Seeing Resonance: On Students' Perception-Based Reasoning in Organic Chemistry

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“[T]he work of abstraction is not exclusively the province of thinking processes alone. Much of thinking turns out to be seeing, if seeing is properly understood.”

(Kellman and Massey, 2013, p. 120)

Kellman P. J. and Massey C. M. (2013). Perceptual Learning, Cognition, and Expertise. In B. H. Ross (Ed.), *The Psychology of Learning and Motivation* (Vol. 58). Elsevier Academic Press, pp. 117-165.

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I. Abstract

Representations are central to conceptual understanding and problem-solving in Organic Chemistry. Resonance, in particular, is a concept that is closely linked to the construction and interpretation of resonance structures. However, understanding these structures as dynamic electron distribution imposes a high cognitive load on learners. While research has emphasized manifold conceptual barriers learners encounter with this concept, little is known about how students perceive resonance structures and use these representations in problem-solving.

To address this gap, a quantitative study with Organic Chemistry (OC) I students investigated how the variation of structural features influences students' consideration of resonance stabilization across different molecular structures. A *k*-means cluster analysis revealed different profiles regarding students' proficiency in recognizing resonance stabilization. It became evident that students' decision-making on resonance was markedly influenced by the visual affordances of the structural features. Students' consideration of resonance was often guided by the visual similarity of features to familiar structural patterns. Yet, students' flexibility in perceiving resonance increased with higher prior conceptual knowledge.

[Braun, I., Lewis, S. E. & Graulich, N. (2025). A question of pattern recognition: investigating the impact of structure variation on students' proficiency in deciding about resonance stabilization, *Chemistry Education Research and Practice*, *26*(1), 158-182.]

Quantitative analysis further revealed that students' recognition of resonance significantly depends on the display of electron lone pairs, as students showed an affirmation bias towards resonance stabilization when electron lone pairs were present.

[Braun, I. & Graulich, N. (2024). The More Explicit, the Better? How the Indication of Electron Lone Pairs Affects Students' Consideration of Resonance in Organic Chemistry, *Journal of Chemical Education*, *101*(11), 4830-4836.]

Extending these findings, a qualitative interview study investigated students' perceptual processes when drawing (un-)productive resonance structures in context. Using eye-tracking, students' connection of visual information and attention distribution to structural features were examined. Analyzing students' verbal drawing rationales further served to triangulate eye-tracking data. While the productivity of resulting resonance structures did not depend on the total amount of integrated and connected visual information, productive drawings were characterized by a more straightforward drawing process transitioning from previous to target drawing. Moreover, the results showcased that flexibility in perceiving interrelated structural features is crucial for constructing valid resonance structures.

[Braun, I., Langner, A. & Graulich, N. (2022). Let's draw molecules: Students' sequential drawing processes of resonance structures in organic chemistry, *Frontiers in Education*, *7*:1055280.]

The interview study also served to investigate students' use of resonance across different task contexts in OC I. Coordination Class Theory was used as an analytical lens to analyze students' problem-solving. Results showed that students' concept use was diverse and shaped by the complex interplay of task affordances and individual factors. However, a more detailed comparison of students' concept use revealed that a more reflective and flexible use of their structural drawings enhanced productive concept use, both in terms of students' task approaches and the activation of task-relevant resources.

[Braun, I. & Graulich, N. (2024). Exploring diversity: student's (un-)productive use of resonance in organic chemistry tasks through the lens of the coordination class theory. *Chemistry Education Research and Practice*, *25*(3), 643-671.]

Thus, this thesis demonstrates that flexibility in perceiving and engaging with representations is crucial for the successful use of resonance in Organic Chemistry. By highlighting the close link between conceptual and perceptual processes in students' reasoning about resonance, it yields new, process-oriented insights into how students perceive, construct, and use resonance structures in problem-solving.

II. Zusammenfassung

Konzeptuelles Verständnis und Problemlösen sind in der Organischen Chemie eng an Repräsentationen gebunden. Insbesondere das Mesomerie-Konzept ist an das Zeichnen und Interpretieren von mesomeren Grenzformeln geknüpft. Mesomere Grenzformeln als dynamische Elektronendichteverteilung zu verstehen, stellt Lernende jedoch vor kognitive Herausforderungen. Während in der Forschung bereits unterschiedliche konzeptuelle Lernschwierigkeiten bezüglich des Mesomerie-Konzepts herausgestellt wurden, ist wenig darüber bekannt, wie Lernende mesomere Grenzformeln wahrnehmen und zum Problemlösen heranziehen.

Um diese Lücke zu schließen, wurde in einer quantitativen Studie mit Studierenden der Organischen Chemie (OC) I untersucht, wie die Variation struktureller Merkmale in Molekülstrukturen das Erkennen von Mesomerie-Stabilisierung beeinflusst. Eine *k*-means Clusteranalyse ergab unterschiedliche Kompetenzprofile hinsichtlich des Erkennens von Mesomerie-Stabilisierung. Es wurde deutlich, dass die Entscheidungsfindung der Studierenden entscheidend von den visuellen Charakteristika struktureller Merkmale beeinflusst war, wobei die visuelle Ähnlichkeit zu vertrauten Strukturmustern eine wichtige Rolle spielte. Allerdings nahm die Flexibilität der Studierenden im Erkennen von Mesomerie mit höherem konzeptuellem Vorwissen zu.

[Braun, I., Lewis, S. E. & Graulich, N. (2025). A question of pattern recognition: investigating the impact of structure variation on students' proficiency in deciding about resonance stabilization, *Chemistry Education Research and Practice*, *26*(1), 158-182.]

Die quantitative Datenanalyse zeigte ferner, dass das Erkennen von Mesomerie signifikant von der Angabe freier Elektronenpaare abhängt. Studierende neigten dazu, Mesomerie-Stabilisierung anzunehmen, wenn freie Elektronenpaare angegeben waren.

[Braun, I. & Graulich, N. (2024). The More Explicit, the Better? How the Indication of Electron Lone Pairs Affects Students' Consideration of Resonance in Organic Chemistry, *Journal of Chemical Education*, *101*(11), 4830-4836.]

Erweiternd wurden in einer qualitativen Interviewstudie die Wahrnehmungsprozesse von Studierenden beim Zeichnen (un-)produktiver mesomerer Grenzformeln, eingebettet in einen Aufgabenkontext, untersucht. Mithilfe von Eye-Tracking wurde die Verknüpfung visueller Informationen sowie die Aufmerksamkeitsverteilung der Studierenden auf strukturelle Merkmale analysiert. Zudem wurden die verbalen Zeichenerklärungen der Studierenden zur Triangulierung der Eye-Tracking-Daten analysiert. Während die Produktivität der Zeichnungen nicht von der Anzahl integrierter und verknüpfter visueller Informationen abhing, waren produktive Zeichnungen durch einen direkteren Zeichenprozess von der Ausgangs- zur Zielstruktur charakterisiert. Zudem wurde deutlich, dass Flexibilität in der Wahrnehmung miteinander zusammenhängender Strukturmerkmale für das Zeichnen korrekter mesomerer Grenzformeln entscheidend ist.

[Braun, I., Langner, A. & Graulich, N. (2022). Let's draw molecules: Students' sequential drawing processes of resonance structures in organic chemistry, *Frontiers in Education*, *7*:1055280.]

Mit der Interviewstudie wurde auch untersucht, wie Studierende Mesomerie in unterschiedlichen Aufgabenkontexten in der OC I nutzen. Mithilfe der Koordinationsklassen-Theorie wurde ihr Problemlösen analysiert. Es wurde deutlich, dass die Konzeptnutzung vielfältig und durch das komplexe Zusammenspiel aus Aufgabenanforderungen und individuellen Faktoren geprägt war. Ein detaillierter Vergleich der Konzeptnutzung zeigte jedoch, dass ein reflektierter und flexibler Umgang mit Strukturzeichnungen sich förderlich auf die produktive Nutzung von Mesomerie auswirkte, sowohl hinsichtlich der Herangehensweise an die Aufgaben als auch bei der Aktivierung relevanter Ressourcen.

[Braun, I. & Graulich, N. (2024). Exploring diversity: student's (un-)productive use of resonance in organic chemistry tasks through the lens of the coordination class theory. *Chemistry Education Research and Practice*, *25*(3), 643-671.]

Damit zeigt diese Dissertation, dass Flexibilität in der Wahrnehmung von und im Umgang mit Repräsentationen für die erfolgreiche Nutzung des Mesomerie-Konzepts in der Organischen Chemie entscheidend ist. Durch die Hervorhebung der engen Verknüpfung von konzeptuellen und perzeptuellen Prozessen bei der Betrachtung von Mesomerie liefert diese Dissertation neue prozessorientierte Erkenntnisse darüber, wie Studierende mesomere Grenzformeln wahrnehmen, konstruieren und im Problemlösen nutzen.

III. List of Publications

Papers in Peer-Reviewed Journals

Braun, I., Lewis, S. E. & Graulich, N. (2025). A question of pattern recognition: investigating the impact of structure variation on students' proficiency in deciding about resonance stabilization, *Chemistry Education Research and Practice*, *26*(1), 158-182.

Braun, I. & Graulich, N. (2024). The More Explicit, the Better? How the Indication of Electron Lone Pairs Affects Students' Consideration of Resonance in Organic Chemistry, *Journal of Chemical Education*, *101*(11), 4830-4836.

Braun, I. & Graulich, N. (2024). Tell Me Why: Raising Student Teachers' Awareness for Elaborate Mechanistic Explanations in Organic Chemistry, *Journal of Chemical Education*, *101*(10), 4485-4494.

Braun, I. & Graulich, N. (2024). Exploring diversity: student's (un-)productive use of resonance in organic chemistry tasks through the lens of the coordination class theory, *Chemistry Education Research and Practice*, *25*(3), 643-671.

Braun, I., Buchczyk, R. & Graulich, N. (2024). Making the connection: The relation of structural and energetic representations in Organic Chemistry, *CHEMKON*, *31*(1), 6-14.

Braun, I., Langner, A. & Graulich, N. (2022). Let's draw molecules: Students' sequential drawing processes of resonance structures in organic chemistry, *Frontiers in Education*, *7*:1055280.

Braun, I. & Graulich, N. (2022). Die Zeichnung im Blick - Nutzung von Eye-Tracking zur Analyse der zeichnerischen Erschließung von Mesomerie-Aufgaben, *CHEMKON*, *29*(S1), 261-266.

Publications in Journals for Teaching Practice

Braun, I., Martin, P. P. & Graulich, N. (2025). Von Biokunststoffen bis zum Verbrennungsmotor. Wie FERMI-Aufgaben Bewertungsprozesse im Chemieunterricht anstoßen können, *Naturwissenschaften im Unterricht – Unterricht Chemie*, Heft 205, *36*(1), 36-39.

Oral Presentations

Braun, I. & Graulich, N. (2024). *Wieso, weshalb, warum? – Nutzung von Lösungsbeispielen zur Förderung der Erklärkompetenz von Lehramtsstudierenden in der Organischen Chemie*, 40. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht, Regensburg.

Braun, I., Lewis, S. E. & Graulich, N. (2024). *Muster erkennen: Analyse der Mesomerie-Wahrnehmung von Studierenden in der Organischen Chemie*, GDCP-Jahrestagung 2024, Bochum.

Braun, I. & Graulich, N. (2024). *Modeling concept use through the Coordination Class Theory: Students' (un-)productive consideration of resonance in organic chemistry tasks*, 28th Biennial Conference on Chemical Education (BCCE), Lexington.

Braun, I. Lewis, S. & Graulich, N. (2024). *Proficiency in structure decoding: Exploring the impact of structural features on students' consideration of resonance*, 28th Biennial Conference on Chemical Education (BCCE), Lexington.

Braun, I. & Graulich, N. (2023). *Kontextbasiertes Problemlösen: Anwendung von Mesomerie in OC-Aufgaben*, GDCP Jahrestagung 2023, Hamburg.

Braun, I. & Graulich, N. (2023). *Von gezeichneten zu mentalen Strukturen – Wie Studierende das Mesomerie-Konzept in organisch-chemischen Aufgaben nutzen*, GDCh-Wissenschaftsforum Chemie 2023: 39. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht, Leipzig.

Braun, I. & Graulich, N. (2023). *The context matters? Exploring students' use of the resonance concept in organic chemistry tasks*, 20th Biennial EARLI Conference, Thessaloniki.

Braun, I. & Graulich, N. (2023). *The context matters? Exploring students' use of the resonance concept in organic chemistry tasks*, JURE 2023, Thessaloniki.

Braun, I. & Graulich, N. (2022). *Wenn die Wahrheit zwischen den Zeichnungen liegt: Analyse der problemlösebezogenen Nutzung mesomerer Grenzformeln in organischen Fallvergleichsaufgaben*, 38. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht, Osnabrück.

Braun, I., Langner, A. & Graulich, N. (2022). *Von Struktur zu Struktur: Untersuchung von Zeichenprozessen in der Organischen Chemie*, GDCP Jahrestagung 2022, Aachen.

Braun, I., Langner, A. & Graulich, N. (2022). *"I've derived them logically": Exploring students' drawing processes of resonance structures in organic chemistry via eye-tracking*, 27th Biennial Conference on Chemical Education (BCCE), West Lafayette.

Poster Presentations

Braun, I. & Graulich, N. (2023). *Den Blick auf das Wesentliche richten: Der Einfluss struktureller Merkmale auf die Anwendung des Mesomerie-Konzepts*, GDCh-Wissenschaftsforum Chemie 2023: 39. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht, Leipzig.

Braun, I. (2022). *It's all in the structures: Investigating students' drawing processes of and perceptual reasoning with resonance structures in organic chemistry*, Qualitative Methods in Science Education, Kopenhagen.

Braun, I. & Graulich, N. (2022). *Diagnostizieren, Fördern, Tutorieren: Ein innovatives Lehramtsmodul zur Anwendung und Vertiefung von Diagnose- und Förderkompetenzen*, Lehrkräftebildung weiterdenken, Leipzig.

Braun, I. & Graulich, N. (2022). *Beyond the drawn structures: Investigating students' reasoning with own resonance drawings in organic case comparison tasks*, 27th Biennial Conference on Chemical Education (BCCE), West Lafayette.

Braun, I., Langner, A. & Graulich, N. (2022). *Quick-Guide to Mobile Eye-Tracking in Chemistry Education Research*, Methods in Chemistry Education Research (MICER), online.

Braun, I. & Graulich, N. (2021). *Die Zeichnung im Blick - Nutzung von Eye-Tracking zur Analyse der zeichnerischen Erschließung von Mesomerie-Aufgaben*, 37. Fortbildungs- und Vortragstagung der Fachgruppe Chemieunterricht, online.

Braun, I. & Graulich, N. (2021). *Analyse der zeichnerischen Nutzung des Mesomerie-Konzepts*, GDCP Jahrestagung 2021, online.

Conference Proceedings

Braun, I., Lewis, S. E. & Graulich, N. (2025). Muster erkennen: Analyse der Mesomerie-Wahrnehmung von Studierenden in der Organischen Chemie. In: van Vorst, H. (Ed.), *Lernen, lehren und forschen im Schülerlabor*, Gesellschaft für Didaktik der Chemie und Physik, Jahrestagung in Bochum 2024 (accepted).

Braun, I. & Graulich, N. (2024). Kontextbasiertes Problemlösen: Anwendung von Mesomerie in OC-Aufgaben, In: van Vorst, H. (Ed.), *Frühe naturwissenschaftliche Bildung,* Gesellschaft für Didaktik der Chemie und Physik, Jahrestagung in Hamburg 2023, 358-361.

Braun, I., Langner, A. & Graulich, N. (2023). Von Struktur zu Struktur: Untersuchung von Zeichenprozessen in der organischen Chemie, In: van Vorst, H. (Ed.), *Lernen, Lehren und Forschen in einer digital geprägten Welt*, Gesellschaft für Didaktik der Chemie und Physik, Jahrestagung in Aachen 2022, 486-489.

1. Review: Tracing the Interplay of Perceptual and Conceptual Processes in Students' Reasoning about Resonance in Organic Chemistry

1.1 Introduction

A central endeavor in teaching Organic Chemistry is to help learners develop a robust understanding of disciplinary core ideas (*e.g.*, bonding and interactions) that enable them to successfully engage in scientific practices, such as predicting and explaining reaction outcomes (Murphy *et al.*, 2012; National Research Council, 2012; Cooper, 2020). This requires not only an understanding of how individual knowledge pieces relate to interconnected larger concepts but also the ability to apply these concepts flexibly across contexts (*e.g.*, engaging in multivariate reasoning) (Ferguson and Bodner, 2008; Crandell *et al.*, 2019; Zaimi *et al.*, 2025). More than in other disciplines, concept understanding in Organic Chemistry is deeply intertwined with the use of representations. Given the abstract character of chemical concepts and the "invisible and untouchable" nature of processes underlying chemical phenomena (Kozma and Russell, 1997, p. 949), representations play a central role in the sense-making and communication of chemical content (Hoffmann and Laszlo, 1991; Talanquer, 2022). Specifically, attending to relevant surface features of a representation builds a critical starting point for accessing implicit electronic properties of a molecule, which helps to draw inferences about reactivity (Chi and VanLehn, 2012; Graulich *et al.*, 2019). Yet, students are often overwhelmed by the discipline's visual language. For instance, they face challenges in predicting molecular properties from representations (Cooper *et al.*, 2010; Cooper *et al.*, 2013; Graulich *et al.*, 2019) and attach different meaning to representational features varying in appropriateness and accuracy (Crandell and Pazicni, 2023; Nelsen *et al.*, 2024; Rotich *et al.*, 2024).

