 2009; Talanquer, 2022).

Representations are not only essential research tools but also valuable educational tools, yet learning *about* and *with* them is not trivial. Learning *about* representations entails knowledge of how to interpret them and of their affordances and limitations, while learning *with* representations involves the use of representations as tools to think about, communicate, and visualize chemical concepts (Kozma and Russell, 2005; Rau, 2017; Talanquer, 2022). Considering the richness of the information presented explicitly or implicitly by representations and the diversity of representations chemists interact with, the effective use of chemical representations requires knowledge of (a) disciplinary conventions, (b) relevant conceptual knowledge, (c) the nature and number of explicit and implicit features that need to be analyzed, and (d) relevant versus irrelevant graphical features (Talanquer, 2022). Similarly, Schönborn and colleagues (2002, 2008) proposed three intersecting factors that affect interpreting and using representations to understand and communicate chemical phenomena: (a) the mode of the given representation—the explicit features of the representation, (b) conceptual knowledge—the knowledge of concepts that are relevant to that representation, and (c) reasoning—the cognitive processes and skills needed to perceive and decode explicit features of a representation and to access and retrieve implicit conceptual information relevant to the representation.

The considerations and requirements outlined above (Schönborn *et al*., 2002; Schönborn and Anderson, 2008; Talanquer, 2022) are cognitively demanding and may lead to novices' difficulties related to learning *about* and *with* representations (Kozma and Russell, 2005; Ainsworth, 2006), especially given learners' rudimentary domain knowledge and disciplinary expertise (Cook, 2006; Talanquer, 2022). Additionally, instructors may overlook explicit instruction about the skills needed to use representations as tools and give more weight to teaching concepts such that representations are a mere 'by-product' of other topics (Linenberger and Holme, 2015; Rau, 2017; Popova and Jones, 2021; Jones *et al*., 2022). As such, students might struggle to effectively use representations to communicate the concepts encoded in their explicit features (Bodner and Domin, 2000; Bhattacharyya and Bodner, 2005; Cooper *et al*., 2010; Grove *et al*., 2012; Popova and Bretz, 2018a; Rodemer *et al*., 2020; Rodriguez *et al*., 2020; Farheen and Lewis, 2021). Given that representations embed rich and abstract information in their varied explicit features, research into how students learn about and use representations to infer different concepts is of high pedagogical importance if we are to support students in developing a robust understanding of chemistry. In this manuscript, we report how organic chemistry students extract information about a fundamental concept (chemical stability) from a commonly used representation across the chemistry curriculum (Lewis structures). Specifically, we characterize the explicit features of Lewis structures that the students analyzed to make inferences about stability, the conceptual resources they activated, and the sophistication of their explanations.

STRUCTURE-PROPERTY RELATIONSHIPS IN THE CONTEXT OF LEWIS STRUCTURES

Structure-property relationships are recognized as a fundamental topic by organic chemistry educators (Duis, 2009), an anchoring concept in organic chemistry (Raker *et al.*, 2013), and a central, crosscutting concept in science and engineering (National Research Council, 2012). Representations are used to depict structure and, therefore, are necessary tools for making inferences about chemical and physical properties.

Lewis structures are among the primary representations of molecular structure that students encounter and are repeatedly exposed to from high school through their undergraduate and even graduate education. They depict a great deal of structural information (e.g., bonding, and nonbonding electrons, atoms, and connectivity) that can be used to explain and predict a molecule's chemical and physical properties. Several studies have investigated students' ability to identify structure-property relationships using Lewis structures in a variety of courses, from general chemistry to graduate-level chemistry subjects (Cooper *et al.*, 2010, 2012b and 2013; Underwood *et al.*, 2016; Kararo *et al.*, 2019). These studies have found that students at all levels are less able to recognize the implicit information (i.e., physical and chemical properties such as boiling points and reactivity) but are more proficient in identifying the explicit information in the representation (i.e., atomic composition and types of bonds) (Cooper *et al.*, 2010, 2012a, 2012b; Underwood *et al.*, 2016). Additionally, students struggle to generate Lewis structures and demonstrate a lack of understanding of this representation's purpose (Shane and Bodner, 2006; Cooper *et al.*, 2010). Promisingly, student performance on predicting boiling points from Lewis structures has been shown to improve with explicit instruction about structure-property relationships and increased scaffolding of prompts (Kararo *et al.*, 2019).

Lewis structures are also commonly used to depict resonance forms to explain the role of electron delocalization in the chemical reactivity and physical properties of molecules. Research on student understanding of resonance structures reported that students commonly think that the major contributor is the resonance hybrid, that resonance structures exist in nature, and that resonance is an equilibrium process (Kim *et al.*, 2019; Petterson *et al.*, 2020; Xue and Stains, 2020; Brandfonbrener *et al.*, 2021; Tetschner and Nedungadi, 2023). Most studies have examined students' conceptualizations of resonance, but not students' reasoning when determining which Lewis structure is the major contributor to the resonance hybrid. Furthermore, in most assessments, students are often asked to identify the major contributor to the resonance hybrid (i.e., the most stable resonance form) but are not prompted to explain their reasoning (Betancourt-Pérez *et.al*, 2010). In summary, while the studies described above investigated *what* structural and conceptual information students could or could not infer from Lewis structures, very few (Cooper *et al.*, 2013; Kararo *et al.*, 2019; Xue and Stains, 2020; Tetschner and Nedungadi, 2023) examined *how* the conceptual information (e.g., melting/boiling points and resonance) was determined from Lewis structures.

Our project adds to the body of literature investigating student understanding of structure-property relationships, with a focus on a previously understudied property in the context of Lewis structures—chemical stability. Chemical stability is a core concept underlying chemical and physical changes in matter (National Research Council, 2012). Studies have elucidated students' conceptualizations of the stability of chemical species (e.g., atoms, ions, molecules, reactants, products, intermediates) in the context of organic chemistry reaction mechanisms and reaction coordinate diagrams (Caspari *et al*., 2018; Popova and Bretz, 2018a, 2018b; 2018c; Bodé, *et al*., 2019; Dood *et al*., 2020; Pölloth *et al*., 2023), ionization energy (Taber, 2009), atomic-molecular interactions (Becker and Cooper, 2014), solvation process of salts in water (Abell and Bretz, 2018), and acid-base chemistry (Demirdö *et al*., 2023). In these studies, findings consistently indicate that students struggle to invoke the concept of chemical stability to explain the impact of structural characteristics on chemical and physical processes.

RESEARCH QUESTIONS

Given that chemical stability is at the heart of understanding the underlying chemical and physical changes in matter (National Research Council, 2012), investigations of how students conceptualize it are necessary for supporting students in developing a robust understanding of structure-property relations. As such, this work aims to characterize how organic chemistry students *use* Lewis structures to make inferences about chemical stability. We focus specifically on student *use* of Lewis structures because Lewis structures are widely employed in the instruction of molecular structure and convey a great deal of conceptual information. Moreover, proficiency in *using* representations as effective tools to visualize and communicate phenomena is at the core of developing representational competence, as highlighted in the definition of representational competence as the "ability to *use* representations and their features in social situations as evidence to support claims, draw inferences, and make predictions" (Kozma and Russell, 2005). As such, we address the following research questions:

When organic chemistry students *use* Lewis structures to make inferences about stability,

1. what features of the representation do they attend to to identify the most stable structure?
2. what conceptual resources (content-specific knowledge elements) do they activate when attending to the specific features?
3. how do students reason when making inferences about stability from Lewis structures?

ANALYTICAL FRAMEWORKS

To investigate how students use Lewis structures to make inferences about stability, we examined the data using three frameworks: the Resource-Based Model of Cognition to capture activated conceptual resources and the features of Lewis structures linked to the conceptual resources (Hammer, 2000; Richards *et al*., 2020), the Dual Process Theory to provide an even deeper analysis of student reasoning that takes into account any reasoning strategies, heuristics and assumptions that students rely on when constructing explanations (Evans and Stanovich, 2013; Talanquer, 2014), and the Modes of Reasoning Framework to characterize the sophistication of student explanations (Sevian and Talanquer, 2014), and determine the relationship between the reasoning processes and sophistication of student explanations (Evans and Stanovich, 2013; Talanquer, 2014). The multiple theoretical perspectives were critical to characterize the variability and nuances of participants' responses.

Resource-Based Model of Cognition. Hammer posited that knowledge comprises fine-grained context-specific knowledge elements, called resources (Hammer, 2000; Elby and Hammer, 2010). Resources can be intuitive or learned through formal instruction. Knowledge elements experienced through formal instruction are referred to as conceptual resources and represent discipline-specific content ideas (Richards *et al*., 2020). Conceptual resources can be productive or unproductive in the context of a specific aim or task (Hammer *et al*., 2005). For instance, while it is productive to invoke the electronegativity of atoms to discuss bond polarity or intermolecular forces, it is typically unproductive to use electronegativity to explain a molecule's stability when using Newman projections (Ward *et al*., 2022). Beyond conceptual resources, the features of representations attended to (explicit resources) can be characterized as relevant or irrelevant to a particular task. Similarly, the reasoning processes (i.e., heuristics and assumptions—reasoning resources) can be examined based on their utility in the specified context.

The resources framework allowed us to capture and frame students' fine-grained knowledge elements as productive or unproductive for the given context as well as the explicit features linked to these knowledge elements. However, this framework alone was not sufficient to explain student reasoning regarding the explicit features and the activated conceptual resources (i.e., why was a particular feature attended to and how was it linked to a conceptual resource). Therefore, we used additional frameworks described below.

Dual Process Theory. In discussing how people reason through problems and make decisions, Evans and Stanovich (2013) proposed the Dual Process Theory that suggests that people can engage in two discrete types of reasoning: Type I and Type II. Type I reasoning is based on intuitive and automated processing that provides a quick response without stimulating deep thinking. On the contrary, Type II reasoning requires critical thinking that overrides intuition to provide a deliberative response needed to make a claim. To characterize student reasoning when evaluating the relative stability of Lewis structures, we analyzed student explanations using the Dual Process Theory. We categorized learners' responses into Type I and Type II reasoning and further characterized students' Type I shortcut reasoning strategies through the lens of Talanquer's (2014) "Ten Heuristics" (explained in more detail in **Table 1**) and Maeyer and Talanquer's (2013) "Valid and Spurious Assumptions." When constructing explanations, learners leverage resources based on assumptions—beliefs or ideas about the properties and behavior of entities or processes (Maeyer and Talanquer, 2013). Chemical assumptions can be valid—well-established and accepted chemical justifications, or spurious—misinterpretation and overgeneralization of chemical principles to fit a particular claim (Maeyer and Talanquer, 2013).