Despite reported difficulties in interpreting representations, research has shown that connecting a representation to a concept is not equally difficult for students. The *proximity* between a representation and the underlying concept influences whether a concept can be readily recognized and used in problem-solving (Graulich *et al.*, 2019; Finkenstaedt-Quinn *et al.*, 2020; Talanquer, 2022). If an implicit property is directly connected to an explicit visual cue in a representation (*e.g.*, inductive effects based on the atom types), it is easier for learners to activate relevant concepts, whereas concepts requiring multiple inferential steps (*e.g.*, manipulation of representations) are much harder to retrieve (Cooper *et al.*, 2012; Finkenstaedt-Quinn *et al.*, 2020). The resonance concept can account for the latter, as the alignment between representation and concept is not directly given. Resonance helps to describe the emergent electronic structure in molecules, which cannot be adequately depicted by a single Lewis structure. Specifically, it illustrates the delocalization of π-electrons of overlapping p-orbitals between multiple atoms in a conjugated system of a molecule. This helps to reason about reaction pathways across many contexts, serves to derive chemical properties (*e.g.*, acid strength), and builds a prerequisite for understanding other concepts (*e.g.*, aromaticity). Unsurprisingly, this concept has often been emphasized as fundamental for learning success in Organic Chemistry (Duis, 2011; Bhattacharyya, 2013; Carle and Flynn, 2020). However, interpreting corresponding representations is cognitively highly demanding, as resonance is "unique in its representational affordances" (Kim *et al.*, 2019, p. 665). Even though different resonance structures display a different spatial arrangement of electrons, one must not adhere to the static structural representations but must interpret the structures in their interplay to infer the actual electron density distribution in the molecule. Doing so entails manipulating given structures into corresponding resonance structures, which requires the concurrent consideration of different concepts (*e.g.*, electronegativity, hybridization) to evaluate the plausibility of possible resonance structures (Betancourt-Pérez *et al.*, 2010; Santos *et al.*, 2024).

Due to its complexity, resonance has garnered increasing attention in chemistry education research in recent years. Studies have extensively explored students' conceptualization of resonance, shedding light on students' operational understanding, their challenges in connecting resonance to other concepts (*e.g.*, stability), and students' diverse interpretations of resonance structures (*e.g.*, Taber, 2002; Xue and Stains, 2020; Brandfonbrener *et al.*, 2021; Barakat, 2024; Santos *et al.*, 2024). While students invoke resonance during problem-solving, research shows that they do not always apply it successfully (*e.g.*, McClary and Talanquer, 2011a; Watts *et al.*, 2020; Demirdöğen *et al.*, 2023). Instead, students tend to rely on heuristics, or disregard resonance unless explicitly prompted (*e.g.*, Ferguson and Bodner, 2008; McClary and Talanquer, 2011a; McClary and Talanquer, 2011b; Finkenstaedt-Quinn *et al.*, 2020). Additional challenges arise in constructing valid resonance structures. Students sometimes simplify rules (Tetschner and Nedungadi, 2023) or overlook critical details, such as atom hybridization (Betancourt-Pérez *et al.*, 2010), eventually creating barriers to the successful use of resonance in problem-solving (Cox *et al.*, 2024). Furthermore, it has been shown that instructional approaches to teaching resonance focus on operational and rule-based strategies, emphasizing what students should *do* with resonance rather than what they should *know* about it (Xue and Stains, 2020; Atieh *et al.*, 2022; Barakat and Orgill, 2024). Given these abundant findings on students' conceptualization of and challenges with resonance, this raises the question of why further research in this area is needed.

When taking a step back and reconsidering existing findings in light of the close link between representations and concept understanding in Organic Chemistry, certain limitations of previous research become apparent. Most studies on students' understanding and use of resonance have primarily adopted a *conceptual* perspective, focusing on students' underlying ideas about resonance. However, these studies often do not consider how students engage with resonance structures when tackling resonance-related tasks. This is despite the unique visual affordances of the concept and the well-documented challenges students face in interpreting representations in Organic Chemistry. While many of students' alternative conceptions are closely linked to their interpretation of depicted resonance structures, few studies explicitly investigate how students derive meaning from these representations (Taber, 2002; Kim *et al.*, 2019; Xue and Stains, 2020). However, these studies are restricted to a narrow range of prominent examples (*e.g.*, benzene) and focus on specific conceptual aspects, such as the resonance hybrid. As such, students' perceptual processes involved in their use of these representations (Schönborn and Anderson, 2008; Rau, 2017) remain largely unexplored.

This gap extends to research on students' construction of resonance structures, a prerequisite skill for successful problem-solving. Although challenges and common errors in constructing resonance structures are often attributed to fragmented concept understanding, little is known about what is actually going on when students are tasked to generate resonance structures. Precisely, it remains unclear how students decode and relate structural information to translate one structure into another. While students' drawings may reveal common mistakes, such artifacts offer limited insight into the underlying development of their drawings. Given existing findings on students' difficulties in constructing Lewis structures due to structure complexity (Cooper *et al.*, 2010; Tiettmeyer *et al.*, 2017; Sandi-Urena *et al.*, 2020), a process-oriented perspective on students' drawing processes becomes necessary, as resonance structures entail the coordination of even more structural features than singular Lewis structures.

Lastly, while several studies have explored students' use of resonance in problem-solving, which provide valuable insights into their concept understanding, most of these investigations are grounded in a single context in the realm of acid-base chemistry or stability considerations. These topics are heavily emphasized in teaching resonance (Carle and Flynn, 2020). Other contexts, such as the consideration of nucleophiles and electrophiles, that are critical in many reactions but often underrepresented in resonance-related teaching materials (Carle and Flynn, 2020), remain scarce. Although research shows that students face challenges in using resonance, reasoning is highly context-dependent and influenced by one's framing (Hammer *et al.*, 2005). Consequently, it cannot be appropriately understood from a single context alone. A fine-grained, resource-based perspective is necessary to gain a more nuanced understanding of students' concept use (DiSessa and Wagner, 2005; Hammer *et al.*, 2005). While some studies have already adopted a resource approach in analyzing their data, students' use of resonance has typically been considered a *singular* resource at a broader grain size, scarcely zooming in on students' thought processes (Watts *et al.*, 2021; Cox *et al.*, 2024). As such, they do not reflect in-depth on the interconnectedness of resonance with other concepts or address students' use and interpretation of provided representations (DiSessa and Wagner, 2005; Rau, 2017). However, focusing on these aspects can deepen our understanding of students' consideration of resonance in context, help explain reasons for students' fragmented concept use, and clarify difficulties in recognizing electron delocalization. Specifically, it can reveal how structural features direct students' attention to resonance.

Overall, reviewing previous research underscores the need for a process-oriented analytical approach to students' use of resonance. Given the unique visual affordances of this concept, focusing on *how* students engage with and make sense of representations of resonance structures can provide new insights into their concept use and related challenges. Hence, incorporating students' representational competence with regard to resonance structures may offer a new perspective on their use of resonance, as different cognitive processes are involved in representation use. These are outlined and synthesized in the following section.

1.2 Theoretical Background

Different theoretical frameworks on representational competence in scientific contexts approach one's learning with and use of representations. While they emphasize different aspects, comparing these frameworks may reveal which factors and processes underlie successful engagement with representations, ultimately informing a process-oriented analysis of students' use of resonance.

Kozma and Russell's (1997; 2005) framework is commonly used in chemistry education to characterize students' competence in dealing with representations. Based on their studies on differences between experts' and students' disciplinary practices (*e.g.*, Kozma and Russell, 1997; Kozma *et al.*, 2000), the authors derive different expert-like skills regarding the use of representations, which may serve as a model for student knowledge development. As such, representational competence encompasses a set of skills enabling the reflective use of representations (*e.g.*, for problem-solving) (Kozma and Russell, 2005). These skills comprise, for instance, the abilities to analyze, interpret, translate, generate, and select appropriate representations, or the ability to describe the affordances and limitations of representations (Kozma and Russell, 1997; 2005). While this framework conceptualizes representational competence in terms of lower- and higher-level skills, which appear interconnected (Ward *et al.*, 2025), overall, it remains at an operational level. It shows *what* students should be able to do with representations, without addressing *how* students develop these skills. Prior knowledge about representations seems to be a prerequisite, implicitly underlying all these skills. But what knowledge underlies this proficiency?

Addressing this gap, Ainsworth's (2006) DeFT framework offers a different perspective on representational competence by focusing on the functions of multiple representations in scientific domains. According to Ainsworth (2006; 2008), multiple representations serve to complement, constrain, and construct concept understanding (*e.g.*, by abstracting underlying principles). Yet, benefitting from the synergies of multiple representations requires students to be able to cognitively engage with *single* representations first. Specifically, each representation includes a *primary notation* (explicit features) and a *secondary notation* (implicitly conveyed information, *e.g.*, electronic properties), which students must learn to connect to interpret representations effectively (Ainsworth, 2006). This entails different *cognitive tasks*: understanding what a representation represents, how a representation encodes information, and how information can be retrieved (Ainsworth, 2006). By emphasizing the processes needed to link *primary* and *secondary notations*, this framework addresses core challenges students face with representations in Organic Chemistry (*i.e.*, deriving implicit features). However, it leaves open the question of how learners develop the skills for visual understanding and what factors determine their ability to connect *primary* and *secondary notations*.

Building on that, Rau (2017) provides a more focused perspective on the learning processes through which learners acquire representational competence. Representational competence is described as the acquisition of "knowledge about how visual representations depict information about the content" (Rau, 2017, p. 717). Rau (2017) distinguishes two broader, interrelated competencies: *sense-making skills* and *perceptual fluency*. *Sense-making skills* refer to one's conceptual and procedural knowledge about representations (*e.g.*, mapping representational features to underlying concepts). This includes visual understanding of individual representations and recognizing relationships among multiple representations, corresponding to Ainsworth's (2006) cognitive tasks and functions of multiple representations. *Perceptual fluency* complements previous frameworks by emphasizing perceptual competencies in dealing with representations. Aligning with cognitive learning theories (see for review Rau, 2017), it refers to one's ability to quickly and effortlessly attach meaning to relevant representational features. That includes the ability to perceive conceptually meaningful visual patterns within an individual representation (visual fluency) as well as to map corresponding visual patterns across different representations (connectional fluency), ultimately enhancing efficiency in information processing (Kellman and Massey, 2013; Rau, 2017). Hence, representational competence requires more than knowledge of how representations encode information; fluency in extracting meaningful visual information is equally important. As such, Rau's (2017) approach extends Ainsworth's (2006) framework by explicitly adding a perceptual dimension, emphasizing the close relationship between conceptual and perceptual processes.

This aspect becomes also evident in Schönborn and Anderson's (2008; 2010) C-R-M model of visual literacy. This framework outlines key factors determining students' ability to interpret and use representations. Specifically, it includes three interrelated main factors influencing the processing of representations: *conceptual* (C), which refers to the students' prior knowledge of concepts of relevance to the representation; *reasoning* (R), which encompasses one's reasoning abilities for interpretation; and *mode* (M), representing the external features of the representation itself. Combined, these factors create four additional dimensions: *conceptual-mode* (C-M), relating to accepted conceptual knowledge conveyed by representations; *reasoning-conceptual* (R-C), addressing how students reason with their conceptual knowledge to interpret representations (*e.g.*, activate representation-specific concepts); *reasoning-mode* (R-M), covering students' ability to process and decode visual information; and the *conceptual-reasoning-mode* (C-R-M), which describes students' ability to successfully interpret representations by using conceptual knowledge of relevance to the representation and making sense of its features (Schönborn and Anderson, 2008). While C-M and M reflect established scientific conventions, reasoning-related factors (R-C, R-M, and C-R-M) are highly learner-dependent and, similar to Rau (2017), point to the close relationship between conceptual and perceptual processes when engaging with representations. However, this model goes further by illustrating that understanding representations is a complex interplay of different factors, not only depending on one's *reasoning* processes with representations (*i.e.*, the activation of appropriate ideas and the ability to decode representations) but being also crucially impacted by the inherent nature and complexity of given representations (*i.e.*, visual affordances).

The comparison of these frameworks offers different perspectives on representational competence, showcasing different aspects underlying successful engagement with and understanding of representations. While learners must be able to operate with representations in various ways and tackle specific visual affordances, their successful use always entails a deeper engagement at a cognitive level. Regardless of framework-specific terminology, this cognitive engagement comprises conceptual and perceptual processes, which mutually influence one another. Figure 1 summarizes these aspects.

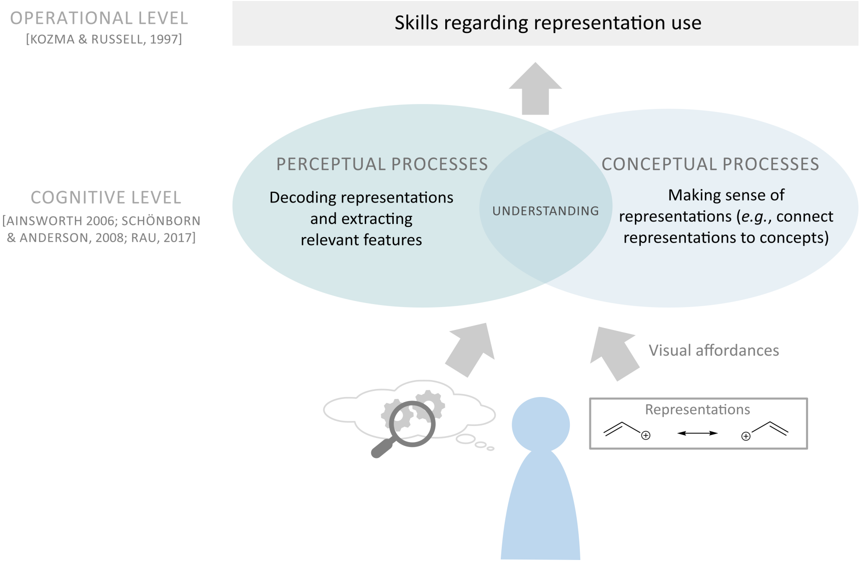


Figure 1. Processes involved in engagement with and understanding of representations.

As such, successful representation use goes beyond solid conceptual understanding; it also includes a perceptual dimension and depends on how students decode and perceive relevant visual features to form and activate relevant concepts, ultimately enabling students to derive meaning from representations. Rau's (2017) and Schönborn and Anderson's (2008; 2010) frameworks, in particular, emphasize the importance of perception in recognizing representational features and accurately extracting information to link it to conceptual understanding. As such, this theoretical perspective underscores that students' conceptual understanding in Organic Chemistry is closely tied to their perceptual processing of representations. Consequently, the interplay between these processes should be more explicitly taken into account to understand students' use of resonance and related challenges in more depth.

1.3 Research Objectives

While much is already known about students' conceptual struggles and challenges with resonance, the actual *use* of resonance and related resonance structures from a process-oriented perspective has only been marginally studied yet. However, given the close connection between conceptual understanding and representation use in Organic Chemistry, "[s]upporting learners in acquiring a solid conceptual understanding requires us to understand how students perceive and deal with representations" (Graulich *et al.*, 2019, p. 925).

Reviewing previous research on students' understanding and use of resonance and synthesizing different theoretical frameworks pertaining to one's engagement with representations (Sections 1.1. and 1.2) reveals that students' reasoning about resonance is multilayered, shaped by various influencing factors and cognitive processes. Their interplay is modeled in Figure 2. Prior research has primarily shed light on instructional practices, students' conceptualization of resonance (*e.g.*, its connection to stability), and its influence on students' problem-solving, ultimately emphasizing a conceptual perspective (Figure 2). Less attention has been given to the impact of visual affordances (*e.g.*, explicitness of structural features) and related cognitive processing of resonance structures on students' use of resonance (Figure 2, A-C). However, given the visual nature of this concept, theoretical considerations suggest that these representational aspects are deeply intertwined with students' understanding and use of resonance (Section 1.2). Consequently, unpacking the representational perspective and investigating how students engage with representations of resonance structures can provide a more comprehensive insight into their concept use (*i.e.*, *how* students' use of representations impacts their use of resonance), thereby complementing and extending existent research.

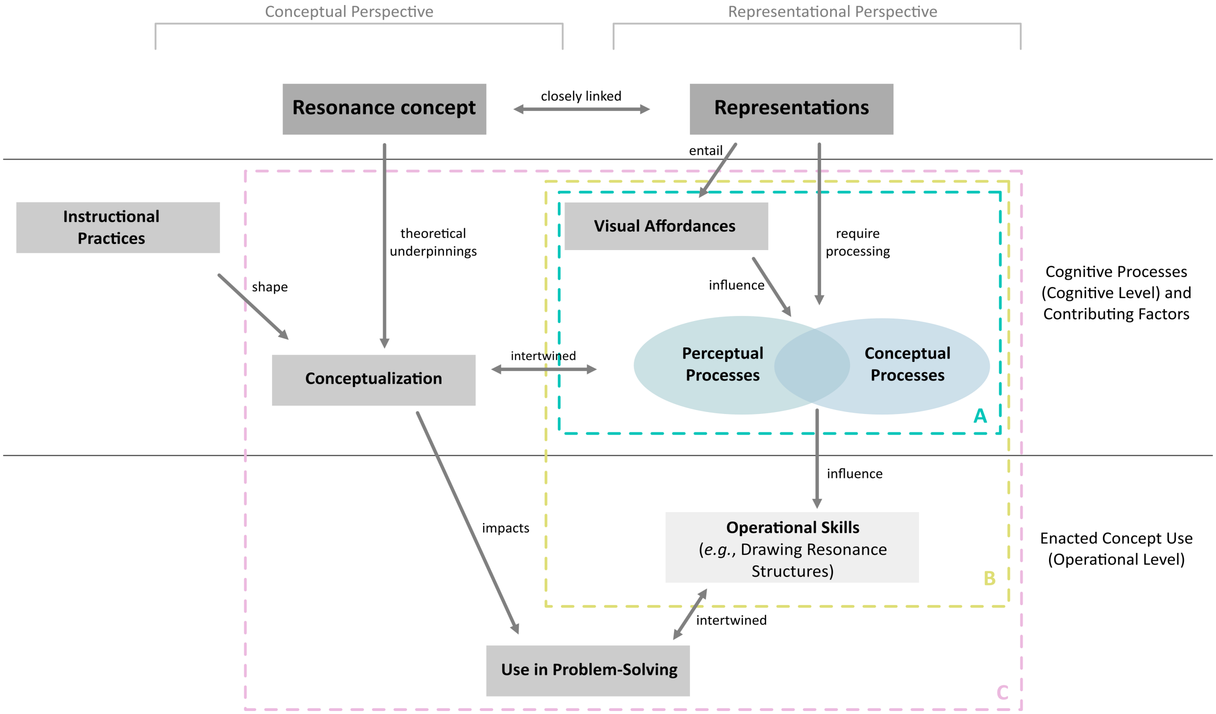


Figure 2. Overview of the different factors, cognitive processes and their interplay influencing students' reasoning about resonance. The highlighted areas (A, B, C) indicate the aspects and relationships addressed within the scope of this dissertation.

Accordingly, this dissertation was driven by different objectives. First, to investigate the interplay of visual affordances and cognitive processes underlying students' consideration of resonance in more depth (Figure 2, A), students' decision-making on resonance stabilization across various molecular structures was examined. Second, shedding light on students' perceptual processes involved in constructing resonance structures served to gain insight into how students' cognitive processes underlying representation use impact their operational skills in using resonance (Figure 2, B). Finally, building on previous research, exploring students' use of resonance across different problem-solving contexts aimed at yielding fine-grained insights into how the interplay between different factors underlying reasoning about resonance impacts students' use of this concept in problem-solving (Figure 2, C). Informed by theoretical considerations on representational competence, three hypotheses guide this dissertation to provide new process-oriented insights into students' reasoning about resonance:

1. The variation of structural features markedly influences students' decision-making on and consideration of resonance in molecular structures.
2. Students' perceptual processing of visual information critically shapes their success in constructing resonance structures.
3. The dynamic interplay between representation use and conceptual considerations accounts for differences in students' use of resonance across different problem-solving contexts.

1.4 Methods

Within this dissertation, two studies were conducted to approach students' use of resonance from different perspectives. While a qualitative study served to investigate students' drawing processes of resonance structures and to examine their concept use across different problem-solving contexts in more depth (Chapters 2 and 3), a quantitative study aimed to explore students' recognition of resonance stabilization across different molecular structures (Chapters 4 and 5) (Figure 3).

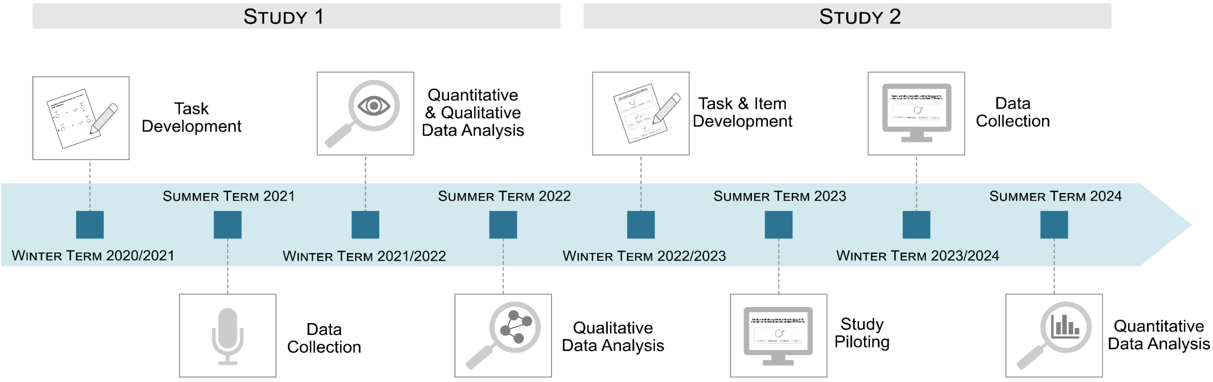


Figure 3. Research design of the complete research project.

Study 1 was a qualitative paper-pencil interview conducted at the Justus-Liebig-University Giessen in summer 2021, subject to the papers presented in Chapters 2 and 3. A total of 21 students from the Organic Chemistry I course voluntarily participated in the study and provided informed consent to the use of their data. Since the study was conducted near the end of the course, it was assumed that the students had a foundational understanding of resonance, having encountered and applied it in various reaction contexts throughout the semester. The study was divided into three parts (warm-up, problem-solving, and general reflection) to elicit students' use of resonance in problem-solving. During the main study part, students were first prompted to solve three case-comparison tasks on their own necessitating resonance considerations in different contexts: (1) an electrophilic aromatic substitution of acetophenone with a bromine ion, (2) a nucleophilic addition of a hydroxide ion in the alkaline hydrolysis of substituted ethyl benzoates, and (3) a leaving group departure step of a nucleophilic substitution reaction (see Appendix 6.1.3). Students' problem-solving was accompanied by mobile eye-tracking (Tobii Pro glasses 3) to capture the perceptual processes underlying their construction of resonance structures. Following each task, a semi-structured retrospective served to gain insight into students' rationale behind their drawing process and to probe students' reasoning for their problem-solving. Besides students' drawings, collected data included video recordings of the interviews and students' eye-gaze data. The original interview protocol, demographic questionnaire, consent form, and the original tasks are provided in Appendix 6.1. As the interviews were conducted in German, students' original quotes with English translations are provided in Appendix 6.1.7.

The corresponding data analysis involved multiple steps tailored to the specific research foci. While described in detail in Chapters 2 and 3, Figure 4 provides an overview of the different analytical approaches, briefly delineating the different methods and coding schemes to facilitate understanding of the subsequent sections. For students' drawing processes, their resonance structures from the third task were first classified into (un-)productive drawings. Furthermore, students' eye-tracking data were manually mapped onto the respective drawings, and various Areas of Interest (AOI) and Times of Interest (TOI) were defined using the software *Tobii Pro Lab*. Different eye-tracking metrics (*i.e.*, fixation duration, transitions) were used and quantitively analyzed using the software *R* with the package *GrpStringR* (Tang *et al.*, 2018) and the *ENA Web Tool* (version 1.7.0) to characterize students' gaze behavior underlying productive and unproductive drawings. Additionally, informed by the theory of visual selection (Theeuwes, 2010), inductive coding was used to qualitatively characterize students' rationale behind their drawings (*i.e.*, the knowledge they draw upon and flexibility in referring to structural features) (Figure 4A).

The analysis of students' reasoning about resonance across different contexts was guided by the Coordination Class Theory (DiSessa and Wagner, 2005). This theory allows an in-depth analysis of students' reasoning during problem-solving as it considers the interplay between extracted visual information and activated resources (DiSessa and Wagner, 2005). Based on the transcribed interviews, students' extraction strategies, extractions of structural features, and activated resonance-related conceptual resources were inductively coded and further analyzed in their granularity and connectivity (*i.e.*, using resource graphs) to reconstruct students' thought processes for each task (Wittmann, 2006; Deng and Flynn, 2021) (Figure 4B). All qualitative data analyses were conducted using *MAXQDA*.

Study 2 was a quantitative online survey conducted at a Southeastern university in the United States in autumn 2023. 699 students enrolled in Organic Chemistry I voluntarily participated, giving informed consent to the use of their data and receiving extra credit worth approximately 0.4% of their course grade upon survey completion. As resonance was introduced and practiced within the first weeks of the semester, students' prior knowledge about this concept was assumed. The survey, implemented in *Qualtrics*, focused on students' proficiency in making decisions about resonance stabilization and consisted of three parts (see Appendix 6.2.1). The first part assessed students' prior conceptual knowledge through self-assessment and tasks focusing on resonance learning outcomes (Carle and Flynn, 2020). In the second part, students were asked to intuitively decide on resonance stabilization for 72 molecular structures varying in their structural features. The third part focused on students' perceived cognitive load while solving the second survey part (Klepsch *et al.*, 2017). For data analysis, students' responses in each survey section were first scored (see Appendices 6.2.2 and 6.2.3 for items). Using *SPSS*, *k*-means cluster analysis and other quantitative tests were performed to elucidate the impact of different structural features on students' ability to recognize resonance (Figure 4C). Chapters 4 and 5 provide a more detailed description of the methodology.

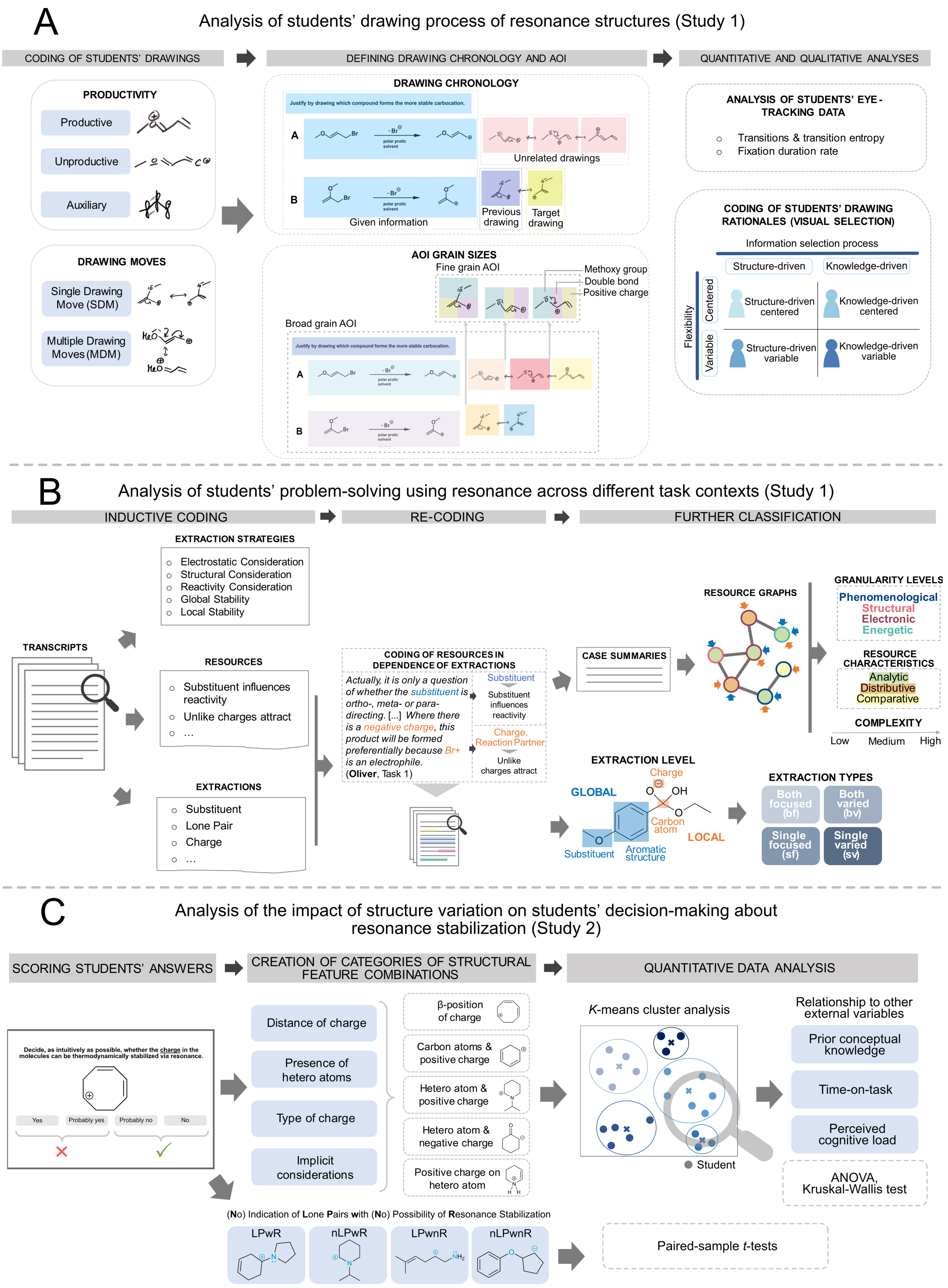


Figure 4. Overview of the analytic steps and coding in both studies. For more details, see Chapters 2-5.

1.5 Results and Discussion

The following section is organized around the three hypotheses guiding this work (Section 1.3). It summarizes the main findings of both studies and situates their contribution to the literature. The first part focuses on students' recognition of resonance and draws on findings from the second study (Chapters 4 and 5). The second part delves into the perceptual processes underlying the construction of resonance structures, recurring to findings from the first study (Chapter 2). Extending these insights, the third part deals with students' use of resonance across different problem-solving contexts, examining the consistency of students' resonance considerations and characteristics impacting the productivity of concept use. This section refers to the first study as well (Chapter 3). To illustrate key findings, student quotes from the first study are reused, unless noted otherwise.

1.5.1 The Impact of Structure Variation on Students' Consideration of Resonance

Proficiency in identifying whether resonance applies in a molecule is a critical prerequisite for generating plausible resonance structures and successfully using this concept in problem-solving (Carle *et al.*, 2021). However, research has shown that students often struggle to recognize whether molecules profit from electron delocalization, resulting in limited integration of this concept in problem-solving (Finkenstaedt-Quinn *et al.*, 2020; Carle *et al.*, 2021). For instance, students struggle to determine the starting point for electron movement (Petterson *et al.*, 2020), invoke resonance when it is not applicable (Farheen *et al.*, 2024), or do not pay attention to details (*e.g.*, breaking sigma bonds) (Betancourt-Pérez *et al.*, 2010). Since the nature and complexity of representations crucially affect students' interpretation and use of representations (M-factor) (Schönborn and Anderson, 2008), examining how the variation of structural features affects students' consideration of resonance may provide new insights into the factors impacting students' decoding of resonance structures and help understand students' operational challenges in more depth (Figure 2, A).

The required cognitive steps to process structural features impact the ease of students' resonance recognition

To investigate how students deal with varying structural features when deciding on resonance, they were shown a sequence of molecular structures with different structural parameters in the second study (Chapter 4). Focusing on combinations of structural features that explicitly need to be considered when deciding on resonance (*e.g.*, charge type, presence of hetero atoms) resulted in five structural feature categories with different overall student mean scores (Table 1).

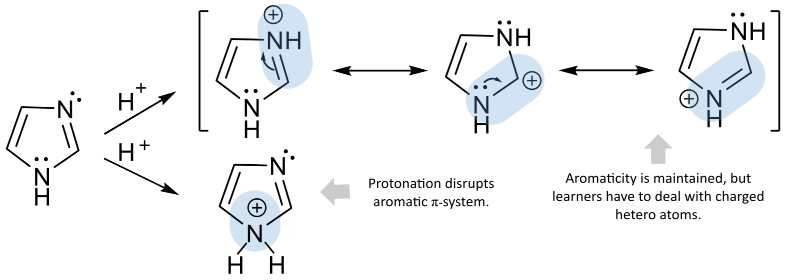
Table 1. Overall mean scores for the different structural feature categories with indication of standard deviations; $N = 681$.

Category	β-position of charge	Carbon atoms & positive charge	Hetero atom & positive charge	Hetero atom & negative charge	Positive charge on hetero atom
Score in %, (*SD*)	65.34 (*25.61*)	75.22 (*28.44*)	55.46 (*27.28*)	54.37 (*32.23*)	43.55 (*28.82*)

While students scored highest for items belonging to the categories *carbon atoms & positive charge* (75%) and *β-position of charge* (65%), their success rate for items involving hetero atoms was lower. Students' scores for *hetero atom & positive charge* and *hetero atom & negative charge* ranged at approximately 55%. When items required the clear consideration of implicit features (*positive charge on hetero atom*), students' performance was the lowest with 44%. A repeated-measures ANOVA revealed significant differences in students' performance scores with a large effect size ($F(3.82, 2599.75) = 123.37, p < 0.001, \eta^2 = 0.15$), along with significant differences in *post-hoc* pairwise comparisons (see Chapter 4).