Apart from enabling us to capture and characterize students' type of reasoning, the Dual Process Theory allowed us to examine the assumptions underlying student reasoning. Moreover, this theory effectively complements the Resource-Based Model of Cognition. Previous research has shown that resource productivity and scientific accuracy continuums can exist as orthogonal axes where chemical assumptions can range in their accuracy but also in their productivity for a particular task (Crandell and Pazicni, 2022). This framework has allowed us to unpack the complexity and diversity of student reasoning elicited by the same prompt, which is a critical step for characterizing student thinking and developing approaches to support students in building a robust chemical understanding.

The Modes of Reasoning Framework. The Modes of Reasoning Framework examines the intricacy of student reasoning based on students' ability to construct explanations, connect ideas, and ground justifications in causality for how and why phenomena occur (Sevian and Talanquer, 2014; Weinrich and Talanquer, 2016). This framework allowed us to characterize the sophistication of student explanations when making inferences about the relative stability of Lewis structures as descriptive, relational, and causal (explained in more detail in **Table 2**). When integrated with Dual Process Theory, this framework enhances our understanding by mapping the link between reasoning types and the depth of student explanations. This link highlights how diverse student reasoning can be, even within the same reasoning mode.

In summary, to investigate how students use Lewis structures to make inferences about relative stability, we characterized students' explanations for explicit (features of the representation), conceptual (content-specific knowledge elements), and reasoning (assumptions and heuristics) resources that guided or constrained their thinking (Evans and Stanovich, 2013; Maeyer and Talanquer, 2013; Talanquer, 2014).

METHODS

Setting and Participants. This study took place at a large public research university in the Southeastern United States, focusing on students enrolled in an Organic Chemistry I course. Organic chemistry students, having initially encountered Lewis structures in General Chemistry, revisit this representation at the onset of their Organic Chemistry course. As the course progresses, they are expected to use this representation to make inferences about more complex topics, such as evaluating the stability of chemical structures for a variety of purposes (e.g., predicting, among other things, the major contributor to the resonance hybrid).

In the Fall of 2020 and Spring of 2021, we recruited participants from four sections of an Organic Chemistry I course taught by four different instructors who used the same curriculum and textbook (Bruice, 2016). Twenty-eight students participated in this study; this sample size allowed us to reach the saturation of data (Glaser *et al.*, 1967). The sample included a range of majors, predominantly in biology (54%) and chemistry and biochemistry (25%). Most (79%) self-identified as females. The sample was ethnically diverse (36% self-identified as Black/African American, 32% as White/Caucasian, 14% as Asian/Pacific Islander, and 18% as other ethnicities) and is representative of the population at the institution from which the sample was drawn.

Ethical considerations. To guarantee the rights and privacy of participants, we obtained approval from the Institutional Review Board prior to the beginning of the study. The students received detailed information regarding the goal of the study, the process of data collection, their right to withdraw from the study without penalty, and assurance of their confidentiality. Recruitment emails were sent to participants detailing that participation in the study was voluntary and informed written consent was obtained prior to their participation. Each participant was assigned a pseudonym to maintain their anonymity and received a $20 gift card in compensation for their time.

Data Collection and Interview Prompts. To collect the data, we employed a semi-structured think-aloud interview protocol, which involved a list of predetermined questions to guide the conversation but with a flexible order of questions based on student responses (Munn and Drever, 1990). We encouraged the participants to verbalize their thought processes as they worked through tasks to elicit their reasoning (Herrington and Daubenmire, 2014), and the think-aloud approach allowed us to ask follow-up questions to probe students' reasoning, providing a deeper understanding of their ideas. We collected data via Zoom, where each task was presented on a PowerPoint slide, one task per slide, to focus students' attention on the question at hand (Chatha and Bretz, 2020). Participants used the Zoom annotation tool to indicate specific features of the representations they were referencing. We captured audio and video recordings and screenshots of student drawings. The data were transcribed verbatim and student drawings augmented the transcripts.

We used organic chemistry textbooks to devise tasks that reflect the questions students typically experience in the course. We presented students with pairs of resonance forms depicted as Lewis structures and asked them to select the more stable structure and justify their choice. We did not tell the participants that the pairs presented are resonance forms as we did not intend to influence the resources they activate when discussing the relative stability of the structures; we simply presented the pairs of representations and asked the participants to comment on their relative stability. It should be noted that studies have suggested that labeling resonance structures as "stable" may be misleading given that resonance structures are not discreet entities (Carle & Flynn, 2020). Instead, a more accurate description would be that the individual structures are major or minor contributors to the hybrid, where the most stable resonance form is the major contributor. For our study, however, the students were familiar with the "one resonance form is more stable than the other" language based on the textbook used for instruction (Bruice, 2016) and the tasks used in this study reflect the questions students typically experience in the course. As such, we designed two case comparison tasks each containing a pair of resonance forms; case comparison tasks have been shown to increase the factors that students consider when constructing explanations (Graulich and Schween, 2018).

Twenty-eight students participated in this study ($N = 28$). Half of the students ($n = 15$) made inferences about the relative stability of structures in Task 1, most of the students ($n = 22$) discussed the pair in Task 2, while a subset of the students ($n = 12$) reasoned with both tasks (

Task 1	**Task 2**

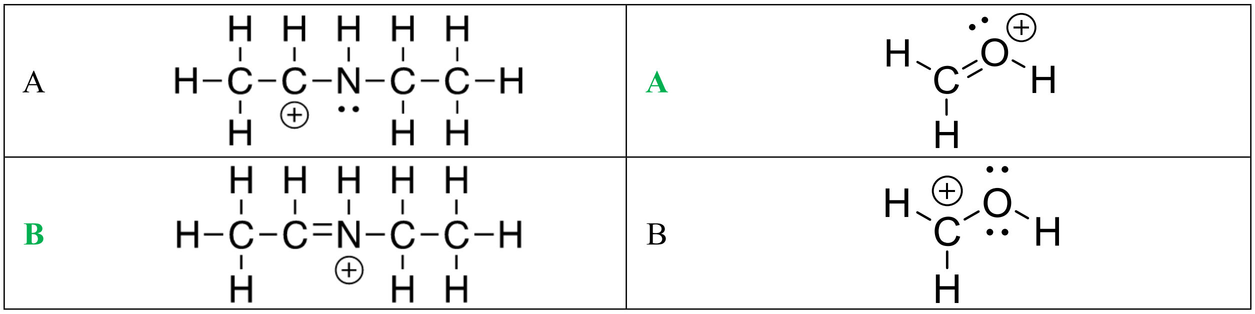

Figure 1). Our analysis revealed similar findings across both sets of prompts, as detailed in the supplementary material. Moreover, most students who completed both tasks (n = 8/12) were consistent in both their mode of reasoning and the accuracy of the claim across the tasks. Consequently, for conciseness, we chose the structures in Task 1 as the primary basis for discussing our findings in this manuscript.

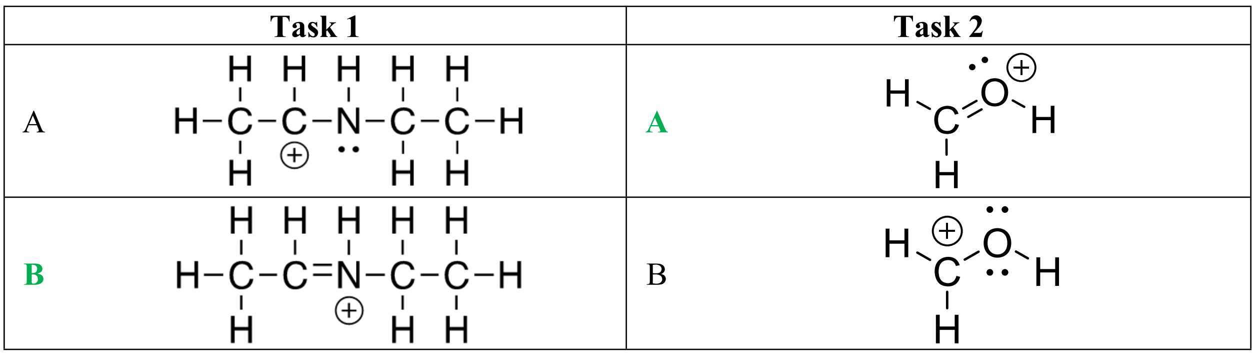

Figure 1. Case comparison tasks of pairs of resonance forms depicted as Lewis structures. Students were presented with these tasks and asked to reason about the relative stability of the Lewis structures. The bold green letters represent the more stable structure/resonance form according to the textbook students used in this study.

Data Analysis. We inductively and deductively coded the transcripts (Saldaña, 2013) using a qualitative data management software, ATLAS.ti (version 9, https://atlasti.com/). Inductive coding was used to capture (a) conceptual resources that students activated, and we further classified them as productive (useful in addressing the prompt) or unproductive (better suited for different contexts) and (b) the explicit features of the structures that students linked to the conceptual resources.

Generating inferences and making conclusions that address a specified prompt involve explicit reasoning strategies. We consider students' reasoning processes (Type I heuristics or Type II reasoning) as resources that guide or constrain individuals to (a) attend to specific aspects of the provided tasks, (b) activate knowledge elements to address the prompt, and (c) apply rules or learned principles to make inferences. As such, we deductively coded the data using the Dual Process Theory and the heuristics applicable to most chemistry education contexts (Talanquer, 2014) to characterize the depth, richness, and diversity of student reasoning. Heuristics can be intuitive or learned to the point of automation such that their application leads to less processing time and quick responses (Type I processing) (Evans and Stanovich, 2013; Talanquer, 2014). Since heuristics are a form of cognitive resources, they are not inherently detrimental; their effectiveness hinges on the context in which they are applied. In fact, experts frequently employ heuristic reasoning—utilizing established patterns and general rules—to quickly and efficiently process complex information. Extensive domain knowledge and disciplinary expertise enable experts to apply heuristics productively (Kahneman and Klein, 2009). This highlights that, when used appropriately, heuristics are valuable tools for problem-solving and decision-making.

We used deductive coding to capture the heuristics used by students (**Table 1**) and determine their impact on students' ability to make inferences about chemical stability. Talanquer (2014) emphasized the significance of examining how students apply heuristics. Understanding the effectiveness of applying heuristics is crucial for educators to reinforce the productive use of heuristics and prevent the unproductive use of heuristics.

Table 1. Cognitive processing strategies (deductive codes) observed in our data (adapted from Talanquer, 2014). Note that some heuristics are highly related to each other, so the same example quote could be categorized as showcasing several heuristics.