Students' varying scores reflect differences in their proficiency in dealing with structural features. This can be tied back to the visual affordances of these features, which entail varying degrees of information processing (see Figure 4C for examples). Specifically, items in the category *β-position of charge* demand learners to estimate the distance of the charge, which can be explicitly read off the representation. Similarly, items in the category *carbon atoms & positive charge* exclusively display allylic carbocations. Given their prevalence as introductory examples in teaching resonance (*e.g.*, Ogilvie *et al.*, 2018; Klein, 2020), this structural motif is likely most familiar to students. As such, familiarity may account for students' higher success rate in this category (Talanquer, 2014; Taskin *et al.*, 2015). The absence of hetero atoms further reduces the required information processing (*i.e.*, intrinsic cognitive load) compared to the remaining categories (Paas and van Merriënboer, 2020). Here, more cognitive steps are required to make correct decisions. Most items in the category *hetero atom & negative charge* comprise double-bonded hetero atoms but require electron delocalization in the reverse direction (*i.e.*, starting from a negative *charge*), involving a greater abundance of delocalized π-electrons. In contrast, items in the category *hetero atom & positive charge* display a different bonding pattern with single bonded hetero atoms. As the conjugated system cannot be directly read off, learners have to infer them by considering hetero atoms' properties (*e.g.*, lone pairs). However, recent work by Cox *et al.* (2024) and Lieber and Cox (2024) highlights that students encounter difficulties surpassing the given depiction of molecules to invoke resonance when features facilitating such inferences are not overtly visible. For the same structural motif (*i.e.*, single-bonded hetero atoms), the authors showed that students often rely on an *electron domain counting* technique to assign atom hybridization, without accounting for conjugation. With regard to our data, the lower mean score for this category suggests that students tend to attribute properties to visible features (*e.g.*, the presence of double bonds) and, therefore, perceive structures rather statically (Shane and Bodner, 2006). Lastly, items in the category positive *charge on hetero atom* necessitate the clear consideration of implicit aspects such as the hetero atoms' hybridization or exceeding octets. Thus, the number of information pieces to infer and connect makes the information processing in this category the most complex (Paas and van Merriënboer, 2020). Following that, students' recognition of resonance is facilitated by the explicitness of information that can be readily perceived and connected. Similar to previous research highlighting the cognitive effort as a difficulty-inducing factor in reasoning with representations (Cooper *et al.*, 2012; Taskin *et al.*, 2015), it becomes evident that the more cognitive steps required to derive relevant information, the more challenging the decision-making on resonance becomes.

This observation offers the possibility to reconsider reported student difficulties with resonance from a different perspective. For instance, Petterson *et al.* (2020) and Finkenstaedt-Quinn *et al.* (2020) showed across two studies that students face challenges in identifying the source of electron delocalization. While the authors primarily attributed these difficulties to alternative conceptions and reliance on surface features (*e.g.*, lone pairs), a closer look at the reactants also points to visual processing complexity. In the study by Petterson *et al.* (2020), for instance, one task involved the protonation of imidazole (Figure 5).



Protonation disrupts aromatic π-system.

Aromaticity is maintained, but learners have to deal with charged hetero atoms.

Figure 5. Protonation of imidazole with respective resonance structures.

Here, students not only had to evaluate multiple potential protonation sites but also had to deal with a relatively high visual complexity of the displayed molecule. First, it comprises multiple double bonds coupled with nitrogen atoms as hetero atoms. Second, the absence of an explicit charge requires students to anticipate the reaction course, further complicating the task by necessitating additional implicit considerations. The lone pair of the nitrogen atom bonded to a hydrogen atom is involved in the molecule's aromaticity, thus, protonating would result in a non-aromatic π-system. Protonating the other nitrogen atom instead would allow resonance stabilization. However, in both cases, charged hetero atoms would result – a motif that students struggled with the most in our study. Combined with alternative conceptions, difficulties in discerning and applying resonance may, thus, stem from an overloaded working memory (Paas and van Merriënboer, 2020), as students must deal with structures' visual affordances and coordinate different implicit considerations to derive the correct protonation site.

The indication of electron lone pairs induces an affirmation bias toward the presence of resonance

Although the number of cognitive steps required to process structural cues accounts for the ease with which students recognize resonance, it raises the question of whether the explicitness of provided information is always helpful for learners. To shed light on this question, students' scores for items displaying or omitting lone pairs with (no) possibility of resonance stabilization were compared in paired-sample *t*-tests (see Chapter 5 for details). Figure 6 summarizes the findings and shows that students' perception of resonance is markedly affected by the visibility of electron lone pairs.

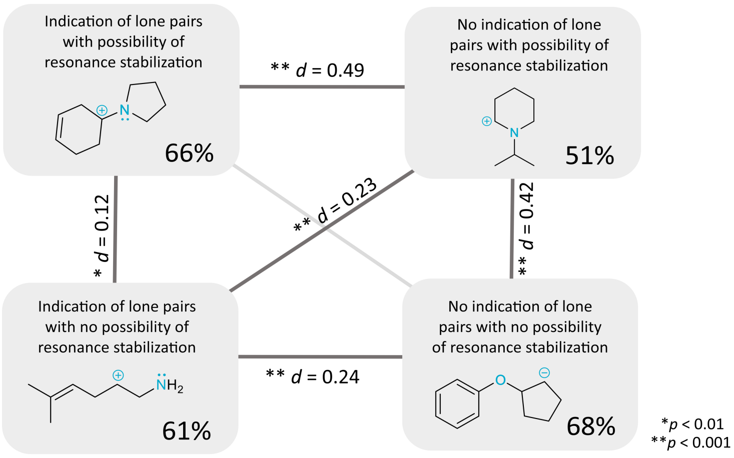


Figure 6. Students' success rates and significant differences for items varying in the indication of lone pairs; $N = 691$. Effect sizes according to Cohen (1992): small ($d = 0.2$), medium ($d = 0.5$), large ($d = 0.8$).

Specifically, the results reveal an affirmation bias toward the indication of lone pairs. Students were prone to misguided decisions when the indication of this feature was incongruent with the possibility of resonance. This suggests that students may pay less attention to structural details when locating conjugated systems but rather rely on easily discernible structural cues when deciding on resonance. Regarding resonance, similar patterns have been observed by Petterson *et al.* (2020) and Finkenstaedt-Quinn *et al.* (2020) in the context of acid-base chemistry and addition reactions, where most students invoked resonance when lone pairs were explicitly shown. Our findings are also congruent to studies in other contexts highlighting that the explicitness of provided cues significantly shapes students' perception and interpretation of representations (*e.g.*, regarding nucleophiles and electrophiles) (Frost *et al.*, 2023; Farheen *et al.*, 2024).

Students' lower performance for items displaying lone pairs and charges in β-position (Figure 6) further suggests that they may struggle to consider structural features in an integrated manner. Instead of interpreting these features in their interplay to decide on the emergent property of conjugated systems, students appear to conceptualize these features in isolation (Talanquer, 2007; DeFever *et al.*, 2015). Stated differently, they seem to add lone pairs and charges to conjugated systems without considering their spatial relationship, such as the distance between them. This may point to a fragmented "relational conceptual understanding" (Graulich *et al.*, 2019, p. 926) in recognizing which structural features are relevant and how they interrelate in specific contexts. Hence, while electron lone pairs may help discern resonance, they require more nuanced and context-dependent consideration.

Visual similarity of structural features to familiar structural motifs serves as a blueprint for students' consideration of resonance

Besides students' performance across the different structural feature categories, a *k*-means cluster analysis was performed to characterize trends and strategies in students' consideration of resonance in more depth. The validity of the resulting clusters was assessed by comparing group differences across external performance metrics (prior conceptual knowledge, time-on-task, cognitive load). Five clusters with distinct profiles regarding the identification of resonance in molecular structures emerged. Their characteristics are summarized in Figure 7. A more detailed description of each cluster, including specific mean values for the external performance metrics, can be found in Chapter 4.

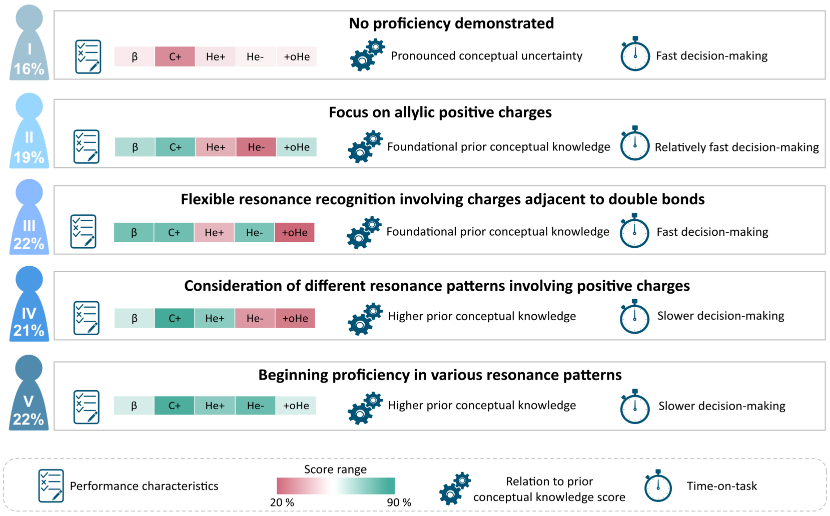


Figure 7. Overview of the different clusters and their characteristics regarding students' decision-making on resonance stabilization. Category abbreviations are: *β* (β-position of charge), *C+* (Carbon atoms & positive charge), *He+* (Hetero atom & positive charge), *He-* (Hetero atom & negative charge), *+oHe* (Positive charge on hetero atom); *N* = 681.

The cluster comparison revealed distinct strategies in how students used features to identify resonance stabilization (Figure 7). Overall, it became apparent that the majority of students based their decisions on double bonds (> 40%) and/or positive charges (≥ 40%) (Figure 7), suggesting that students' decision-making was markedly influenced by the structural motif of allylic carbocations, further leveraged by students' overall highest score in the category *carbon atoms & positive charge* (75%) (Table 1). This pattern seems a guiding principle for students. Serving as a structural blueprint for resonance considerations, the mere visual resemblance of structural features to allylic carbocations activated resonance-specific associations, even in cases where resonance stabilization does not apply (*positive charge on hetero atom*). This may be due to the lower cognitive load associated with this pattern and its familiarity from teaching contexts, ultimately enhancing its perceptual saliency (Kellman and Garrigan, 2009; Theeuwes, 2010). The emerging reliance on familiar patterns aligns with research in chemistry education emphasizing familiarity as a reoccurring theme in student reasoning approaches. For instance, students often use case-based or 'memory-bank' reasoning in problem-solving, matching new problems to stored representations and modifying them to fit with familiar steps (Kraft *et al.*, 2010; Weinrich and Sevian, 2017). Similarly, due to their familiarity, students favor line-angle diagrams over other representations when solving problems (DeCocq and Bhattacharyya, 2019) and draw upon familiar structures when constructing Lewis structures (Kaufmann *et al.*, 2017). Likewise, conceptualizing resonance stabilization as the compensation of positive charge for some students (clusters II, IV; Figure 7) could stem from the accustomed source-to-sink flow of electron density encountered in organic reactions (Bhattacharyya, 2013).

Considering familiarity may also complement previous findings on students' operational descriptions of resonance, which often involve listing individual structural features like double bonds and lone pairs as prerequisites (*e.g.*, Tetschner and Nedungadi, 2023). While prior studies attribute "cherry-pick[ing] bits and pieces of these patterns" (Barakat, 2024, p. 303) to limited conceptual understanding (Xue and Stains, 2020), our findings suggest that this focus may be more closely tied to the familiarity of certain features emphasized in teaching. Anchoring specific features may function as a shortcut heuristic, helping students navigate the concept's visual affordances (Talanquer, 2014). Nevertheless, a constrained perception of molecular structures may limit students' ability to recognize the interplay of structural features. Specifically, most students' challenges with items belonging to *positive charges on hetero atoms* in our study (Figure 7) indicate a surface-level focus on resonance. Aligning with the operational approach previously reported (*e.g.*, Xue and Stains, 2020; Brandfonbrener *et al.*, 2021), it seems that students in our study focus on explicit features, such as positive charges and double bonds, to decide on resonance stabilization without invoking implicit aspects in their decision-making (*e.g.*, electronegativity, atom hybridization). Hence, students seem to simplify the complexity inherent to resonance considerations. While this surface-level approach corroborates previous studies highlighting student difficulties in linking structural to more granular considerations when dealing with chemical reactions and Lewis structures (*e.g.*, Cooper *et al.*, 2010; Caspari *et al.*, 2018; Pölloth *et al.*, 2023), it also reinforces previous studies emphasizing students' fragmented understanding of the relationship between structural and electronic levels in resonance contexts. Similar to our results, Carle *et al.* (2021) observed that students often employ simplified rules, such as counting electron domains in depicted structures, rather than considering p-orbitals, to determine atom hybridization.

Flexibility in discerning resonance patterns increases with higher prior conceptual knowledge

Even though Figure 7 shows that the majority of students were guided by certain structural features when considering resonance, students' flexibility in dealing with varying structural patterns increased with higher prior conceptual knowledge. While students in the first cluster (*No proficiency demonstrated*) exhibited below-average scores for (nearly) all categories and showed the lowest prior knowledge score among all clusters (Figure 7), students in cluster V (*Beginning proficiency in various resonance patterns*) significantly outperformed other clusters in their prior conceptual knowledge (see Chapter 4). They showed pronounced above-average scores for most categories (Figure 7), indicating proficiency in dealing with various resonance patterns. This suggests that the competency to flexibly decode different structural motifs encompassing varying atom connectivity increases with conceptual understanding. This finding is consistent with various studies showing that a higher degree of prior knowledge facilitates flexibility in processing representations and abstracting the deep structure of representations (Chi *et al.*, 1981; Keig and Rubba, 1993; Cook, 2006).

While higher prior knowledge enhanced a more thorough engagement with the molecular structures as further denoted by the positive correlation with the time spent on tasks ($r = 0.24$, $p < 0.001$), more proficiency in handling different structural features did not correspond to a decrease in cognitive load (see Chapter 4). For instance, students in clusters IV and V performed weaker than clusters II and III for the category *β-position of charge* (Figure 7), suggesting that the consideration and weighing of *multiple* structural features may also induce overthinking and uncertainty (Linn, 2005).

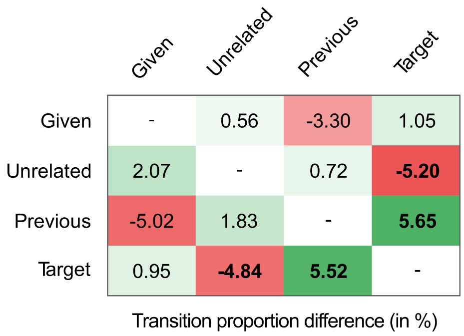
Thus far, it becomes evident that the visual affordances imposed by the variation of structural features crucially impact students' consideration of resonance in molecular structures (Figure 2, A). Students first seem to rely on simpler, familiar patterns when considering resonance before more thoroughly paying attention to and including other features, such as hetero atoms and negative charges, comprising a higher degree of processing complexity. However, the analysis also showed that the ability to identify resonance across various molecular structures is influenced by the interplay of perceptual and conceptual processes (Schönborn and Anderson, 2008; Rau, 2017). While students' strategies in identifying resonance varied (*e.g.*, focusing on double bonds), higher prior knowledge facilitated recognition across different resonance patterns, highlighting the role of conceptual understanding in using representations (Ainsworth, 2006; Rau, 2017). Despite valuable insights into students' recognition of resonance in terms of visual affordances, these findings are detached from students' concept consideration in problem-solving contexts. Therefore, analyzing the perceptual processes governing students' construction of resonance structures via eye-tracking extends these findings and provides insights into how students' engagement with representations influences their operational skills (Kozma and Russell, 1997) (see Figure 2, B).

1.5.2 The Role of Perceptual Processes in Students' Construction of Resonance Structures

Constructing resonance structures comprises various skills related to representational competence (Kozma and Russell, 1997). In addition to identifying relevant features (*e.g.*, conjugated systems), students must connect selected visual information, translate it into corresponding resonance structures, and evaluate their plausibility (*e.g.*, charge separation). While drawing resonance structures requires an understanding of related concepts (*e.g.*, electronegativity, hybridization) (Betancourt-Pérez *et al.*, 2010), it is also closely tied to visually coordinating different structural features. Consequently, students' processing and decoding of representations play a pivotal role in such tasks (R-M-factor) (Schönborn and Anderson, 2008). Given the various challenges students face in constructing resonance structures (Section 1.1), examining their perceptual processes may offer a new perspective on how students engage with resonance structures and how they relate to the construction of (un-) productive drawings.

The types of connection, not the amount of integrated visual information, determine the productivity of students' constructed resonance structures

Research in STEM education shows that high- and low-achievers differ in their problem-solving behavior, exhibiting pronounced differences in how they process and integrate visual information (*e.g.*, Susac *et al.*, 2023). For instance, eye-tracking studies in physics and biology task contexts have shown that novices make significantly more transitions between representations than experts (Cook *et al.*, 2008; Kohl and Finkelstein, 2008). Building on these findings, we explored how students connect visual information (*i.e.*, the drawing elements *previous drawing*, *target drawing*, *unrelated drawings*, and *given information*[1] (see Figure 4)) when constructing resonance structures. An Epistemic Network Analysis (ENA) (Shaffer *et al.*, 2016) based on students' AOI hits on the drawing elements was performed to model the structure and strength of connections between drawing elements underlying the construction of (un-)productive drawings. Contrary to findings in STEM fields outlined above, the ENA revealed a similar global gaze behavior for productive and unproductive drawings concerning visual information retrieval and integration; no significant differences in the absolute *number* of connections between drawing elements emerged, with a predominant connection of *previous* and *target* drawings for all constructed resonance structures (see Chapter 2 for detailed results). However, significant differences in the types of transitions between drawing elements (*i.e.*, the direction of information linkage) could be observed. Figure 8 depicts the subtracted transition matrix for productive and unproductive drawings, showing differences in the frequency of students' transitions between pairs of drawing elements.



	Given	Unrelated	Previous	Target
Given	-	0.56	-3.30	1.05
Unrelated	2.07	-	0.72	**-5.20**
Previous	-5.02	1.83	-	**5.65**
Target	0.95	**-4.84**	**5.52**	-

Transition proportion difference (in %)

Figure 8. Subtracted transition matrix indicating characteristic transitions regarding the construction of productive (green cells) and unproductive drawings (red cells); Positive values indicate a higher degree of transitions for productive drawings, negative values for unproductive drawings. Significant differences in transition types are displayed in bold ($p < 0.05$). [Reproduced from Braun *et al.* (2022).]

Productive drawings were characterized by more frequent transitions between the *previous* and *target* drawing ($p = 0.043$, $r = 0.26$) and vice versa ($p = 0.025$, $r = 0.29$), indicating a more straightforward drawing process. Conversely, unproductive drawings involved significantly more transitions between *unrelated* and *target* drawings ($p = 0.005$, $r = 0.36$) and vice versa ($p = 0.008$, $r = 0.34$). As such, not

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[1] The drawing elements characterize the relevance of different (student) drawings for the construction of resonance structures. The *target drawing* is the structure of interest, which results from the *previous drawing*. While *unrelated drawings* represent structures and auxiliary drawings that are not necessary for the construction of the target drawing, *given information* comprises all printed structures and text in the task prompt (see Figure 4 for an example).

the *amount* of visual information integration but the directionality of information connection accounted for differences between productive and unproductive drawings. Since transitions play a critical role in information processing (Schmidt-Weigand *et al.*, 2010), integrating less relevant information to a greater extent suggests that students may exhibit searching processes and uncertainty when constructing unproductive resonance structures. This is further supported by existing eye-tracking research in chemistry education comparing high- and low-performers' problem-solving behavior. While experts (or high-performing participants) usually display a more focused, goal-oriented gaze behavior (*e.g.*, transitions between or focus on relevant task components), novice learners (or low-performers) frequently exhibit less effective search strategies and focus on less relevant representational features (*e.g.*, Baluyut and Holme, 2019; Rodemer *et al.*, 2020; Connor *et al.*, 2021).

Constructing productive resonance structures involves flexible attention distribution to interrelated, relevant structural features

Due to the predominant focus on *previous* and *target drawings* for all resonance structures, a more fine-grained comparison considered the transition between these two drawing elements by focusing on students' fixation duration rates on smaller AOI units (*i.e.*, methoxy group, double bond, positive charge) during the construction process (Figure 9).

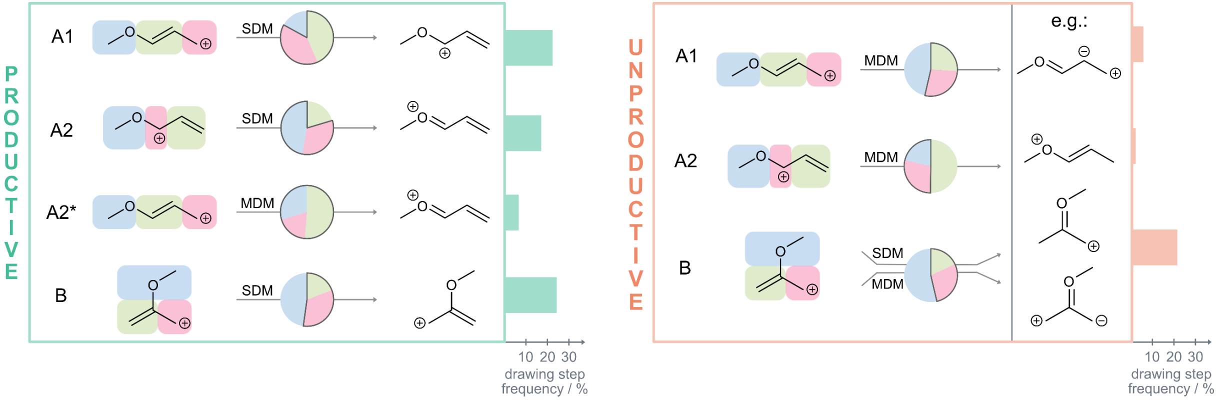


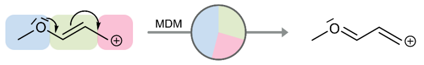
Figure 9. Relative drawing step frequency ($N = 57$) and fixation duration rates (pie charts) on the structural features (blue = methoxy group, green = double bond, pink = positive charge) in the construction of productive (green frame) or unproductive drawings (orange frame). Necessary structural features for the drawing step are highlighted by framing. SDM = single drawing move, MDM = multiple drawing moves (see Figure 4). A1 and A2 represent drawings necessary for reaction A, B for reaction B (see Chapter 2). A2* denotes students' drawings in case of skipping A1. [Reproduced from Braun *et al.* (2022).]

Figure 9 shows that productive drawings involved a more sequential fixation on interrelated, relevant features (> 80% of attention distribution in structures A1 and A2). Like other emergent properties, resonance requires a broader consideration of representations to successfully discern and use this concept (Bhattacharyya, 2014; Tümay, 2016). Aligning with that, students' successive consideration of interrelated, adjacent features resulted in sequential, productive single drawing moves (SDM) (Figure 9). In contrast, unproductive drawings were characterized by a focus on single, unrelated structural features to a greater extent, often inducing multiple drawing moves (MDM) at once (Figure 9). While these differences were pronounced for linear structures (structures A1, A2), students' attention distribution for the branched, spatially more complex structure (structure B) was more convergent across all drawings (Figure 9).

Reconsidering these findings in light of the results from Study 2 on students' resonance recognition (Section 1.5.1) further illuminates students' drawing steps and attention distribution. First, as shown in

Figure 9, students encountered less difficulty with structure A1, which involved electron delocalization in familiar allylic carbocations (*i.e.*, the motif *carbon atoms & positive charge*), whereas most unproductive drawings in A1 and A2 entailed changes to the double bond (*e.g.*, shifting the electrons of the double bond onto a carbon atom; see Figure 9). Together, this reaffirms the critical role of double bonds in decoding and translating resonance structures. Second, unlike the linear structures in A, the branched, visually more complex structure in B required broader visual processing. The conjugated system in B is less easily discernable due to the spatial proximity of the different structural features. As more information needs to be weighed (*e.g.*, connectivity and electronic effect of the oxygen atom), this may have possibly contributed to students' more even attention distribution across the entire molecule for structure B. Given the highest rate of unproductive drawings observed for structure B (Figure 9), this suggests that students may find it easier to decode and process *linear* structures when considering resonance. As such, students' increased challenge with the visually more complex structure contributes to existing research in Organic Chemistry education emphasizing the impact of visual complexity on student reasoning (DeFever *et al.*, 2015; Olimpo *et al.*, 2015). For instance, Flynn and Featherstone (2017) showed in the realm of the electron-pushing formalism that students had more difficulties and lower scores when dealing with visually more demanding molecules (*e.g.*, intramolecular reactions). Similarly, Rodemer *et al.* (2020) demonstrated that the number of explicit differences between reactions, such as leaving groups and substrates, impacted novice students' attention distribution in Organic Chemistry case comparison tasks, leading to more transitions.

While eye fixations indicate where students allocate their attention, they do not reveal why or how students use certain parts of representations. Analyzing students' verbal drawing rationales complements and fills this gap (Stieff *et al.*, 2011). Aligning with students' varying attention distribution for (un-)productive drawings, coding students' drawing explanations regarding their visual selection (Figure 4) showed that the *flexibility* in visual selection accounted for the productivity of resulting drawings. Students who explained in a *centered* manner (*i.e.*, focusing on single structural features) more often produced unproductive drawings. Such a narrowed drawing rationale was often coupled with trial-and-error approaches and the application of overgeneralized rules. Catherine's *knowledge-driven centered approach* for structure A can serve as an example (Figure 10).

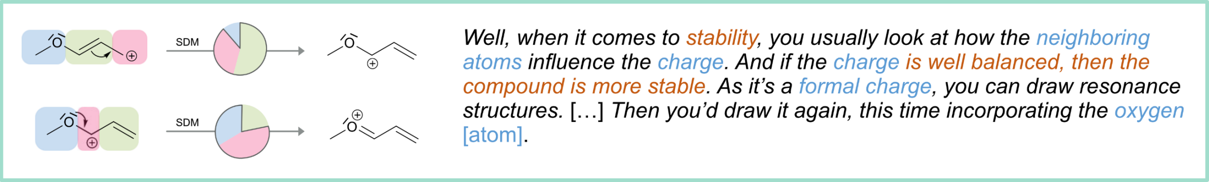


If oxygen has two lone pairs, then it can be assumed that it does something with them, or that resonance structures can be formed.

Figure 10. Catherine's drawing move, fixation duration rate on the structural features and rationale for her drawing in reaction A. The orange frame indicates the unproductivity of the resulting drawing. The orange highlighting in the text refers to the knowledge she applies when explaining her drawing step, whereas the blue highlighting denotes the features she focuses on. [Reproduced from Braun *et al.* (2022).]

Catherine attributes the lone pairs a central role in the translation of resonance structures, which is mirrored by her attention distribution, predominantly directed toward the methoxy group (46%). Accordingly, her drawing reveals that she manipulated the methoxy group and double bond without actually delocalizing the positive charge and paying less attention to details like implicit hydrogen atoms (Figure 10). This narrowed approach limited her ability to link structural elements, revealing challenges in accurately using visual information. As such, Catherine's case supports findings from Study 2 on students' affirmation bias toward lone pairs and limited attention to implicit aspects when considering resonance. In general, students' *centered* visual selection corresponds to prior studies (Betancourt-Pérez *et al.*, 2010; Cooper *et al.*, 2010), emphasizing students' reliance on overgeneralized rules and trial-and-error approaches when constructing and using Lewis structures for problem-solving.

Contrary to that, drawings underlying *variable* visual selection were frequently associated with a more holistic consideration of multiple interrelated features. Oliver's *knowledge-driven variable approach* for the structures A1 and A2 illustrates that (Figure 11, not discussed in Chapter 2). Guided by stability considerations, Oliver's analytical approach involved evaluating properties of structural features in their interplay in order to delocalize the positive charge. This led to a sequential construction of resonance structures, with a more focused attention distribution on relevant, adjacent features for each step.

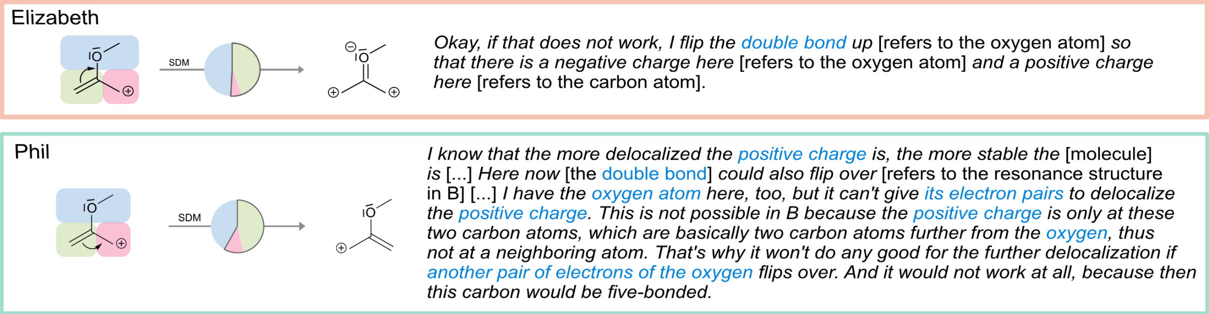


Well, when it comes to stability, you usually look at how the neighboring atoms influence the charge. And if the charge is well balanced, then the compound is more stable. As it's a formal charge, you can draw resonance structures. […] Then you'd draw it again, this time incorporating the oxygen [atom].

Figure 11. Oliver's drawing moves, fixation duration rates on the structural features and rationale for his drawings in reaction A. The green frame indicates the productivity of the resulting drawings. The orange highlighting in the text refers to the knowledge he applies when explaining his drawing steps, whereas the blue highlighting denotes the features he focuses on.

Students attach varying meaning to structural features despite comparable attention distribution

Even though differences in students' attention distribution converged for the more branched structure B (Figure 9), comparing students' drawing rationales revealed differences in their processing of visual information by applying their resonance-related knowledge in different ways. To illustrate, consider Phil's and Elizabeth's drawing rationales (Figure 12).



Okay, if that does not work, I flip the double bond up [refers to the oxygen atom] *so that there is a negative charge here* [refers to the oxygen atom] *and a positive charge here* [refers to the carbon atom].

I know that the more delocalized the positive charge is, the more stable the [molecule] *is* [...] *Here now* [the double bond] *could also flip over* [refers to the resonance structure in B] [...] *I have the oxygen atom here, too, but it can't give its electron pairs to delocalize the positive charge. This is not possible in B because the positive charge is only at these two carbon atoms, which are basically two carbon atoms further from the oxygen, thus not at a neighboring atom. That's why it won't do any good for the further delocalization if another pair of electrons of the oxygen flips over. And it would not work at all, because then this carbon would be five-bonded.*

Figure 12. Comparison of Elizabeth's and Phil's drawing moves, fixation duration rates and drawing rationales for their drawings in reaction B. The frames indicate the productivity of the resulting drawings (orange = unproductive, green = productive). The blue highlighting in the text refers to the structural features the students focus on. [Adapted from Braun *et al.* (2022).]

Elizabeth only refers to the electron-donating features (*i.e.*, double bond). The creation of two additional charges, while preserving the initial positive charge in her drawing (Figure 12), shows that she is primarily concerned with the re-location of electrons (Taber, 2002). This indicates that she tends to perceive the structure statically and apply rules thereon. In contrast, Phil's approach is more nuanced and aligns with the task affordances (*i.e.*, stabilizing the positive charge through electron density distribution). He centers his drawing steps around the positive charge and takes an analytic, holistic approach by considering adjacent structural features and analyzing their contribution to the delocalization of the positive charge. As such, he explicitly takes the electron flow from areas of high to low electron density into account. The higher gaze distribution for productive drawings may, thus, stem from a more thorough weighing of the different structural features.

Hence, while students may perceive the same structural features and allocate their attention similarly, they still attach varying meaning to these features (*e.g.*, the starting point for delocalization), which may influence how they rationalize their drawing steps. Students who narrowly focus on single, salient features, such as lone pairs, may miss the bigger picture, resulting in more static approaches when constructing resonance structures. This is congruent with recent findings by Rotich *et al.* (2024), showing that students encountered various features when assessing the stability of Lewis structures but attributed stability only to the most salient feature. Thus, it becomes clear that constructing correct resonance structures requires a sound conceptual understanding of electron delocalization, that allows students to perceive and connect visual features meaningfully (Ainsworth, 2006; Rau, 2017). This aligns with Keig and Rubba's (1993) findings, which emphasize that solving information-processing tasks, such as translating between structures, requires a thorough understanding of the underlying concept.

Overall, this section highlighted that perceptual processes play a crucial role in students' construction of (un-)productive drawings (*i.e.*, their operational skills in using resonance) (Figure 2, B). Flexibility in structure decoding (*i.e.*, focusing on broader areas of structural features surpassing single features or functional groups) enhanced the construction of productive resonance structures, as students perceived the structures more globally. In contrast, a more constrained focus was hindering. However, analyzing students' drawing rationales also underscores the intertwined nature of perceptual and conceptual processes (Figures 1 and 2) (Schönborn and Anderson, 2008; Rau, 2017), as meaning attribution to structural features shaped students' ability to generate valid representations. Consequently, conceptual understanding affects students' perception of resonance structures as well.