Reasoning heuristic	**Definition**	**Example quote**
Processing fluency	Use of easy-to-access cues to facilitate a fast search and decision-making.	*"B (Task 1) is more stable because the positive charge is on a nitrogen instead of on a carbon."* — Evans
Associative activation	Mental association of objects, properties, or events frequently seen or experienced together.	*"Because the nitrogen is more like electronegative, so the [positive] charge should be on the more electronegative element."* — Brenda.
Attribute substitution	A more readily accessible attribute is used as a replacement for the more difficult target query.	*"The presence of a double bond (A in Task 2) makes it more stable because it'd be harder for a change in nature to break it."* — Paula
Surface similarity	Objects that resemble each other are taken to be members of the same category and, hence, share similar properties.	*"Since they both (A and B in Task 1) have a formal charge, so it's not like all of them have their outer shells completely filled."* — Sally
Recognition	Familiar objects are given higher value in decision-making.	*"Nitrogen is more stable in this spot (A in Task 1) ... It typically has two unpaired electrons."* — Mori

One-reason decision making	A single cue or factor, frequently the first feature, is used to provide a plausible answer	*"Electronegative atoms are well-suited to deal with charge compared to like less electronegative atoms. So, I'll choose that one (A in Task 2)."* — Jorge
Generalization	Applying learned rules/patterns in situations that they do not hold.	*"Nitrogen doesn't have all the bonds that it wants to have. It doesn't fill its octet... that's why it has the plus charge on it."* — Maggy

Additionally, we categorized how students leveraged conceptual resources as valid (well-established and accepted chemical principles) or spurious (misinterpreted and overgeneralized chemical principles) (Maeyer and Talanquer, 2013). This further characterization occurred once we noticed that some students could activate productive resources yet express scientifically nonnormative chemical assumptions. This observation is in line with Crandell and Pazicni's (2022) account that resource productivity and scientific accuracy continuums can exist as orthogonal axes where ideas can range in their accuracy but also in their productivity for a particular task.

Finally, we deductively coded the data using the Modes of Reasoning Framework (**Table 2**) to capture the levels of complexity in students' reasoning by characterizing their explanations about stability. Descriptive explanations involve citing explicit features of the representation as the only evidence to support claims. Relational explanations establish connections between explicit features of the representation and the activated conceptual resources (implicit properties), but the connections are not justified. Causal explanations justify the claim using an explicit feature and conceptual resource in addition to explaining how and why that explicit feature/conceptual resource contributes to the effect observed. The two reasoning frameworks (Dual Process Theory and Modes of Reasoning Framework) revealed the relationship between the type of reasoning (i.e., heuristics applied) and sophistication of student explanations (i.e., modes of reasoning), providing a rich analysis of student reasoning.

Table 2. Modes of reasoning (deductive codes) illustrating different levels of sophistication in student explanations (adapted from Sevian and Talanquer, 2014).

Mode of reasoning	**Definition**	**Example quote**
Descriptive	Explicit features or the properties of entities are given without further explanations	*"B (Task 1) would be more stable due to double bonding."* — Brenda
Relational	Explicit features and implicit properties are highlighted in a correlative fashion	*"A (Task 2) is stable because double bonds, in general, are more stable than*

		single bonds because they don't rotate as much." — Delila
Causal	Explicit features and implicit properties are highlighted, and additional reasoning explains why or how they are relevant	*"A (Task 1) is more stable because the lone pair from the nitrogen helps to stabilize that carbon because it can donate electron density that could help alleviate that strain."* — Nate

To ensure the trustworthiness of our findings, the first and the third authors collaboratively coded all the data and discussed every case of coding disagreement until a 100% interrater agreement was achieved (McAlister *et al.*, 2017). To synthesize the central ideas in the data and capture the similarities and differences in student response patterns, we employed constant comparative analysis and thematic analysis (Lincoln and Guba, 1986; Saldaña, 2013; Creswell, 2014). All four authors held weekly debriefing sessions dedicated to interpreting the data. Throughout this process, we maintained reflective memos to capture our thoughts about the data. The memos helped with the communication between the investigators about the coding process, how the process of inquiry was taking shape, and the emergent patterns, categories, and themes in the data (Birks *et al.*, 2008; Saldaña, 2013). This careful record of memos ensured the confirmability and dependability of the analysis (Shenton, 2004; Anney, 2014) and the frequent debriefing sessions between the researchers helped address biases and assumptions brought to the interpretive analysis and ensured the credibility of the results (Lincoln and Guba, 1986; Pandey and Patnaik, 2014).

Results and Discussion

Deciding which resonance form is more stable and contributes more to the nature of the resonance hybrid is not necessarily straightforward for learners, as several factors need to be considered and weighed simultaneously (e.g., charge, octet, electronegativity, etc.). Overall, half of the participants (n = 8) who worked on Task 1 correctly selected B as the more stable structure, while the other half (n = 7) selected A. For Task 2, more than half (15/22) of the students selected the correct structure as the more stable. Given our goal to characterize student explanations when using Lewis structures to make inferences about stability, we delve into the explicit features attended to, the conceptual resources activated, and the reasoning strategies used in judging the relative stability of the provided structures. The section below is organized around the main themes developed from the data:

I. While students noted all explicit features of the representations, they predominantly linked stability to particularly striking features unique to each structure.
II. The discrete explicit features of representations that students attended to impacted the conceptual resources they activated.
III. Students relied on various heuristics and lower-level reasoning modes when constructing explanations about stability.

IV. Many students misapplied chemical principles to make justifications that fit their correct or incorrect claims about stability.

In the findings, the frequencies correspond to the number of responses within each category (e.g., features, concepts, or reasoning strategies) rather than the number of participants because one participant could express several ideas spanning multiple categories. Unless explicitly noted, all example quotes and data pertain to Task 1, as we found similar patterns across the tasks. For clarity, quotes are highlighted in italics.

Theme I: While students noted all explicit features of the representations, they predominantly linked stability to particularly striking features unique to each structure.

Explicit (visible) features of a representation (e.g., atoms, bonds, lone pairs of electrons, and formal charges) influenced the information students decoded and used to make judgments. Different students attended to different explicit features, meaning that certain features were more readily noticed and thus processed (*processing fluency* heuristic) to infer the relative stability of the structures. For example, some students quickly recognized the difference in the number of bonds (single vs. double) in each structure and settled for a response based on that first-noticed feature. This was the case with Charlie, who attended to a singular feature—bonds—and reasoned that "*B [is more stable than A] because it has a double bond.*" Other students noted the difference in the types of atoms bearing the charge, attending to a combination of features—atoms and charge. This was the case with Evans, who highlighted that "*the positive charge is on a nitrogen instead of on a carbon"* (**Table 1**). Donna focused on a different combination of features—atoms and lone pair of electrons: "*The two dots [lone pairs] on the nitrogen fills the octet of nitrogen*." Across the participants, every explicit feature of the provided structures was attended to (singularly or in combination) and deemed relevant in making inferences about stability (**Figure 2**).

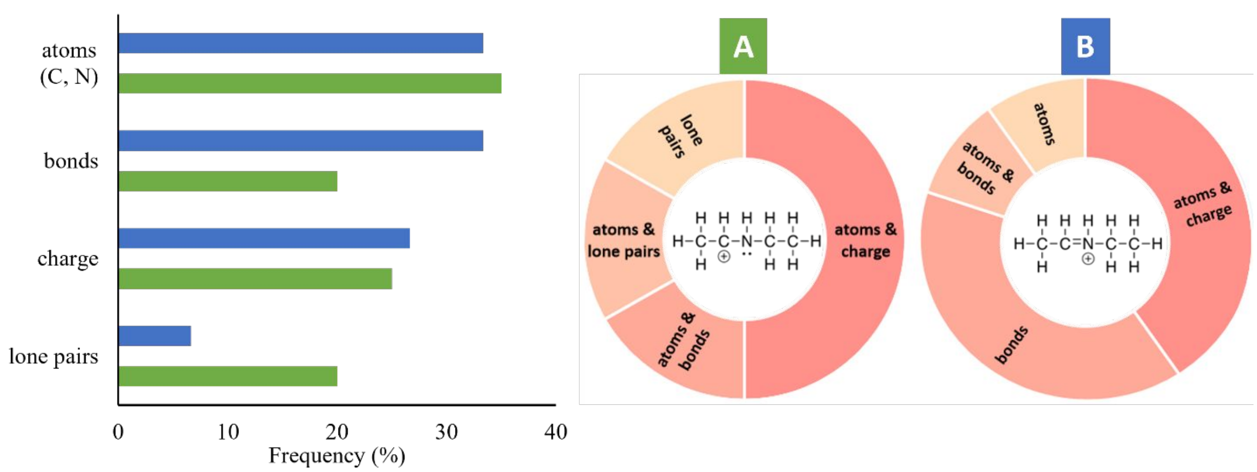

Figure 2. The frequency with which the students attended to the explicit features of the representations when comparing the relative stability of Lewis structures A (green) and B (blue). The bar graph represents individual features, whereas the donut chart highlights instances when

students relied on more than one feature. The size of the arc in the donut charts indicates the frequency with which the feature(s) was mentioned.

Atoms, specifically carbons and nitrogen, were the most frequently referenced feature in both structures, singularly or in combinations with charge, bonds, or lone pairs (**Figure 2**). Bonds, especially double bonds, were the next most frequently noted feature, considered singularly or in combination with atoms to determine the overall number of bonds surrounding a particular atom. The positive charge was always mentioned in relation to the atom bearing it, while the lone pair of electrons was the least referenced feature, whether considered singularly or in combination with the corresponding atom (**Figure 2**). Notably, none of the students discussed hydrogen atoms, indicating a degree of understanding of the relevant vs. irrelevant information to process. It is also possible that the hydrogen atoms may not have captured students' attention, given their similar arrangements in both structures. A similar trend was observed for responses to Task 2, where students most frequently attended to atoms in combination with charge, followed by bonds, and lastly, lone pairs of electrons (**Figure 2S**).

Interestingly, while students collectively considered all the singular external features, they frequently emphasized the unique characteristics of each structure, such as the double bond in structure B and the lone pair of electrons in structure A. For instance, a similar proportion of students referenced features present in both structures, like the charge, in their justifications (e.g., 25% referencing the charge for structure A compared to 27% for structure B, as shown in **Figure 2**). However, students who favored a specific structure as the more stable tended to highlight that structure's unique feature more frequently. For example, students choosing structure A referenced its lone pair of electrons more often (20%) than students selecting structure B (7%) (**Figure 2**). In the rare cases where students mentioned a lone pair of electrons when examining structure B, they did so to note its absence in that structure, as illustrated by Sybil's response: "*B is more stable because it doesn't have any leftover lone pair [of electrons].*" Bonds were another unique feature of selective focus—20% of students who chose structure A and 35% who chose B mentioned bonds, where a significant proportion of responses favoring structure B specifically pointed to the double bond (25%). The correct structure in Task 2 was also favored largely due to the double bond (**Figure 2S**). In associating stability with the unique features of the structures, our participants relied heavily on these distinctive features of representations that stood out more prominently and caught their attention. Instead of making inferences based on the underlying principles, which would have directed students' attention to all the relevant features, many associated stability with the unique, eye-catching features of each structure. Our findings support previous research conducted in the context of other representations, which shows that rather than relying on underpinning principles, learners heavily rely on salient features of representations to rapidly and easily process the information conveyed by representations (Chi *et al*., 1981; Graulich *et al*., 2019; Talanquer, 2022).