1.5.3 New Insights into Students' Use of Resonance across Different Problem-Solving Contexts

Subsections 1.5.1 and 1.5.2 revealed that perceptual processes play a critical role in students' consideration of resonance. Molecular structures' varying visual affordances and students' strategies in structure decoding markedly influenced their recognition of electron delocalization. These perceptual processes also affected how students constructed resonance structures. However, the accurate use of structural features plays an important role in problem-solving as well. Several studies demonstrated that students' perception and use of representations crucially shape their reasoning in chemistry (*e.g.*, Anzovino and Bretz, 2015; Graulich *et al.*, 2019; Rodriguez *et al.*, 2020; Nelsen *et al.*, 2024). For instance, bond-line structures, ball-stick-representations, and electrostatic potential maps cued students to different concepts (*e.g.*, charge separation, electronegativity, resonance) when predicting partial charges and nucleophiles (Farheen *et al.*, 2024). Similarly, Carle and colleagues (2021) noted that the competencies to identify and construct resonance structures build prerequisites for successfully applying resonance across different task contexts. Hence, to address students' fragmented consideration of resonance in problem-solving (*e.g.*, Finkenstaedt-Quinn *et al.*, 2020; Demirdöğen *et al.*, 2023), a more thorough understanding of how students engage with resonance structures during problem-solving is necessary. Accounting for the strong influence of representations on reasoning processes, Coordination Class Theory models concept understanding as a complex and interacting system of three components: (1) extraction strategies (*i.e.*, task approaches), (2) knowledge elements (*i.e.*, activated resources[2]), and (3) extractions (*i.e.*, features attended to within representations). Together, these components form

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[2] Following fine-grained constructivism, *resources* are cognitive components varying in grain size (*e.g.*, p-prims) and characterizing one's knowledge and reasoning. Their activation is context-dependent and sensitive to one's framing (Hammer *et al.*, 2005).

concept projections, representing how students consider a concept in a given context (DiSessa and Wagner, 2005; for a theoretical overview, see Chapter 3). Analyzing students' problem-solving through this lens can illuminate the interplay between representation use and resource activation, offering a more comprehensive understanding of student reasoning about resonance across different task contexts (Figure 2, C).

Students' use of resonance in problem-solving is diverse and context-dependent

Qualitatively comparing students' concept use revealed diverse concept projections across the three task contexts (*i.e.*, electrophilic aromatic substitution, nucleophilic addition step, leaving group departure step) (see Appendix 6.1.5 for an overview). There was not *one* unique way of considering resonance in problem-solving. Instead, a variety of approaches permitted productive concept use, which was highly influenced by the task affordances and the complex and individual interplay of the different coordination class components (*i.e.*, extraction strategies, extractions, activated resources). This accounted for differences in students' reasoning in problem-solving. Mary's and Audrey's problem-solving for the third task (not discussed in Chapter 3) can serve as an example. It shows that even the same coordination class components do not lead *per se* to the same problem-solving outcome (Figure 13).

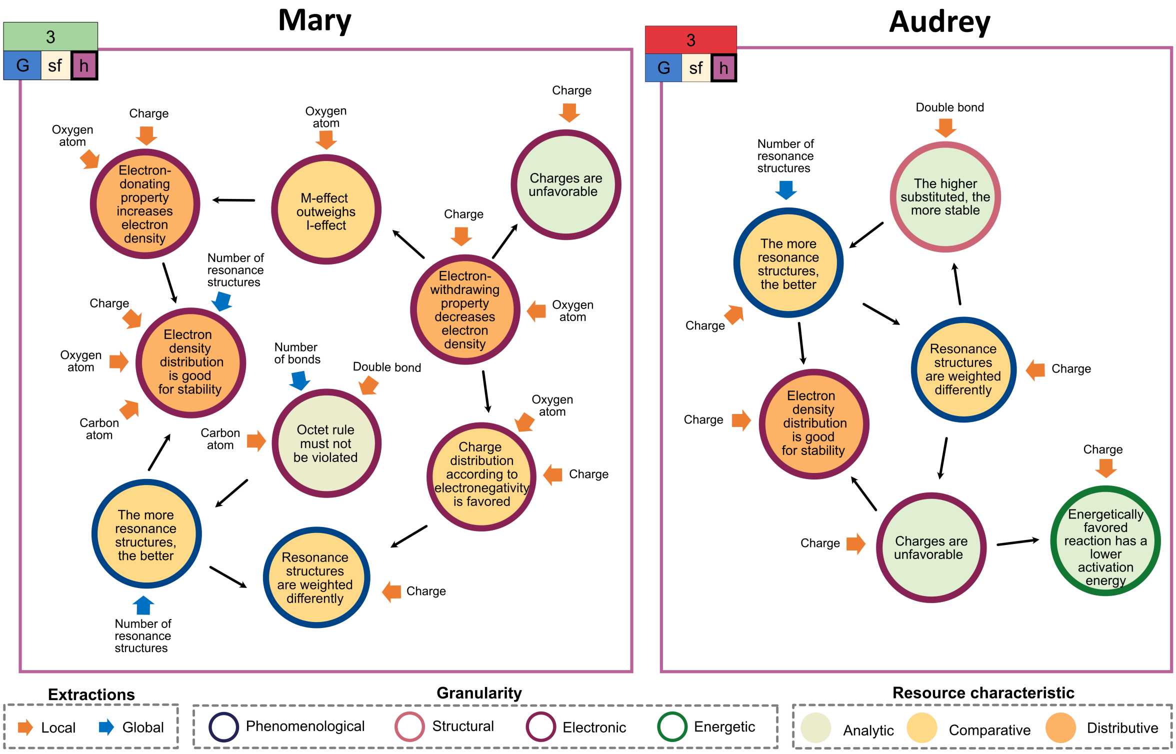


Figure 13. Mary's and Audrey's concept projection for the third task, illustrating the respective resource graphs and indicating their readout strategy (G = *global stability*), extraction types (sf = *single-focused*), and complexity of resulting resource graphs (h = *high*).

Despite convergent task approaches in comparing the overall number of resonance structures (*i.e.*, *global stability*) and exhibiting the same extraction types and complexity of connected resources, Audrey and Mary dealt with the task differently, pointing to more subtle differences in how they used and interpreted representations. Specifically, the task context cued them to different structural features, evoking different ideas about resonance (Figure 13), which, as a whole, contributed to different problem-solving solutions. This emphasizes that the intertwined nature of the Coordination Class components makes students' use of resonance in problem-solving diverse. Accordingly, Figure 13 also illustrates that activating suitable resources matching the task affordances proved more beneficial for productive concept use than the overall complexity of students' resource graphs.

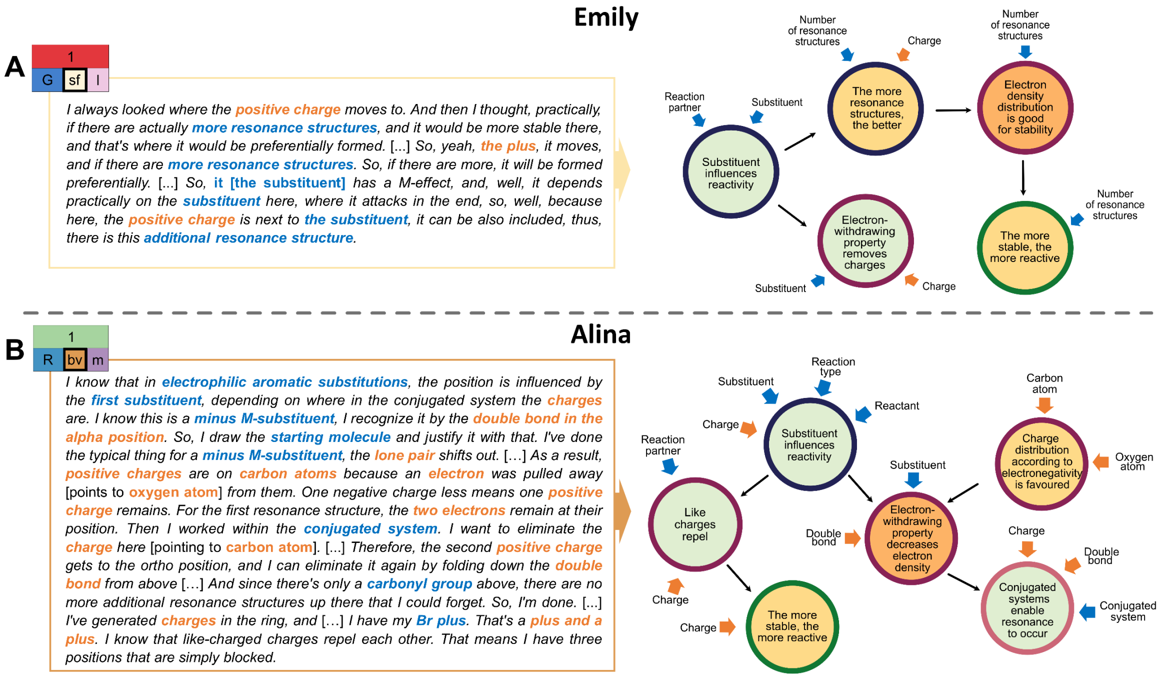
Following the diversity of students' concept projections, there was no clear trend in the activation of specific extraction strategies, extraction types, or resources that were*, per se,* associated with successful problem-solving. Nevertheless, the different task contexts and related task affordances accounted for some differences in students' concept use. Students' extraction strategies within and across the tasks exemplify this. While, ideally, the first and second tasks demand the comparison of reactive sites corresponding to *reactivity considerations*, the third task asks students to compare the molecules' *global stability* (Chapter 3). However, students' extraction strategies varied and occasionally even underwent multiple changes within a task (see Appendix 6.1.5). The fact that many students approached the first two tasks, which required similar considerations, differently (Appendix 6.1.5), underscores that even similar contexts may elicit different framing (Hammer *et al.*, 2005). Furthermore, connecting to studies on learner struggles with unfamiliar representations and reactions in problem-solving (Grove *et al.*, 2012; DeFever *et al.*, 2015; Taskin *et al.*, 2015; Houchlei *et al.*, 2021), familiarity seemed to influence students' extraction strategies as well. In fact, students changed their extraction strategies twice as often in the second task compared to the first and third task (Appendix 6.1.5). Since the second task involved more complex structures (*i.e.*, substituted ethyl benzoates) and was embedded in a seemingly unfamiliar context, students possibly needed more time to figure out a suitable approach, leading to more changes in their extraction strategies.

Similar to the extraction strategies, students' resource activation was diverse. While some resources were activated with similar frequency across tasks (*e.g.*, *conjugated systems enable resonance to occur*), others were more task-specific (Chapter 3). Resources pertaining to reactivity and electron flow were more present in the first and second tasks (*e.g.*, *electron-withdrawing property decreases electron density*; *substituent influences reactivity*), whereas resources targeting local considerations were more frequent in the third task (*e.g.*, *charges are unfavorable*; *the higher substituted, the more stable*). Despite differences in resource activation, it is noteworthy that resources directly related to electron distribution, central to resonance, were infrequently invoked in student reasoning. For example, while most students chose a *global stability* approach for the third task, a higher percentage of activated resources focused on local factors in this task (*e.g.*, *the higher substituted, the more stable; charges are unfavorable*). This suggests that students may encounter challenges in dynamically conceptualizing resonance in varying contexts and, thus, recur to the local interpretation of resonance structures. This observation aligns with recent studies. While students in the study by Rotich *et al.* (2024) did not identify given Lewis structures as corresponding resonance structures and recurred to resources such as the octet rule or electronegativity to reason about stability, students in the study by Cox and coworkers (2024) did not invoke resonance as a resource but relied on ideas pertaining to formal charges or electronegativity when reasoning about acid-base properties.

Overall, the variety of activated resources suggests that students do adjust their consideration of resonance across task contexts, which challenges previous studies reporting limited resonance use (*e.g.*, Cartrette and Mayo, 2011; Brandfonbrener *et al.*, 2021; Demirdöğen *et al.*, 2023). While these studies consistently suggest that students rely on rules and heuristics, our findings present a more nuanced perspective. Students may indeed activate heuristic-like resources but integrate them in a broader network with other (productive) resources, leading to context-dependent differences in concept use. As such, this finding contributes to a growing number of asset-based studies emphasizing the diversity of student reasoning in problem-solving in chemistry (*e.g.*, Rodriguez *et al.*, 2019; Crandell and Pazicni, 2023; García Ramos and Towns, 2024; Liang-Lin *et al.*, 2024). However, despite this diversity in concept use, a detailed comparison of students' problem-solving revealed distinct characteristics underlying (un-)productive concept projections, which were closely tied to students' engagement with their constructed drawings.

Analytical and reflective engagement with one's structural drawings enhances the productive use of resonance in problem-solving

Research in psychology and chemistry education has repeatedly emphasized the importance of encountering the multiplicity of structural features for successful problem-solving, particularly when inferring emergent properties (Chi and VanLehn, 2012; Bhattacharyya, 2014; Tümay, 2016). In accordance with that, the comparison of students' concept projections revealed that the holistic consideration of structural features, *i.e.*, considering and combining structural features in their variety and across global and local levels, often proved beneficial for successful problem-solving. Consider as an example Emily's and Alina's problem-solving in the first task (Figure 14). Despite showcasing similar task approaches, the students refer to different structural features (*i.e.*, extraction types), which influenced their overall problem-solving success.



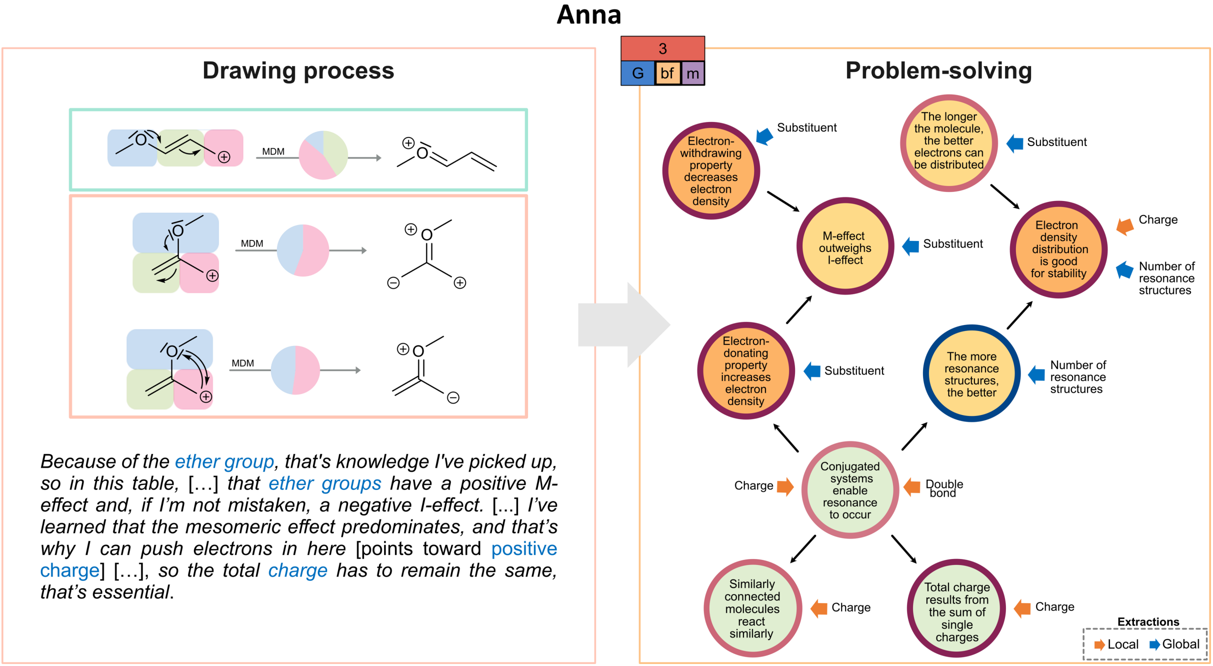
I always looked where the ***positive charge*** *moves to. And then I thought, practically, if there are actually* ***more resonance structures****, and it would be more stable there, and that's where it would be preferentially formed. [...] So, yeah,* ***the plus****, it moves, and if there are* ***more resonance structures****. So, if there are more, it will be formed preferentially. [...] So,* **it [the substituent]** *has a M-effect, and, well, it depends practically on the* ***substituent*** *here, where it attacks in the end, so, well, because here, the* ***positive charge*** *is next to* ***the substituent****, it can be also included, thus, there is this* ***additional resonance structure****.*

I know that in ***electrophilic aromatic substitutions****, the position is influenced by the* ***first substituent****, depending on where in the conjugated system the* ***charges*** *are. I know this is a* ***minus M-substituent****, I recognize it by the* ***double bond in the alpha position****. So, I draw the* ***starting molecule*** *and justify it with that. I've done the typical thing for a* ***minus M-substituent****, the* ***lone pair*** *shifts out. […] As a result,* ***positive charges*** *are on* ***carbon atoms*** *because an* ***electron*** *was pulled away* [points to **oxygen atom**] *from them. One negative charge less means one* ***positive charge*** *remains. For the first resonance structure, the* ***two electrons*** *remain at their position. Then I worked within the* ***conjugated system****. I want to eliminate the* ***charge*** *here* [pointing to **carbon atom**]. *[…] Therefore, the second* ***positive charge*** *gets to the ortho position, and I can eliminate it again by folding down the* ***double bond*** *from above […] And since there's only a* ***carbonyl group*** *above, there are no more additional resonance structures up there that I could forget. So, I'm done. […] I've generated* ***charges*** *in the ring, and […] I have my* ***Br plus****. That's a* ***plus and a plus****. I know that like-charged charges repel each other. That means I have three positions that are simply blocked.*

Figure 14. Comparison of Emily's and Alina's extraction types (*single-focused* [sf], *both-varied* [bv]) with an illustration of their overall resulting resource graphs (*low* [l] and *medium* [m] complexity) in the first task. While Emily's concept projection is unproductive and exhibits a *global stability* (G) extraction strategy, Alina's concept projection is productive and involves a *reactivity* (R) extraction strategy. The orange highlighting in the quotes indicates local extractions, the blue highlighting global extractions. [Reproduced from Braun & Graulich (2024) with permission from the Royal Society of Chemistry.]

Emily primarily centered on few structural features at a global level (*i.e.*, the number of resonance structures and the substituent), while paying limited attention to local features like positive charges. Ultimately, the *single-focused* extraction type (Figure 14) restricted her analysis of the constructed resonance structures. This constrained her ability to activate relevant resources (*e.g.*, leaving her uncertain about the carbonyl's electronic properties), and led to unproductive problem-solving strategies overall (*i.e.*, getting stuck with *global stability* considerations). In contrast, Alina demonstrated a more thorough structural analysis, integrating multiple structural features across both local and global levels (Figure 14). By zooming in and out her drawings, she employed a *both-varied* extraction type. Her ability to transition between structural features and view the drawings as a coherent system allowed her to activate more productive resources for the task at hand, such as determining the electronic effect of the carbonyl group, ultimately facilitating productive concept use.

The productivity of considering structural features in their variety aligns with our findings on students' drawing processes, where flexibility in visual selection also supported the construction of productive resonance structures (see Subsection 1.5.2). Relatedly, comparing students' drawing processes and subsequent use of structural features in problem-solving reveals further similarities. Overall, 12 of the 18 unproductive concept projections involved a *focused* extraction type, where students paid attention to a limited number of structural features during problem-solving (Appendix 6.1.5). Qualitatively comparing students' drawing process of resonance structures to their subsequent problem-solving in the third task showed that in four of five unproductive concept projections, *focused* extraction types were associated with *centered* drawing approaches (see Figure 4 for codes). Stated differently, when students narrowly focused on structural features during drawing, they also tended to base their activation of resources in problem-solving on single structural features in this task. Anna's engagement with her resonance structures exemplifies this observation (Figure 15, not discussed in Chapters 2).

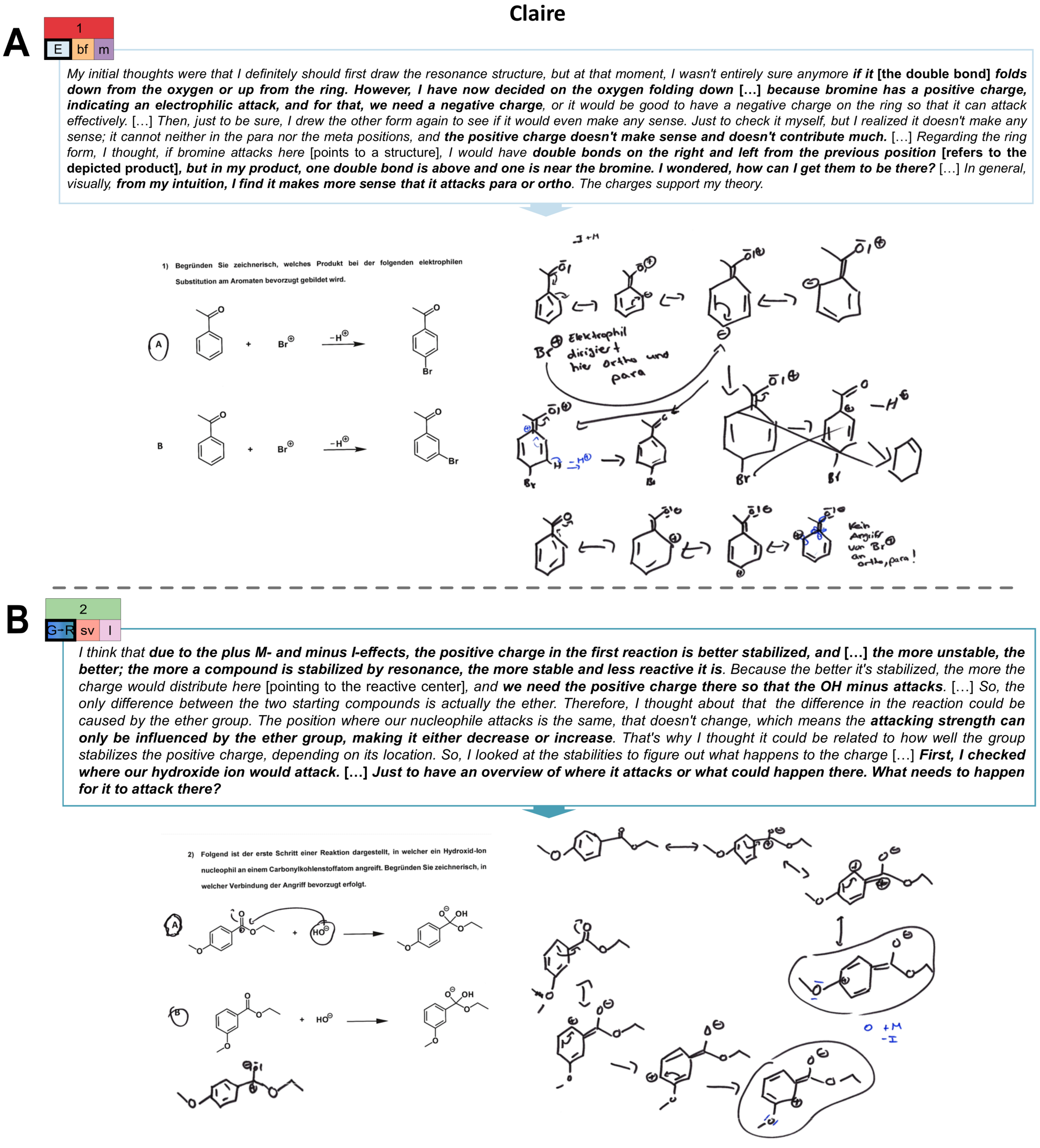


Because of the ether group, that's knowledge I've picked up, so in this table, […] that ether groups have a positive M-effect and, if I'm not mistaken, a negative I-effect. [...] I've learned that the mesomeric effect predominates, and that's why I can push electrons in here [points toward *positive charge*] […], *so the total charge has to remain the same, that's essential.*

Figure 15. Comparison of Anna's drawing process and subsequent reasoning (*i.e.*, resource graph) in the third task. See Figures 10 and 13 for explanation of the color meanings.

Apart from one productive drawing in reaction A (green frame), Anna's attention distribution is mainly placed on the methoxy group and the charge for the remaining resonance structures (Figure 15). Her extractions in her resource graph further mirror this narrowed representation use, as most resources are invoked based on these single structural features. Even though she activated task-relevant resources (*e.g.*, *the more resonance structures, the better*), her restricted reference to single structural features also gave rise to simplified ideas (*e.g.*, *similarly connected molecules react similarly* based on the encountered charges). Consequently, at least for the third task, this observation suggests that students' perception of representations might affect their overall reasoning process. While recent work by Cox *et* *al.* (2024) emphasizes that drawing difficulties hinder students' productive use of resonance during problem-solving, the observation regarding the third task extends these results by underscoring the close link between drawing processes and concept use: narrowing one's attention to single structural features not only increases the likelihood of generating unproductive drawings but also seem to impact how students use these drawings during problem-solving. As such, our findings contribute to the body of research in chemistry education emphasizing students' limited focus on salient surface features in problem-solving (DeFever *et al.*, 2015; Galloway *et al.*, 2017; Galloway *et al.*, 2018; Popova and Bretz, 2018).

Students' analytical engagement with drawings also shaped their approaches to the tasks. In unproductive concept projections, students' extraction strategies were often characterized by a static focus on isolated structural features (*e.g.*, presence of charges), showcasing limited use of (constructed) drawings as problem-solving tools to infer properties (Cooper *et al.*, 2017). Consider Claire's *electrostatic considerations* in the first task (Figure 16A).



My initial thoughts were that I definitely should first draw the resonance structure, but at that moment, I wasn't entirely sure anymore ***if it*** **[the double bond]** ***folds down from the oxygen or up from the ring. However, I have now decided on the oxygen folding down*** **[…]** ***because bromine has a positive charge, indicating an electrophilic attack, and for that, we need a negative charge****, or it would be good to have a negative charge on the ring so that it can attack effectively.* […] *Then, just to be sure, I drew the other form again to see if it would even make any sense. Just to check it myself, but I realized it doesn't make any sense; it cannot neither in the para nor the meta positions, and* ***the positive charge doesn't make sense and doesn't contribute much.*** […] *Regarding the ring form, I thought, if bromine attacks here* [points to a structure], *I would have* ***double bonds on the right and left from the previous position*** **[refers to the depicted product]*****, but in my product, one double bond is above and one is near the bromine. I wondered, how can I get them to be there?*** […] *In general, visually,* ***from my intuition, I find it makes more sense that it attacks para or ortho****. The charges support my theory.*

1) Begründen Sie zeichnerisch, welches Produkt bei der folgenden elektrophilen Substitution am Aromaten bevorzugt gebildet wird.

I think that ***due to the plus M- and minus I-effects, the positive charge in the first reaction is better stabilized, and*** **[…]** ***the more unstable, the better; the more a compound is stabilized by resonance, the more stable and less reactive it is****. Because the better it's stabilized, the more the charge would distribute here* [pointing to the reactive center], *and* ***we need the positive charge there so that the OH minus attacks****.* […] *So, the only difference between the two starting compounds is actually the ether. Therefore, I thought about that the difference in the reaction could be caused by the ether group. The position where our nucleophile attacks is the same, that doesn't change, which means the* ***attacking strength can only be influenced by the ether group, making it either decrease or increase****. That's why I thought it could be related to how well the group stabilizes the positive charge, depending on its location. So, I looked at the stabilities to figure out what happens to the charge* […] ***First, I checked where our hydroxide ion would attack.*** **[…]** ***Just to have an overview of where it attacks or what could happen there. What needs to happen for it to attack there?***

2) Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.

Figure 16. Claire's extraction strategies in the first (unproductive concept projection, A) and second task (productive concept projection, B) (E = *electrostatic considerations*, G = *global stability*, R = *reactivity considerations*) along with her drawings. [Reproduced from Braun & Graulich (2024) with permission from the Royal Society of Chemistry.]

Instead of reasoning based on her drawings to infer implicit properties, Claire constructed competing structures (*i.e.*, ketone group as electron-withdrawing and electron-donating). She perceived the resonance structures as discrete entities and projected her preconceived idea of charge attraction onto the task, ultimately deciding on the electron-donating effect of the ketone to make the solution fit to the task (Kraft *et al.*, 2010). This approach concurs with numerous studies in chemistry education, stating that students often rely on explicit surface features when struggling to derive implicit properties, resulting in less successful problem-solving strategies (McClary and Talanquer, 2011a; Anzovino and Bretz, 2015; Graulich and Bhattacharyya, 2017; Graulich *et al.*, 2019).

Conversely, productive concept projections often stemmed from reflective, inductive approaches, where students slowed down their reasoning, carefully analyzed the task requirements, and aligned their strategies with the task affordances (Airey and Linder, 2009). This deliberate process fostered nuanced and analytical reasoning, as exemplified by Claire's reactivity extraction strategy in the second task (Figure 16B). After reconstructing the reaction step and thoroughly examining the reaction conditions, Claire explicitly considered the structural differences between the reactants in both reaction pathways. She constructed resonance structures to reflect on the influence of the substituents on the reactive center. This process-oriented, analytical approach allowed her to draw context-specific inferences, with her drawings playing a central role as problem-solving tools (*i.e.*, linking varying charge stabilization to reactivity). Aligning with our findings, the benefit of careful examination of reaction conditions and task prerequisites for successful problem-solving has been previously reported in chemistry education research (Yuriev *et al.*, 2017; Caspari and Graulich, 2019; Rodriguez *et al.*, 2019).

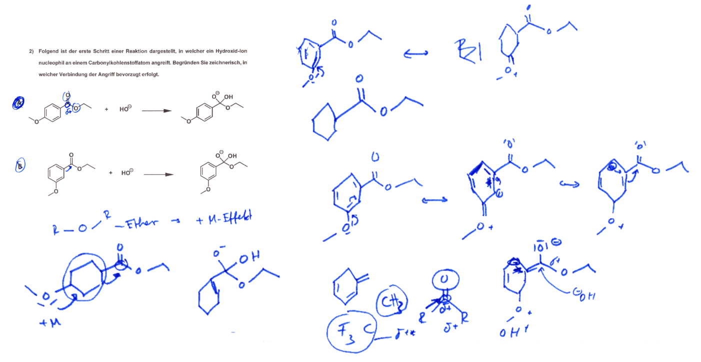
As illustrated in Claire's problem-solving for the second task, students often changed their task approaches within a task due to new insights during their problem-solving. Here, the extent of analytical engagement with one's drawings (*i.e.*, a thorough structural analysis of the structures) decided upon the productivity of extraction strategy changes as well. While Claire initially used a *global stability* approach, she productively shifted to *reactivity considerations* after critically reconsidering her drawings in light of the task affordances (Figure 16B). This is in contrast to few unproductive changes in extraction strategies, which either resulted due to drawing difficulties or limited analytical engagement with constructed structures. Consider Anna's change of *reactivity* to *structural considerations* in the second task, not discussed in Chapter 3 (Figure 17).

Anna

2

R→S | bv | m

I think it is B because I thought that by pushing electrons here [refers to reactive center in A]*, it is possible that the delta positive charge is at the carbonyl group.* ***If the benzene ring can push its charge here*** **[refers to reactive center in A]*****, I would have lower reactivity than if it were in the meta-position.*** [...] *I'm reconsidering, sorry.* [...] *I'll stick with answer A.* [...] *By redrawing it* [resonance structures in reaction A] *and thinking about it again,* ***I realized that both paths, A and B, show that it is possible to push electrons to this carbonyl group. The question now is, which of the two, they differ in the ether position, the ether group is in meta-position here*** **[in B]** ***and in para-position there*** **[in A]** ***to this carbonyl group. Now the question is, which one can better activate it. And that's when I thought about the aromatics again and realized that we have an activating group, which is usually in the para-position.***



2) Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.

Figure 17. Anna's change in extraction strategy from *reactivity* (R) to *structural* (S) *considerations* in the second task along with her drawings as task solution. (bv = *both-varied* extraction type, m = resource graph of *medium* complexity).

Initially, Anna reasoned productively about electrophilicity differences. However, as a result of resource activation, her approach shifted to focusing on the position of the ether substituents due to their activating function in electrophilic aromatic substitutions. Despite initially assuming electrophilicity differences, she only constructed (partially) incorrect structures for reaction B, skipped those for reaction A, and did not further elaborate on her drawings. Instead, Anna globally attributed the same electron-donating effect of the ether substituent to the reactive center in both reaction steps. This suggests that she did not use her drawings as a problem-solving tool. As she relied on her knowledge of the substituent independent of the structures at hand, the provided representations "fail[ed] to represent" (Strickland *et al.*, 2010, p. 293).

Overall, students' concept use is closely tied to their analytical engagement with resonance structures. The flexibility in considering structural features not only influenced their task approaches but also played a key role in the activation of resources. This reinforces the strong relationship between the use of representations and concept understanding (Ainsworth, 2006; Rau, 2017). Given the reciprocal nature of this relationship, understanding students' interpretation of these representations is essential. This entails both the conceptual processes involved in making sense of resonance structures and students' conceptualization of resonance (see Figure 2, C). Mirrored by students' activation of conceptual resources during problem-solving, examining the nature of activated resources can, thus, provide a more comprehensive account of student reasoning about resonance.

The depth and connectivity of activated resources impact productive concept use in problem-solving

Students' reasoning encompassed a wide range of conceptual resources across the different task contexts. However, subtle differences emerged in the types of activated resources. In unproductive concept projections, resources were more often characterized by static ideas (*e.g.*, *unlike charges attract*), alternative conceptions (*e.g.*, *electron-withdrawing property removes charges*), or ideas not directly linked to the resonance concept (*e.g.*, *steric hindrance makes attack more difficult*). Not touching upon the consideration of electron-density distribution, thus, not corresponding to the actual meaning of electron delocalization, may have hampered productive concept use. This is consistent with the literature on students' use of resonance in problem-solving, emphasizing that reliance on heuristics and overgeneralized rules is often coupled with unsuccessful task outcomes (*e.g.*, McClary and Talanquer, 2011a; Demirdöğen *et al.*, 2023). In contrast, students demonstrating productive concept projections more often invoked analytical-comparative resources (*e.g.*, *charge distribution according to electronegativity is favored*; *conjugated systems enable resonance to occur*). These resources reflected a deeper consideration of resonance prerequisites and the plausibility of resonance structures, reinforcing a more analytical engagement with constructed structures. Despite these differences, students activated many resources with comparable frequency, regardless of their concept projection productivity (see Chapter 3 for an overview).

Further comparison revealed that not the mere activation of resources but their (inter-)connectedness and organization often contributed to a productive concept use. Specifically, the overall complexity of resource graphs was less important than students' ability to transition across different levels of granularity (*i.e.*, phenomenological, structural, electronic, energetic) and to jointly activate different types of resources (see Appendix 6.1.6 for all student resource graphs). To illustrate, consider Audrey's and Louis' resource graphs for the first task as contrasting examples (Figure 18).