Recognizing relevant explicit or implicit features is essential to properly decode information conveyed by representations because a dynamic relationship exists between specific features attended to by an individual and the conceptual resources they activate (Rodriguez *et al*., 2020). As such, in the section below, we delve deeper into the conceptual resources that students activated in connection with the explicit features they focused on.

Theme II: The discrete explicit features of representations that students attended to impacted the conceptual resources they activated.

Students' justifications for why their selected Lewis structure was more stable depended on the explicit features they attended to and the conceptual resources activated, including how these resources were used to support their claims about stability.

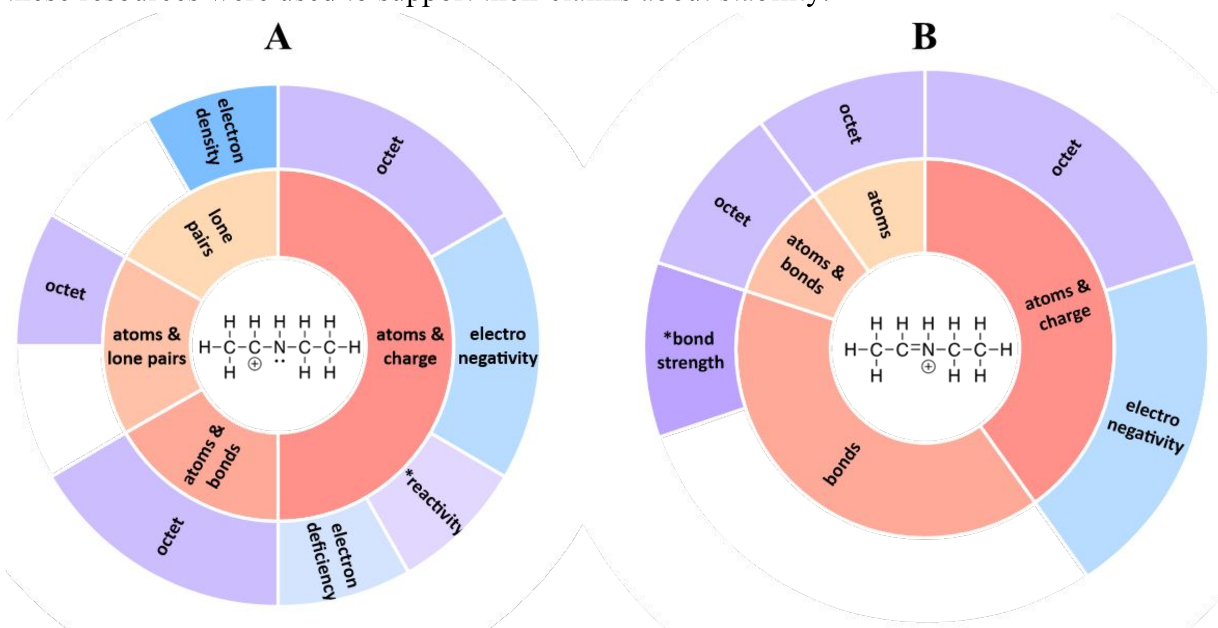

Figure 3. The explicit features of representations (inner ring) and the conceptual resources activated (outer ring) regarding the relative stability of structure A (left) or B (right). The size of the arc indicates the frequency with which the feature/conceptual resource was mentioned. * is used to depict conceptual resources that are not productive for the context.

Students who selected the correct structure B activated fewer but more relevant conceptual resources than those who selected structure A (**Figure 3**). Those selecting B frequently discussed octet and electronegativity of the atoms bearing the positive charge—both relevant in this context (**Figure 3**). In Task 2, students selecting the correct structure A considered additional factors, such as atom size, reactivity, and charge delocalization (**Figure 3S**). However, some students highlighted less pertinent features, such as the presence of a double bond, without justifying how double bonds impact stability (as indicated by the absence of outer rings associated with *bonds* in **Figure 3B** and **Figure 3SA**). A few students argued that double bonds, being stronger and more difficult to break than single bonds, contribute to greater structural stability. Sally encapsulated this perspective, stating, "*B is more stable because it has a double bond [which is] stronger and harder to break.*" In responses favoring the correct answer for Task 2, additional conceptual resources in relation to the double bond—such as bond length and bond rotation—were discussed (**Figure 3S**). Although students favored structures with double bonds as more stable than those with single bonds, as has been observed in other studies (Tetschner and Nedungadi, 2023), the explicit feature—double bond, as well as the activated conceptual resources—bond strength, length, and rotation, are less relevant for justifying stability in the context of tasks in this study (**Figure 1**).

In addition to discussing octet and electronegativity, students who selected A also considered reactivity, electron deficiency, and electron density (**Figure 3A**), which echoed the conceptual resources observed in responses to Task 2 (**Figure 3S**). In discussing reactivity, students pointed to specific structural elements—such as positive charges, lone pairs, and double bonds—as indicators of reactivity. For instance, Betty commented on the double bond's implications, stating, "*that pi bond there would just be somewhat reactive with other things… And so based on that, the alkene would be not so stable.*" This argument suggests that double bonds heighten reactivity, thereby lowering stability. As has been observed elsewhere (Brandfonbrener *et al*., 2021), students discussed how the structural features related to reactivity, hence stability, in isolation of the conditions for a reaction. This approach to discussing reactivity without contextualizing it is less productive. Interestingly, some students who selected structure A claimed that it possesses the structural features that will cause the chemical species to undergo a change (break and form new bonds) to become more stable. For example, Irene speculated, "*Maybe [A] is more stable because I feel like the carbon is like an easy fix. Something else could have been added to that carbon to make it stable*". These ideas were based on the structure's potential to become stable rather than considering aspects that make it stable or unstable as is.

Notably, none of the students recognized that the two Lewis structures provided were resonance structures, and, therefore, they did not discuss ideas related to major and minor contributors to the resonance hybrid. Instead, they viewed the two structures as separate entities with distinct structural features and properties. This observation aligns with findings from other studies that have examined student challenges with understanding resonance structures (Kim *et al*., 2019; Petterson *et al*., 2020; Xue and Stains, 2020).

Theme III: Students relied on various heuristics and lower-level reasoning modes when constructing explanations about stability.

When investigating how students integrate the information available (explicit features of representations and the activated conceptual resources) to address the prompt, we observed variability in their explanations, both in the reasoning processes utilized and their sophistication. In this section, we report the heuristics and reasoning processes students employed when making inferences about stability, as well as how these approaches relate to different modes of reasoning. These findings shed light on the diverse cognitive mechanisms students engage in during problem-solving, highlighting the complexity of their thought processes in the context of chemical stability.

Reliance on Heuristics when Constructing Explanations. To explain the diversity of student thinking in determining which structure would be more stable, we turned to the Dual-

Process Theory, which distinguished between Type I heuristics (intuitive, fast-thinking processes) and Type II reasoning (deliberate, analytical thinking). This framework helped us explain why students focused on different explicit features and how these features were connected to specific conceptual resources when making inferences about stability.

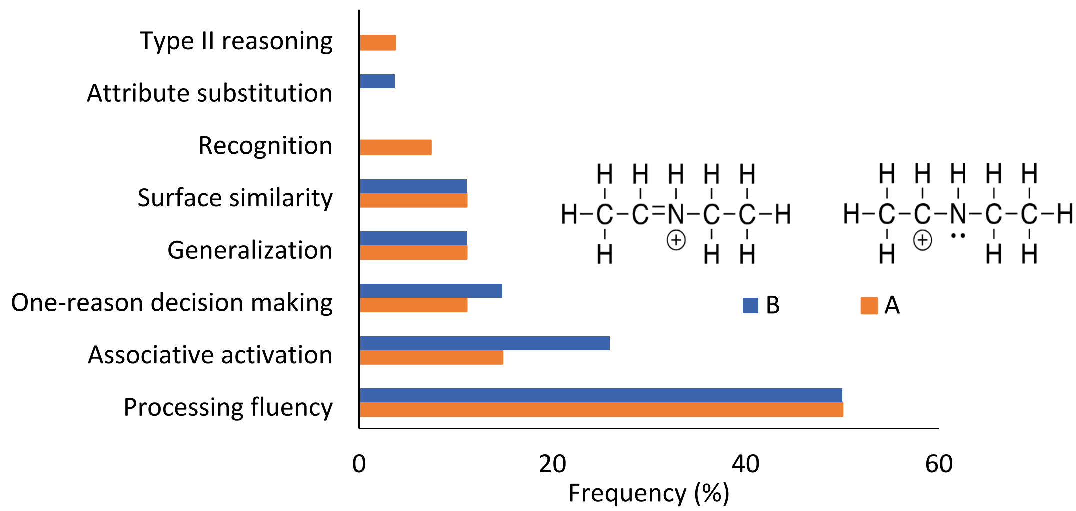

Figure 4. The frequency of various heuristics and reasoning processes in student explanations.

Heuristics (Type I reasoning strategies) strongly influenced our participants' performance on both tasks (**Figure 4** and **Figure 4S**). Key heuristics used include *processing fluency*, *associative activation*, and *one-reason decision-making*, regardless of whether justifications were for the correct or incorrect structure. As explored under Theme 1, students readily noticed and processed different features (*processing fluency*)—some observed differences in bond types, others noted the presence or absence of lone pairs of electrons, and some recognized variations in the types of atoms bearing the charge (**Figure 2** and **Figure 2S**). Although processing fluency can guide attention to relevant visual cues in a representation, minimizing cognitive load, this heuristic may be influenced by the most salient feature which might be irrelevant for a given context, resulting in non-normative responses (Talanquer, 2022), as was observed with responses regarding double bonds. Attention to salient features triggered associations (*associative activation*) between the feature and the property frequently linked to that feature (e.g., the association between an atom bearing a charge and electronegativity) (**Figure 3**).

Some participants replaced the target attribute (molecular stability) with a more readily accessible attribute like bond strength or bond rotation (**Figure 3** and **Figure 3S**) (*attribute substitution*). Rather than evaluating factors that impact stability at the molecular level, they focused on what was most accessible to them—energy at the bond level. Intuitively, one can associate stability with strength (i.e., things that are rigid and strong must be stable), and, in our case, students found those attributes in double bonds (they are stronger than single bonds, and they do not rotate). These students made inferences about stability based on identifying a single differentiating characteristic between the structures (*one-reason decision-making*) that allowed them to make justifications that fit their claims about stability. Other instances of *one-reason decision-making* included the narrow focus on the lone pair of electrons—a prominent feature in structure A. For instance, when Sybil noticed the absence of a lone pair of electrons in B, she settled on a response based on this feature alone, concluding that "*B is more stable because it doesn't have any leftover [lone pair of electrons]. They all have something to bond to.*"

Other students' responses reflected the application of heuristics like *generalization* and *surface similarity*. For example, as has been observed in other studies (Tetschner and Nedungadi, 2023), some students believed that a formal charge indicates an atom's incomplete octet, even for the nitrogen atom in B, which has a complete octet (e.g., Maggy in **Table 1**). These students saw cases where the atom with a formal charge (e.g., a positively charged carbon atom in A) did not have a complete octet and *generalized* this pattern to all contexts where a formal charge is present. These students claimed that both structures did not have a complete octet and, therefore, were equally unstable because of the resemblance in possessing a positive formal charge (*surface similarity*, Sally in **Table 1**). They, therefore, looked for other features (e.g., double bonds) that differentiated the structures enough to make justifications that fit their claims about stability.

Some students also relied on the *recognition* heuristic. Mori, for example, chose structure A as the more stable (**Table 1**) because he was more familiar with a nitrogen atom with three bonds and a lone pair (as is the case in structure A) and less familiar with a positively charged nitrogen with four bonds (as is the case in structure B). Similarly, Irene selected structure A as the more stable; she expressed her unease about the "nonnormal" nitrogen in structure B, perceiving it as more unstable due to its bonding: "*Nitrogen usually only makes three bonds, but right now (in B) it has four. So it's got extra [bonds], like more than normal… making the nitrogen more unstable than it was before*." Some students ignored the charged nitrogen, focusing instead on the necessity for carbon atoms in the chain to have full octets. They reasoned that the main chain primarily dictates the structure and reactivity, emphasizing that organic chemistry predominantly concerns carbon atoms. These examples reflect a common heuristic where students may prioritize more familiar or seemingly central aspects of a molecule, neglecting other important features and their impacts. Recognizing patterns is a useful cognitive tool in learning, yet it can sometimes lead students astray by causing them to focus solely on familiar features and eliminate or ignore less familiar information.

Lastly, very few students used analytical Type II reasoning, which involves deeper, more deliberate consideration of multiple factors. For instance, Nate initially cited a learned pattern that *"nitrogen is more stable with three bonds and carbon is stable with four."* He then recognized that this pattern does not hold for either of the structures, which pushed him to consider the electron density contributions from lone pairs to stabilize the charged carbon, explaining that "*the lone pair from the nitrogen helps to stabilize that carbon because it can donate electron density that could help alleviate that strain."* Even though Nate demonstrated deeper thinking in his analysis of structure A, he did not apply the same depth of reasoning to structure B or recognize that his analyses of structure A supported events that resulted in structure B. He ultimately chose the incorrect structure A as the more stable, demonstrating that even more analytical reasoning does not always lead to correct inferences. This pattern of not fully integrating analytical reasoning was similarly observed in students' responses to Task 2 (**Figure 4S**).

The Dual-Process Theory and Heuristics Framework shed light on students' heavy reliance on the salient explicit features and the implicit properties they readily associate with those structural features. This dependence varies significantly among students due to the interplay between the specific features of a representation and each student's background knowledge and prior experiences (Talanquer, 2022). As depicted in **Figures 2** and **3**, what stands out to one learner may not be salient to another, explaining why our students focused on all explicit features of the Lewis structures to make inferences about relative stability and engaged various conceptual resources linked to these features. Overall, our study corroborates the findings of other studies which also have highlighted chemistry students' over-reliance on heuristics across various chemistry tasks (Maeyer and Talanquer, 2010, 2013; McClary and Talanquer, 2011; Talanquer, 2014; Graulich, 2015; Miller and Kim, 2017).

Reliance on Lower Level Modes of Reasoning when Constructing Explanations. In the previous sections, we have detailed how students focused on particular features—driven by *processing fluency* where salient explicit features of representations captured their attention. We have also explored how conceptual resources are linked to these features and the reasoning behind these associations, whether through *associative activation*, *generalization*, or *analytical reasoning*. In this section, we delve into the sophistication of student explanations through the lens of the Modes of Reasoning Framework. The majority of students' explanations in both tasks were relational (72%), followed by descriptive (33%), and causal (6%) (**Figure 5** and **Figure 5S**). No clear trends were identified between the accuracy of the selected Lewis structure and the sophistication of student reasoning in support of their claims.

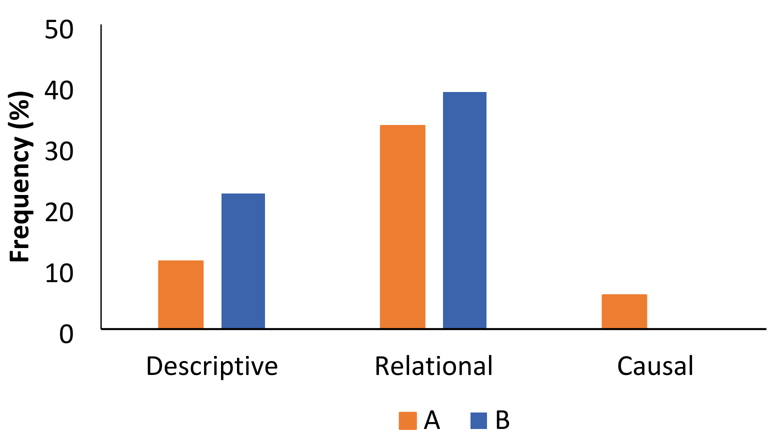

Figure 5. The frequency with which students provided descriptive, relational, or casual explanations. The total frequency is slightly above 100%, as several students argued about both structures, and their responses were counted twice (once for each structure).

The students who provided descriptive explanations (33%) often mentioned explicit features without connecting them to conceptual resources. This type of response typically lacked depth as it did not demonstrate an understanding of how features influence stability. For example, explicit features such as double bonds and lone pairs of electrons were simply noted for their contribution to the stability of a specific structure without further justification (as indicated by the absence of outer rings associated with explicit features in **Figures 3** and **3S**). The *processing fluency* heuristic significantly influenced the construction of descriptive responses, where the most visually salient features were quickly and effortlessly noted. Additionally, the *recognition* heuristic and *one-reason decision-making* were prevalent, where students often relied on a single, recognized feature to make inferences. Moreover, *surface similarity* and *generalization* could result in descriptive responses, as students could judge the degree of similarity based on features of two structures that resemble each other and generalize some learned patterns about their properties (Weinrich and Talanquer, 2016).

A high proportion of students provided relational explanations (72%) by noting the relationships between explicit features and implicit properties (conceptual resources) (**Figure 5** and **Figure 5S**). For instance, discussions often centered around electronegativity and its relation to the type of atom bearing the positive charge. In his response, Evans stated that "*B is more stable because the positive charge is on a nitrogen instead of on a carbon, and the nitrogen being more electronegative… it can more easily house the positive charge than the carbon can*." In contrast, Ivy chose structure A as more stable by attending to the same features and properties, but with a different interpretation: "*Because nitrogen is a lot more electronegative and if it has a charge on it, the balance of the molecule might be off*." Both students identified and linked features (atoms and charge) with the conceptual resource of electronegativity through *associative activation*, yet they arrived at opposite conclusions. This discrepancy highlights a common issue with relational explanations—making connections based on frequently observed associations without a deeper understanding of the underlying reasons or implications (e.g., the rationale for why a positive charge should reside on a more or less electronegative atom).

Causal explanations (6%) involve a deeper level of reasoning, where students provide comprehensive explanations about *how* and *why* specific, explicit features and associated conceptual resources influence a given outcome. This type of causal reasoning was rare, observed in only one student's response for Task 1 and two for Task 2. For example, Nate discussed the role of a lone pair of electrons in donating electron density to alleviate electron deficiency on the charged carbon atom (**Table 2**). However, in Task 2, he initially chose the correct structure but later changed his answer, selecting a structure with two lone pairs of electrons and justifying it by arguing that more lone pairs imply greater electron density, potentially stabilizing the structure. He supported this choice with the *recognition* heuristic that carbocations, which he perceived as more common than oxonium ions, are more stable. This example illustrates that more sophisticated reasoning does not guarantee the accuracy of inferences. At the same time, compared to students who provided relational explanations, those who constructed causal explanations demonstrated the ability to consider and evaluate the contributions from multiple external features and internal properties. This integration included not just the visible features and associated properties but also a deeper understanding of how multiple characteristics interact to affect stability. These differences between the three types of explanations in the context of our tasks are depicted in **Figure 6**.

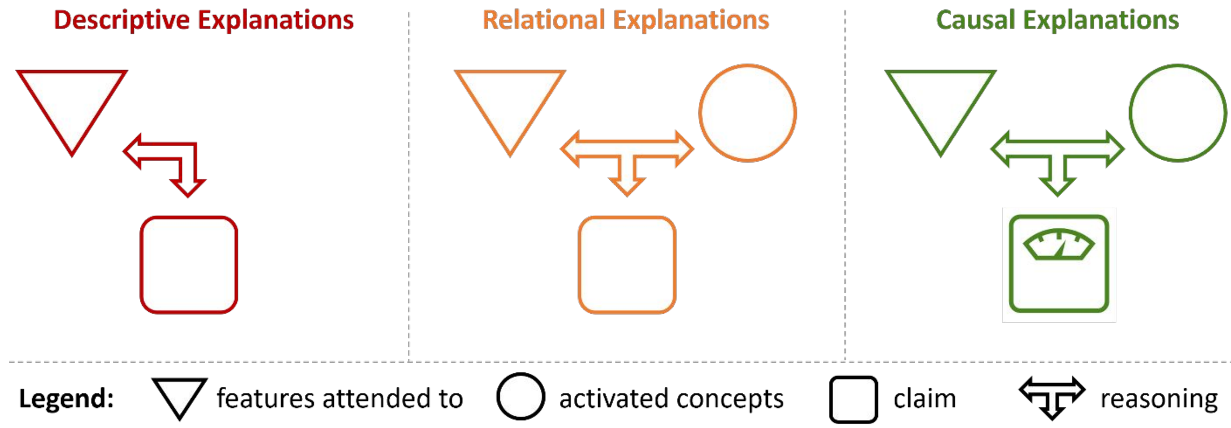

Figure 6. The differences in the three types of explanations that students constructed to make inferences about the relative stability of the provided Lewis structures. The scale in the third frame represents the ability to weigh the contributions of multiple visible features and associated concepts to make a claim.

Contrary to our findings, some studies have reported a higher proportion of causal modes of reasoning demonstrated by organic chemistry students from other institutional contexts and with other tasks (Becker et al., 2016; Bodé *et al.*, 2019). We believe that our participants' explanations for the presented task were primarily relational, given that many practice problems in the textbook used by our sample (Bruice, 2016) and common tasks in this topic (Betancourt-Pérez *et al.*, 2010) only ask students to identify the most stable structure without requiring justification or explanation. Additionally, the textbook used by our participants and several others presents delocalization as a set of rules that include limited causal explanations of the contribution of resonance structures to the hybrid (Carle and Flynn, 2020). Such tasks and presentation of topics using a set of rules may promote lower-level reasoning modes and errors as students tend to overgeneralize rules. Explicitly teaching and intentionally assessing concepts supported with higher-level reasoning, hence moving beyond the mere evaluation of factual content knowledge, provides opportunities for students to practice constructing explanations and arguments using evidence and better supports productive chemical thinking (Talanquer, 2014; Carle and Flynn, 2020).

Theme IV: Many students misapplied chemical principles to make justifications that fit their correct or incorrect claims about stability.

In addition to capturing the explicit features students attended to and conceptual resources they activated, we evaluated students' application of chemical principles in their justifications as valid or spurious. **Figure 7** represents all these analyses by adding to the layers from **Figure 3**. **Table 3** includes example quotes to support the data for each scenario in **Figure 7**.

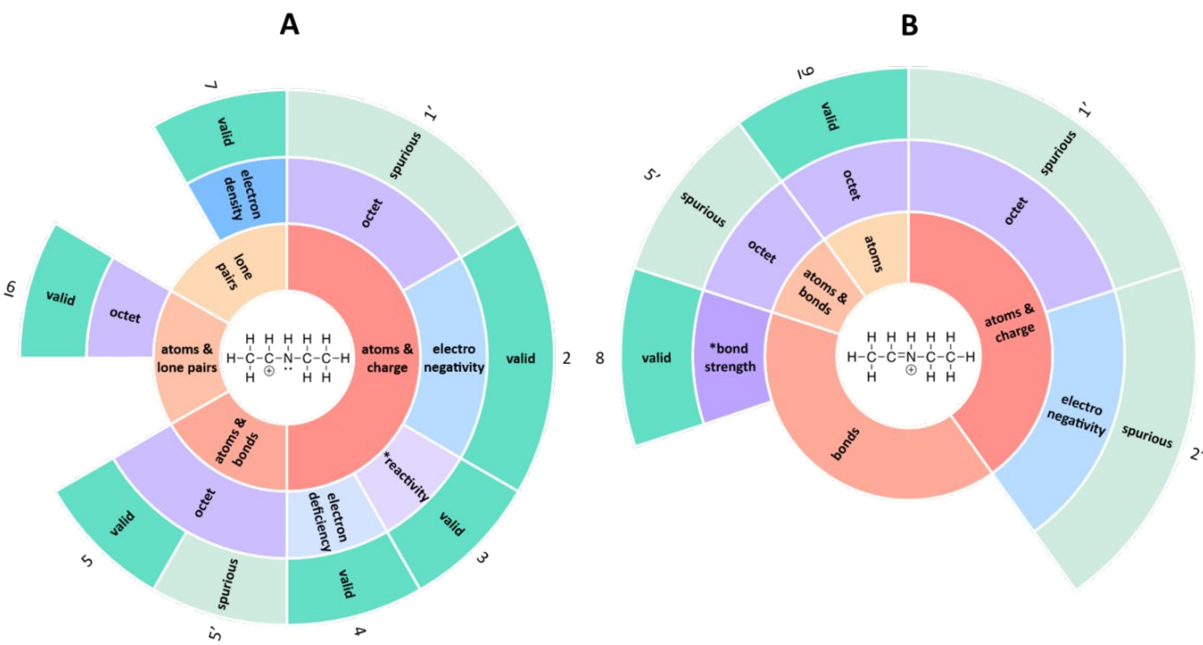

Figure 7. The explicit features of representations (inner ring), the conceptual resources activated (middle ring), and the validity of assumptions (outer ring) by students who selected A (left) or B (right) as the more stable Lewis structure. Legend: The size of the arc indicates the frequency with which the feature/conceptual resource was mentioned. The numbers on the outer ring indicate the unique combinations of features, resources, and validity of assumptions (a total of 9) used to justify claims about stability, where * is used to depict conceptual resources that are not productive for the context, whereas ' to depict spurious chemical assumptions, and an 'underline' to differentiate between numbers 6 and 9.

Table 3. Student responses illustrating the conceptual resources activated based on the explicit features attended to and whether explanations reflected the appropriate application of chemical principles/rules. Legend: Orange text = explicit features. Green text = activated conceptual resource. Italicized text = spurious assumptions. Plain text = valid assumptions. * = knowledge elements that are not productive for the context.

No.	Student response
1'	*"Nitrogen [in B] doesn't fill its octet... that's why it has the plus charge on it."* — Maggy
2	"A looks more stable because I don't like the idea of having a nitrogen with a positive charge because nitrogen is more electronegative than a carbon." — Victor
2'	"B is more stable because the positive charge is on a nitrogen instead of on a carbon and the *nitrogen being more electronegative, having more protons on it can more easily house the positive charge than the carbon can.*" — Evans

3	“[in A], the positive [charge], would affect the stability because [carbon] would really want to *make a new bond. So then it [carbon] would be really high energy and trying to like *react with other molecules or atoms.” — Irsa
7 4	“The lone pair [in A] can donate electron density that could help stabilize that electron-deficient carbon, electron-poor carbon.” — Nate
5 5’	“Carbon normally has four bonds to complete the octet, but now [in A] it's missing a bond… nitrogen usually only makes three bonds, but right now (in B) it has four. *So it’s got extra, like more than normal…* Maybe [A] is more stable because I feel like the carbon is like an easy fix, something else could have been added to that carbon to make it stable. That wouldn’t really affect anything else. *Whereas using the nitrogen to fill [complete octet on] that carbon is making the nitrogen more unstable than it was before*.” — Irene
<u>6</u>	“The two dots [lone pairs] on the nitrogen from the left [A] fills the octet of nitrogen.” — Donna
8	“B is more stable because it has double bonds (which) are *stronger and harder to break.” —Sally
<u>9</u>	“B is more stable because the main chain of carbons all has satisfied the octet rule now and the carbon chain is what's most responsible for structure and the reactivity in a molecule” — Paula

Unexpectedly, students who selected the correct structure mostly displayed spurious chemical assumptions compared to their counterparts (**Figure 7** and **Figure 3S**). For instance, when discussing octet and electronegativity (productive conceptual resources), students expressed that a positive formal charge indicates an atom’s incomplete octet (1’ in **Table 3**) or that the positive charge should reside on a more electronegative atom (2’ in **Table 3**) (spurious assumptions) (Tetschner and Nedungadi, 2023). Spurious assumptions regarding the octet were expressed by students selecting structure A to a lesser extent, but the students additionally argued that the positive charge was needed to make the atom with fewer bonds “happy,” meaning that the positive charge fills an atom’s octet (Waldrip and Prain, 2012). Furthermore, some students who selected A claimed that the nitrogen atom in B violated the octet rule due to the presence of four instead of three bonds that it should typically have (5’in **Table 3**). Spurious assumptions could result from the *generalization* heuristic, as in the case of charge and an atom’s octet (1’ in **Table 3**), or they can be hastily formulated to support a previously made claim. For example, a student might choose a structure with a positive charge on a more electronegative atom and then justify it by altering a chemical rule to argue that the positive charge should be on the most electronegative atom, thereby tailoring the rule to fit their claim.

In general, even though students who selected the correct structure activated fewer but more relevant conceptual resources compared to their counterparts whose ideas were more wide-ranging, their leverage of these conceptual resources to justify why structure B is more stable demonstrated misinterpretation of chemical principles, leading to spurious chemical assumptions. These students were drawn to structure B, favoring structures with more bonds as more stable (Tetschner and Nedungadi, 2023); coincidentally, this was the correct answer for the designed task. In their justifications, students reframed chemical rules to fit their selection, resulting in a correct answer supported by inappropriate reasoning. Students focused on the unique features of the representations, activated conceptual resources related to these features, and, similar to the findings of Abell and Bretz (2018), misapplied chemical principles to make justifications that fit their claims. At the same time, our findings contrast with other studies examining student reasoning in which correct claims were more frequently supported by relevant concepts and valid assumptions (Bodé *et al*., 2019; Deng and Flynn, 2021; Kararo *et al*., 2019).

Altogether, our findings indicate that student responses to similar prompts can be varied and complex (Bodé, *et al*., 2019; Caspari and Graulich, 2019; Deng and Flynn, 2021; Watts *et al*., 2021; Kranz *et al*., 2022). On one hand, students can make a correct claim (select the appropriate structure) supported by spurious assumptions or unproductive conceptual resources and lower-level modes of reasoning. On the other hand, students can make an incorrect claim and support the claim with valid chemical assumptions, relevant conceptual resources, and more sophisticated reasoning. Students may activate similar knowledge elements but focus on different explicit features when analyzing structures. For example, in determining an atom's octet, some participants might count the number of bonds around the atom to ensure this matches the typical appearance of particular atoms, such as nitrogen typically having three bonds and a lone pair of electrons (Irene in **Table 3**). Conversely, others would assume an incomplete octet due to the presence of a positive charge (Maggy in **Table 3**). This diversity in approach shows how students selectively apply their understanding of chemical concepts to the features they deem most significant.

When using representations to make inferences about chemical concepts, several important factors are at play: explicit features of the representation, conceptual resources associated with these features, and chemical principles applicable to the context. The use of heuristics to focus attention on relevant aspects of the prompt can result in quick and efficient solutions, but given learners' tendency to overgeneralize rules, the use of heuristics can be misleading and result in errors in decision-making. To better support students in making accurate chemical inferences, explicit instruction that covers all relevant factors is essential. This includes teaching students how to assess the contribution of each factor and understand how these factors interconnect. Additionally, aligning instruction and assessment practices, such that prompts explicitly direct students to consider different aspects—such as features, conceptual resources, and chemical principles—and evaluate their relevance in solving the task, can enhance students' ability to provide relevant and sophisticated explanations about structure-property relationships. Promisingly, one study found that intentional instruction about structure-property relations and explicit prompting—asking students to provide directed explanations—resulted in more sophisticated and complete explanations of implicit properties (boiling point trends) of Lewis structures (Kararo *et al*., 2019).

Limitations

The findings from this study are specific to the student population at a single institution and may not be universally applicable to other educational contexts. Students using different curricula or textbooks might engage with the prompts in this study differently. While our data provides detailed insights into student reasoning patterns, we do not extrapolate these findings to broader populations. This underlines the need for further research to explore how diverse student groups interpret and utilize chemical representations across various educational settings.

Additionally, it is important to note the specificity of our investigation, focusing on the use of Lewis structures to draw inferences about stability. There's a wealth of potential insights to be uncovered beyond this singular context, considering that the "use" skill represents just one aspect of representational competence, "Lewis structures" constitute one of the numerous representations employed in organic chemistry, and "stability" is just one of many concepts. Nevertheless, this study adds to the existing literature by investigating previously unexplored property of stability in the context of Lewis structures.

Furthermore, while interviews provide deep insights into students' reasoning, this data collection method may limit our understanding to what students choose to verbalize, potentially overlooking some cognitive processes and explicit features of representations they attend to but do not explicitly name.

Lastly, while staying true to the type of tasks students typically engage in within the course, the tasks designed may not necessitate Type II or causal reasoning. This could partly explain why our participants relied on lower-level reasoning modes to make claims. Moreover, the prompt asked students to justify their selection but did not explicitly require students to provide a more sophisticated argument. While the tasks reflect typical classroom activities, they may not fully challenge students to demonstrate deeper levels of understanding. Nonetheless, we have shown that even with simple tasks that require the use of a representation, students pay attention to different structural features, activate various conceptual resources, and misapply chemical principles to craft explanations that fit their claims.

CONCLUSIONS

We investigated how organic chemistry students reason when making structure-property predictions by noting which features of representations they paid attention to and what conceptual resources they included in their explanations. We also characterized the depth of their explanations and the influence of heuristics in their decision-making. By adding a justification aspect to a task that students commonly engage in within the course, we uncovered diverse ideas and processes that students apply to the same prompt. These findings are summarized in **Table 4**.

Table 4. Summary of key aspects (explicit features, conceptual resources, and reasoning) observed in student responses.

		Correct claim (structure B)	**Incorrect claim (structure A)**
Unique features attended to		Mostly double bond	Mostly lone pair of electrons
Conceptual resources activated		Fewer, mostly relevant	More, mostly relevant
	Assumptions	More spurious	More valid

Reasoning	**Modes of reasoning**	Less sophisticated	More sophisticated
	Heuristics	More associative activation and attribute substitution (relational reasoning)	A variety of Type I heuristics, including Type II reasoning

Students referenced different explicit features and primarily attributed chemical stability to the unique, eye-catching features of each structure. Notably, learners favored structures with double bonds as more stable than those with single bonds (Tetschner and Nedungadi, 2023), or structures with structural arrangements they were more familiar with (nitrogen atom with three bonds and a lone pair of electrons) (Talanquer, 2014), as they could easily and quickly decode the information conveyed through such salient features (Chi *et al.*, 1981; Graulich *et al.*, 2019; Talanquer, 2022). Additionally, students associated the explicit features with various implicit properties, and their explanations varied in sophistication based on assumptions and heuristics applied (Maeyer and Talanquer, 2010, 2013; McClary and Talanquer, 2011; Talanquer, 2014; Graulich, 2015; Miller and Kim, 2017). Importantly, students' success on tasks was not associated simply with attending to fewer or more explicit features of representations. Productive decision-making resulted from several factors other than combinations of structural features such as activation of productive resources and whether assumptions held regarding these resources were valid or spurious. Overall, we found that productive decision-making entails paying attention to relevant information and considering and weighing contributions from as many variables as possible.

The diversity in responses could result from the instruction that students received. For example, the textbook resource students used presents the topic of delocalization as a set of rules, and the practice problems students encounter ask them to identify the most stable structure without requiring justification or explanation (Betancourt-Pérez et.al, 2010; Bruice, 2016; Carle and Flynn, 2020). This instructional approach might foster a surface-level engagement with the material, where students may correctly identify more stable structures without truly understanding the underlying chemical principles. As such, students may form intuitive patterns or overgeneralize chemical rules that lead to errors in solving tasks. Our results show that regardless of whether students activated productive or unproductive conceptual resources, some misapplied chemical principles to fit their claims about the relative stability of the provided structures (Maeyer and Talanquer, 2013; Abell and Bretz, 2018).

Overall, our investigation of various aspects (explicit features of representations, conceptual resources, depth of explanations, and validity of assumptions) challenges the assumption that correct answers necessarily reflect a deep understanding (**Table 4**). Notably, selecting the wrong structure was associated with more sophisticated reasoning, suggesting that correct answers do not always reflect sophisticated chemical thinking or appropriate use of chemical knowledge, as has been observed in other studies (Miller and Kim, 2017). Consequently, researchers and instructors should consistently investigate how students arrive at a given answer by asking both the *what* and the *why* behind a phenomenon (Cooper *et al.*, 2016;

Ward *et al.*, 2022) instead of assuming that when students arrive at a correct answer, they have grasped the concepts or have reasoned appropriately.

Implications

The findings necessitate two important educational objectives: eliciting student reasoning and fostering the development of productive chemical thinking. Instructors should prioritize nurturing students' ability to reason effectively by integrating these goals into their learning objectives and aligning them with both instructional strategies and assessment methods. By consistently employing thoughtfully designed activities that compel students to articulate not only *what* occurs but also *why* it occurs, instructors can create numerous opportunities for students to practice and be evaluated on their critical thinking skills concerning the phenomena under study.

The students in our study used a textbook that only asked for the *what* in the tasks related to our topic of interest. As evidenced in the investigation, the students relied on lower-level reasoning to decipher which structure would be more stable. Our study underscores the notable impact that the nature of tasks commonly found in educational materials can have on students' reasoning processes. Through our analysis of students' reasoning about relatively simple tasks involving Lewis structures, we observed a predominant reliance on heuristics and relational thinking, which are often sufficient for such tasks. This finding highlights a potential limitation of common textbook tasks, which may not encourage the development of deeper, more sophisticated reasoning abilities and representational competence. This finding has been previously reported in the context of many other chemistry tasks commonly found in chemistry textbooks (Carle & Flynn, 2020; Dávila & Talanquer, 2010; Gurung et al., 2022; Thompson et al., 2023). To cultivate a more sophisticated conceptual understanding, it is crucial for educators and curriculum developers to integrate tasks that challenge students to engage more deeply with the material. By incorporating tasks that require causal reasoning, educational materials can better promote higher-order cognitive skills and enrich students' understanding of stability and other fundamental chemical concepts.

To facilitate this deeper engagement, instructors could employ scaffolding—breaking down complex tasks into manageable steps and requiring extensive explanations with each step (Caspari *et al.*, 2018; Caspari and Graulich, 2019; Lieber and Graulich, 2020; Kranz *et al.*, 2022). It is equally important that instructors choose instructional materials that help students understand the *why* behind chemical rules so they do not make intuitive connections and overgeneralize rules to avoid errors and the development of lower-level reasoning (Carle and Flynn, 2020; Thompson *et al.*, 2023). Explicitly instruction about different representations and the selection of instructional resources that support the development of representational competence (Kozma and Russell, 2005; Gurung *et al.*, 2022) may lead to student success in inferring chemical concepts from representations, thereby improving their overall success in chemistry.

Eliciting student reasoning is half the battle; what one does with the elicited information will determine whether students develop productive chemical thinking. Our study used a case comparison to increase the factors students consider when constructing explanations (Graulich and Schween, 2018). This task revealed what students deemed relevant or irrelevant in making inferences about chemical concepts and the various heuristics and assumptions that constrained their thinking. Instructors can use similar case comparison tasks to elicit students' diverse ideas, then compile all the ideas and have students work in groups to review other students' responses. While reviewing other students' responses, group members can reflect and discuss relevant and irrelevant aspects of the explanations and normative and non-normative reasoning. This evaluation of several alternative explanations that may be contradictory to their own will be helpful in promoting a more meaningful analytical approach, as students will have to think deeply about the many alternatives and decide which ones are more plausible (Lieber and Graulich, 2020). Attending to student reasoning is important. It helps researchers and instructors design strategies that challenge low-level reasoning by pushing students to reflectively find and use all the relevant information for a given context. This will, in turn, support the development of productive chemical reasoning.

The work on eliciting student reasoning and supporting students to develop more sophisticated thinking need not rely on instructors only. Researchers can perform fine-grained analysis of student reasoning utilizing multiple frameworks in tandem to provide a holistic understanding of student reasoning. When investigating how students reasoned when making inferences about stability through the lenses of the Modes of Reasoning Framework and the Dual-Process Theory (Type I heuristics and Type II reasoning), we found that heuristics played a dual role—in some contexts, they supported students in quickly making sense of the representations (e.g., processing fluency, recognition, associative activation), whereas in other cases they led to biased decisions even for the most sophisticated student responses. Researchers can design evidence-based tasks and intervention activities, as well as quality assessments that promote the development and evaluation of productive chemical thinking. An example can be shown in our prior work, in which we demonstrated how to use student reasoning to develop distractors for multiple-choice items (Ward *et al.*, 2022). Researchers can also facilitate instructor professional development in designing tasks and assessments that elicit student thinking about representations or utilize the researched intervention activities to support meaningful learning. This professional development is critical because previous studies have found that chemistry instructors lack knowledge about effective teaching regarding representations (Linenberger and Holme, 2015; Popova and Jones, 2021; Jones *et al.*, 2022). Such training needs to help instructors take cognizance of relevant theories of learning and the key factors affecting students' ability to reason with representations.

CONFLICTS OF INTEREST

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Author Contributions

MP conceptualized the study, obtained the funding for the project, and led project administration. FR collected and analyzed the data with assistance from LWW, CB, and MP. FR wrote the original draft of this article. MP and LWW reviewed and edited the article. All authors approved the submitted version of the article.

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Supplementary information

ATTENTION IS CURRENCY: HOW SURFACE FEATURES OF LEWIS STRUCTURES INFLUENCE ORGANIC CHEMISTRY STUDENT REASONING ABOUT STABILITY

Fridah Rotich, Lyniesha Ward, Carly Beck, and Maia Popova*

Below are the two case comparison tasks used in this study (Figure 1S). Because similar patterns were observed in the context of both tasks, the main document discusses Task 1 in detail.

Twenty-two students (n = 22) were presented with Task 2 and asked to reason about the relative stability of the two Lewis structures. When deciding which resonance form is more stable, 15 students selected A, 5 selected B, and 2 reasoned that both forms are equally stable.

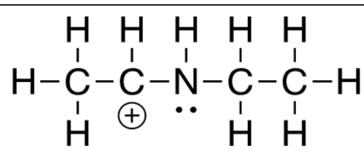
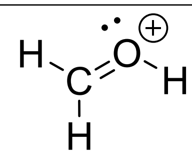
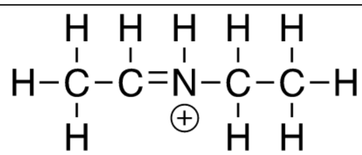
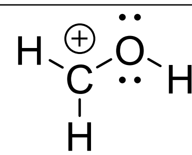
	Task 1		**Task 2**
A		**A**	
B		B	

Figure 1S. Case comparison tasks of pairs of resonance forms depicted as Lewis structures. The bold green letters represent the more stable structure/resonance form based on the textbook used by students in this study.

Below are the patterns identified for Task 2, organized by research question.

RQ1: What features of Lewis structures do students attend to to identify the most stable structure?

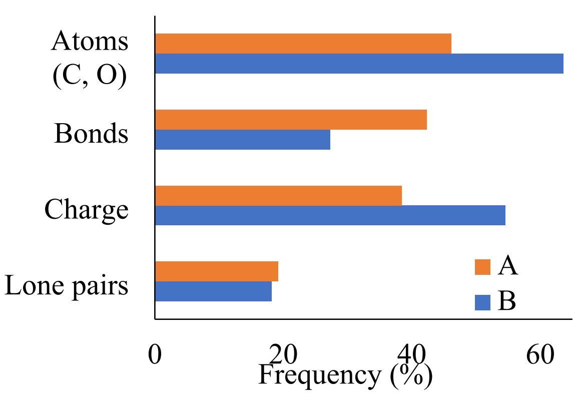


Figure 2S. The frequency with which the students attended to the explicit features of the representations when comparing the relative stability of Lewis structure A (orange) and B (blue).

Similar to Task 1, participants referenced all the explicit features of the provided representations but primarily attributed chemical stability to the unique, eye-catching features of each structure. Structure A was favored as more stable due to double bonds (which is why students who selected A attended to bonds more frequently, Figure 2S), and structure B was thought to be more stable given the charge on the carbon atom (which is why in Figure 2S there are higher frequencies associated with atoms (carbon) and charge for structure B compared to A).

RQ2: What conceptual resources (content-specific knowledge elements) do students activate when attending to the specific features?

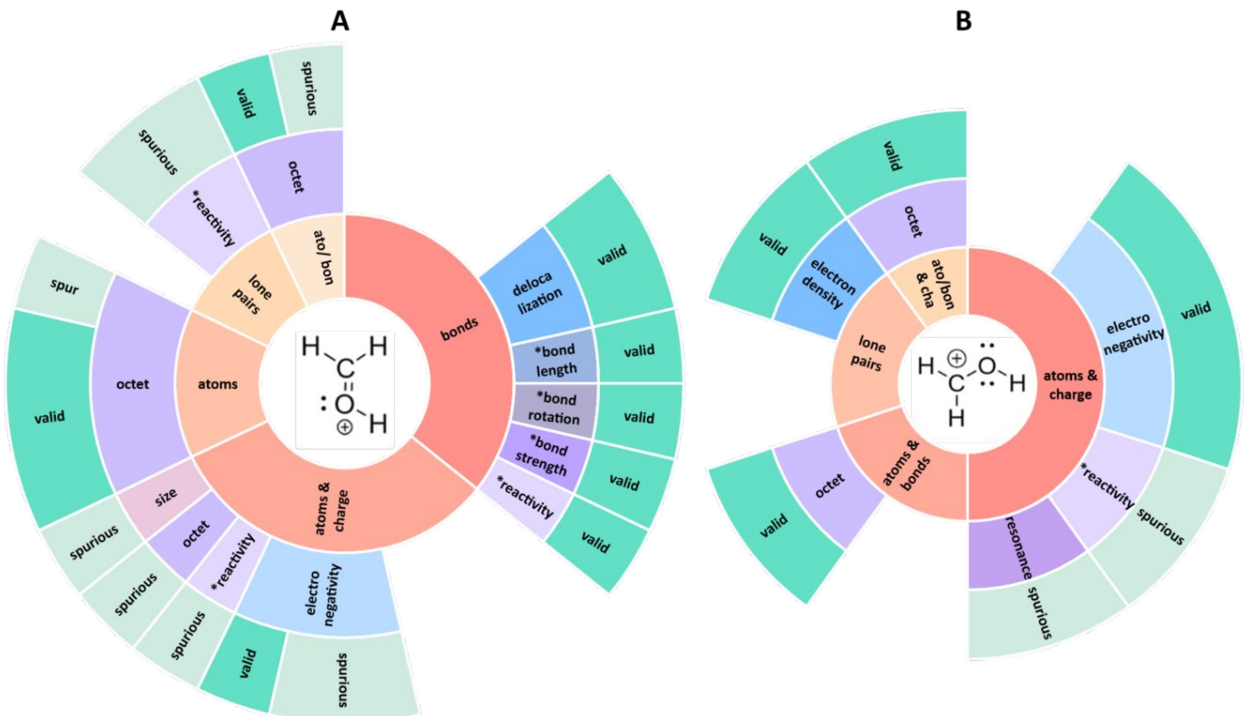


Figure 3S. The surface features of representations (inner ring), the conceptual resources activated (middle ring), and the validity of assumptions (outer ring) associated with the relative stability of the two Lewis structures. Legend: The size of the arc indicates the frequency with which the feature/conceptual resource/assumption was mentioned and not the number of students since one student could mention several features/conceptual resources/assumptions. ‘ato/bon’ (inner ring in A) stands for ‘atoms & bonds.’ ‘ato/bon & cha’ (inner ring in B) represent ‘atoms, bonds & charge.’

In considering the factors that contribute to the stability of structure A, students activated conceptual resources related to the double bond (i.e., bond strength, bond length, bond rotation), similar to the findings of comparison Task 1. In both tasks, these conceptual resources were validly referenced but are not productive for this context. Additionally, other conceptual resources such as reactivity, electronegativity, and octet were activated. In all instances for both tasks, reactivity was coded as unproductive as students only discussed explicit features rather than explained the context in which the given structure would undergo a reaction. Similar ideas were discussed related to electronegativity in both tasks but some students mentioned that the size of an atom bearing the charge was an important consideration (Figure 3S). Overall, while the majority of the students selected the correct answer for Task 2, similar to responses to Task 1, some of their conceptual resources were unproductive, and some of their interpretations of chemical principles were nonnormative (Figure 7 and Figure 3S), indicating that correct answers do not always correspond to productive thinking.

When discussing what makes structure B more stable, students activated conceptual resources such as electronegativity, reactivity, and octet and considered the role of lone pairs of electrons in donating electron density to bring about stability (Figure 3S), as had been reported with the comparison Task 1 (Figure 3).

Finally, similar to Task 1, some students only cited explicit features without including any conceptual resources in their explanations (illustrated by the absence of outer rings in Figure 3 and Figure 3S). Additionally, none of the students recognized that the two Lewis structures provided were resonance structures and instead treated the two structures as distinct entities with different structural features and properties. As such, they did not discuss ideas related to major/minor contributors to the resonance hybrid.

RQ3: How do students reason when making inferences about stability from Lewis structures?

Heuristics

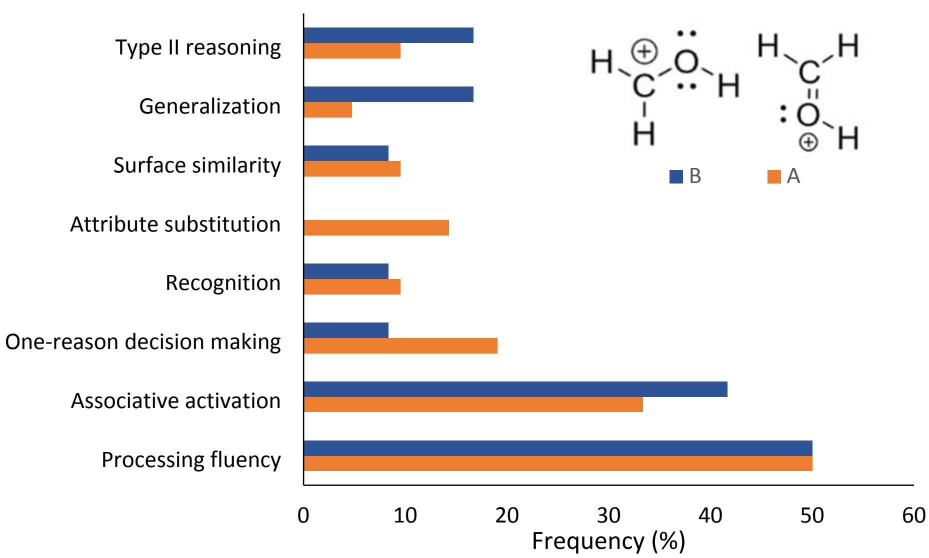


Figure 4S. The frequency of various heuristics and reasoning processes in student explanations.

As observed in responses to Task 1, *processing fluency* and *associative activation* were prevalent heuristics, while other heuristics and Type II reasoning were less common in student explanations to justify what makes a particular structure more stable. In summary, regardless of whether students selected the correct or the incorrect structure as the more stable structure, their explanations included primarily *processing fluency* and *associative activation* heuristics.

Modes of reasoning

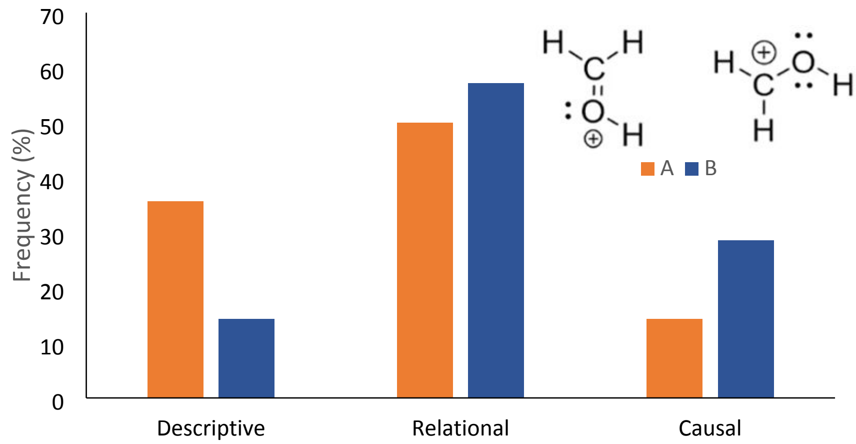


Figure 5S. The frequency with which students provided descriptive, relational, or casual explanations.

Relational explanations were the most frequent and included simple associations between explicit and implicit features without a discussion of *why* or *how* the implicit concepts affect stability. Descriptive explanations were the next most prevalent mode of reasoning, in which students justified their choices by solely referencing explicit features of the provided structures. Additionally, causal explanations were the least common and incorporated discussions of *how* or *why* a particular feature or conceptual resource contributed to stability. Similar patterns were observed for responses to Task 1. Note that even though it looks like students provided more causal explanations for Task 2 (Figure 5S), these causal explanations were expressed by only two students in comparison to one student in Task 1.