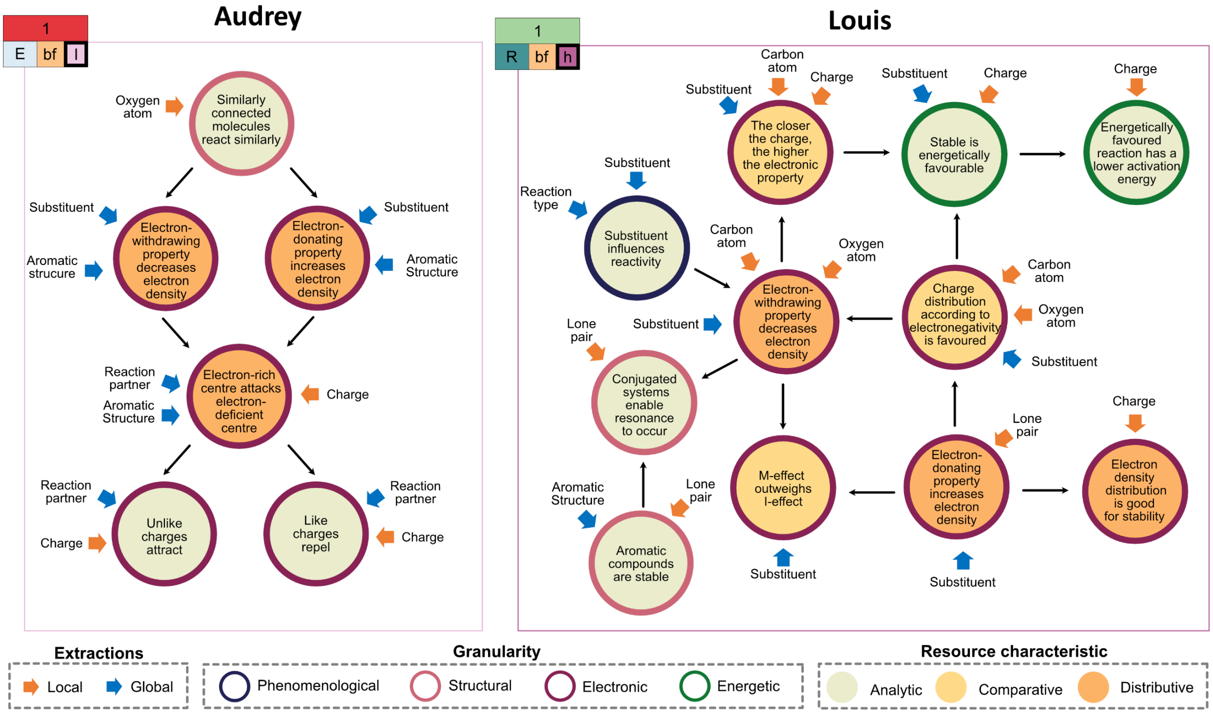


Figure 18. Resource graphs for Audrey's and Louis' problem-solving in the first task. Louis exhibits a productive concept projection with a *reactivity* (R) extraction strategy, a *both-focused* (bf) extraction type and a resource graph of *high* (h) complexity. Audrey's concept projection is unproductive and encompasses an *electrostatic considerations* (E) extraction strategy, a *both-focused* (bf) extraction type and a resource graph of *low* (l) complexity. [Reproduced from Braun & Graulich (2024) with permission from the Royal Society of Chemistry.]

While both students activate similar resources to some extent (*i.e.*, electronic properties of the substituent), their organization differs. Audrey demonstrates a dualistic thought process attributing both electron-withdrawing and -donating properties to the substituent. While she activates different (electronic) resources and links them back to structural features of the representations (*i.e.*, charge interactions), her reasoning is only characterized by *analytical* and *distributive* resources (*i.e.*, targeting the distribution or flow of electrons). In contrast, Louis' reasoning is more differentiated and reflective, combining multiple granularity levels. He links structural to electronic ideas, which are further connected to energetic considerations in order to draw conclusions about the reaction pathway. Consequently, he connects electron density distribution to other concepts. In doing so, he integrates *comparative* (*i.e.*, weighing) resources, making his reasoning more nuanced. Altogether, Louis considers the resonance concept more holistically, using his drawings as a starting point to infer more implicit and abstract aspects. As such, a more thorough conceptual consideration supports the productive use of resonance. This aligns with a body of research emphasizing the importance of connecting different concepts and incorporating energetic considerations into reasoning (Caspari *et al.*, 2018; Asmussen *et al.*, 2022; Pölloth *et al.*, 2023). Although all students invoked electronic resources in our study, those with unproductive concept projections often did not include various granularity levels. This corroborates reported challenges in linking resonance to energetic considerations (Brandfonbrener *et al.*, 2021; Demirdöğen *et al.*, 2023), leaving student ideas about resonance unconnected fragments (DiSessa and Wagner, 2005). The greater extent of missing comparative resources in unproductive concept projections indicates that students may not always reflect on resonance plausibility. This reaffirms our findings in Study 2, where all students struggled, to a varying extent, with the correct decision-making on resonance in items requiring more implicit considerations (*e.g.*, atom hybridization) (Section 1.5.1). Yet, our analysis demonstrates that students' reasoning about resonance encompasses numerous (relevant) fine-grained ideas, whose coordination primarily accounted for the productivity of concept use.

It becomes clear that, beyond reflective and analytical use of representations, students' ideas about resonance, whether in the depth of their reasoning or the presence of alternative conceptions, significantly influence their sense-making of resonance structures (Ainsworth, 2006; Rau, 2017). Hence, students' use of resonance in problem-solving is deeply shaped by the interplay between conceptual considerations and the use of representations (Figure 2, C).

1.6 Conclusions

This dissertation demonstrates that students' consideration of resonance in Organic Chemistry is deeply intertwined with their engagement with representations. Building on theories that emphasize the interplay of conceptual and perceptual processes underlying representational competence (Schönborn and Anderson, 2008; Rau, 2017), this work yielded new insights into students' use of resonance. By adopting a process-oriented perspective, this dissertation showed that students' perception of visual information markedly impacted their consideration of resonance in multiple facets, from recognizing and constructing resonance structures, to successfully using this concept in problem-solving. As such, the hypotheses guiding this dissertation could be confirmed (Section 1.3).

Specifically, it became evident that the molecular structures' visual affordances critically shaped students' recognition of resonance stabilization. The findings revealed that the cognitive steps required to process structural features accounted for students' varying success in deciding on resonance. Familiarity with structural motifs (*e.g.*, resemblance to allylic carbocations) often guided students' decision-making, eventually leading to affirmation biases. As such, students initially rely on simpler patterns before thoroughly including other features (*e.g.*, hetero atoms) in their consideration of resonance. Despite varied decision-making strategies and persistent cognitive load, increased prior conceptual knowledge accounted for more flexibility in successfully dealing with different structural motifs, highlighting the role of conceptual understanding in flexible information processing.

Perceptual processes also significantly influenced students' construction of resonance structures in problem-solving contexts. Eye-tracking data revealed that allocated visual attention accounted for the productivity of constructed resonance structures. Productive drawings were characterized by a more direct connection between previous and target drawings, further supported by a sequential and broader focus on relevant, interrelated structural features. In contrast, unproductive drawings often stemmed from a static focus on single, unrelated features, reflected by students' meaning attribution to the most salient structural features. Thus, flexibility in perception, selection, and integration of visual information was key to generating productive resonance structures.

Finally, a fine-grained qualitative analysis of students' reasoning about resonance across different problem-solving contexts showed that students' concept use was diverse, shaped by the task affordances and the dynamic and complex interplay of various factors (*e.g.*, activated resources). Consequently, no clear trends emerged, suggesting that there is not only *one* way of considering resonance in problem-solving. Still, students' concept use markedly depended on their engagement with constructed resonance structures. While drawing difficulties hampered students' concept use, a holistic consideration of structures (*i.e.*, considering and combining structural features across local and global levels) supported successful problem-solving. A thorough structural analysis not only facilitated nuanced, productive task approaches, but also supported the activation of relevant conceptual resources. Relatedly, even though students activated various resources, activating and connecting resources across different granularity levels, spanning from phenomenological to energetic considerations, and jointly combining analytical and comparative resources, were beneficial for productive concept use.

Unpacking the interleaved nature of conceptual and perceptual processes underlying students' use of resonance (Figure 2) provides a new perspective to characterize students' understanding and consideration of resonance. Much is going on when students consider resonance (*e.g.*, constructing resonance structures and interpreting the structures). While prior studies primarily emphasized the role of conceptual understanding for appropriate concept use, this dissertation advances these works by showcasing that proficiency and flexibility in processing visual information proved equally critical for successful resonance use, which may also account for related learning challenges.

As such, this dissertation also contributes to broader chemistry education research by emphasizing the central role of representations in student reasoning. Reliance on surface features often poses a barrier to successful problem-solving, linked to challenges connecting explicit features to implicit properties (*e.g.*, DeFever *et al.*, 2015; Graulich *et al.*, 2019). However, as shown in the realm of resonance, this dissertation suggests that these challenges may be rooted more deeply, possibly stemming from a narrow, constrained perception of representations. This hinders the recognition of emergent properties and impacts not only the construction of representations but also their successful consideration in problem-solving. While both studies revealed that students do encounter different structural features, they do not necessarily consider and interpret them in an interrelated manner, emphasizing that students may not view these features as part of an interconnected system. Successful concept use in Organic Chemistry is not only tied to identifying relevant explicit features but also depends on the *flexibility* with which these features are perceived (*i.e.*, recognize their interplay). Engagement with representations shapes students' concept use; hence, fostering students' proficiency in perceiving and engaging with representations proves critical to enhancing students' use of resonance and problem-solving abilities.

While this dissertation has unpacked the role of representations in students' reasoning about resonance, not all factors impacting students' understanding and use of resonance could be addressed (Figure 2). For instance, instructional practices crucially shape students' concept use (Xue and Stains, 2020). Therefore, effective approaches to support students' nuanced perception and use of representations for resonance considerations warrant future investigation. Similarly, while frameworks on representational competence stress the importance of developing different skills and competencies to flexibly deal with representations in problem-solving, such as perceptual fluency (Section 1.2) (Ainsworth, 2006; Rau, 2017), this work did not delve deeper into how students' proficiency in dealing with resonance structures evolves. Together with the abundant insights gained in this dissertation, these aspects lay a rich foundation for different directions for future research and teaching.

1.7 Outlook and Suggestions for Future Research

Resonance, like many other concepts in chemistry, requires students to integrate explicit structural features with implicit electronic considerations while navigating the visual affordances of specific representations. Our work highlights the diversity in students' use of resonance, yet underscores that flexible engagement with structural representations is a key prerequisite for productive concept use. This raises the question of how one can effectively support students' flexible and dynamic consideration of resonance. Building on our findings, different directions for research and instruction emerge. On the one hand, fostering students' flexibility in perceiving and utilizing interrelated structural features (*i.e.*, looking beyond single features or functional groups to perceive structures more globally) suggests a valuable avenue for future investigation. On the other hand, the diversity in students' concept use underscores the need for adaptive instructional approaches tailored to students' individual learning needs. The following subsections outline in greater detail different exemplary directions of how the findings of this dissertation could inform future research.

1.7.1 Supporting Students' Flexibility in Perceiving Resonance Structures through Visual Chunking

More than in other disciplines, reasoning in Organic Chemistry is intricately linked to domain-specific representations. However, one's ability to keep things in mind while performing complex tasks such as problem-solving is constrained by working memory capacity (Baddeley, 2012). Visual working memory, in particular, plays a critical role when reasoning with representations, whose capacity is limited to approximately four visual items, irrespective of singular features or linked groupings of information (Luck and Vogel, 1997; Zhang *et al.*, 2012). In our studies, students often focused narrowly on singular structural features. As such, simultaneously processing and coordinating multiple interrelated features required for resonance considerations may exceed visual working memory capacity. This increases cognitive demands and leads to a higher intrinsic cognitive load, ultimately limiting meaningful engagement with representations and hampering successful problem-solving (Sweller, 2010). Cognitive psychology research suggests that *chunking*, where related structural features are encoded as a single unit, can enhance visual working memory capacity (Miller, 1956). Notably, a recent study by Stieff *et al.* (2020) found that even naïve and beginner Organic Chemistry students implicitly identify common groupings and patterns of atoms in domain representations, highlighting the critical role of visual chunking in representation processing. Consequently, *visual chunking* offers a promising avenue for enhancing learners' flexibility in perceiving resonance structures. By compressing information into higher-order structures, students can achieve more efficient and holistic information processing. This reduction in cognitive load could facilitate the perception of emergent properties and enable students to simultaneously consider multiple, interrelated structural features (Chi and VanLehn, 2012). Ultimately, such an approach could help students more easily perceive conjugated systems as perceptual units, thereby supporting their ability to consider resonance in problem-solving.

While instruction typically emphasizes the semantic information encoded in domain-specific chunks (Stieff *et al.*, 2020), the effectiveness of learning interventions to help students encode these chunks in Organic Chemistry could be explored. Previous results in mathematics education are promising. In different studies, Zhang *et al.* (2012; 2020) showed that visual chunking of interrelated features in geometry diagrams via highlighting positively affected students' problem-solving performance. It supported information integration in complex problems and in representations of pronounced complexity. Similarly, Parnafes (2007) demonstrated that using representations that explicitly highlight features helped students to reason about natural harmonic oscillation in physics contexts.

To support students in developing greater flexibility in the perception of structural features, the impact of visual chunking on their consideration of resonance structures could be investigated in more depth. Specifically, research could explore whether visual chunking strategies broaden students' perception of structural features and conjugated systems. Drawing on research in chemistry education and beyond, which demonstrates the effectiveness of highlighting in enhancing student reasoning and visual understanding (*e.g.*, Ratwani *et al.*, 2008; Zhang *et al.*, 2020; Rodemer *et al.*, 2021), future studies could investigate the impact of highlighting techniques, varying in informational detail and explicitness, on student chunking of interrelated features and developing proficiency. For instance, three intervention groups could be created: (1) no highlighting, (2) highlighting of interrelated features via color coding, and (3) highlighting via indication of electron density (*e.g.*, highlighting electron deficiency and richness to hint electron flow, and, when suitable, indicating partial charges) (Figure 19A).

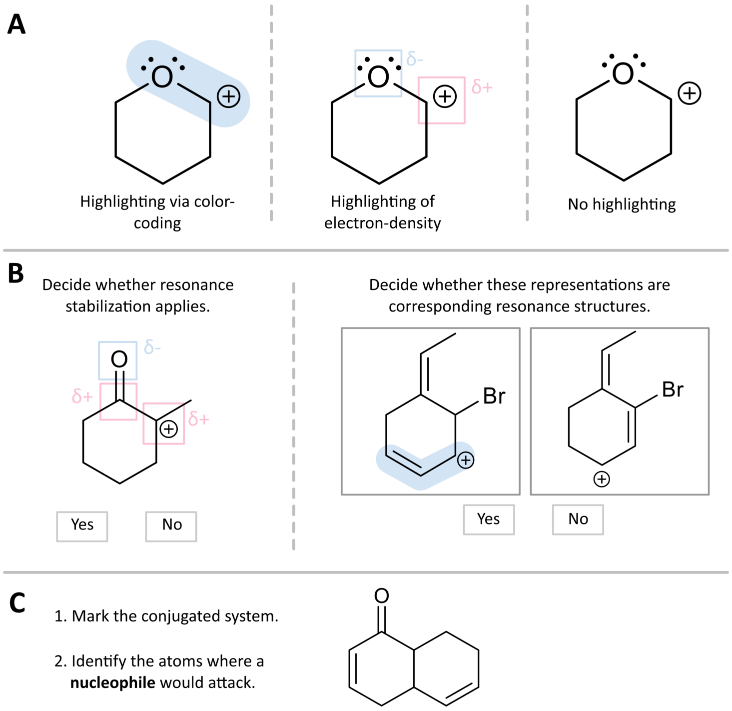


Figure 19. (A) Different highlighting techniques for visual chunking; (B) Exemplary tasks to foster visual chunking; (C) Exemplary task to include fading in visual chunking.

In line with Rau (2017), a learning environment could be designed to train Organic Chemistry beginner students' recognition of resonance. While earlier studies denote that fluency-building activities are most beneficial for learners with advanced prior knowledge (*e.g.*, Rau, 2018), more recent research (Rau *et al.*, 2019) has demonstrated that even learners with limited prior knowledge can benefit from such activities when they explicitly direct students' attention to visual features, *i.e.*, train their efficiency in *perceiving* these features (*e.g.*, via mapping activities), while reducing cognitive load (Rau *et al.*, 2019). Based on that, various exercises could be developed to promote the recognition and encoding of conjugated systems as larger chunks, helping students perceive their semantic interrelatedness (*e.g.*, via comparisons, error detection, and sorting tasks) (Figure 19B). To prevent overreliance on highlighting, which may hinder meaningful chunk recognition in the absence of visual cues (Seufert, 2003; Bhattacharyya and Bodner, 2005), fading could be integrated into the exercises as well. Tasks could be designed to have students progressively identify and apply chunked features on their own (*e.g.*, expanding structures and marking electrophilic sites (Figure 19C).

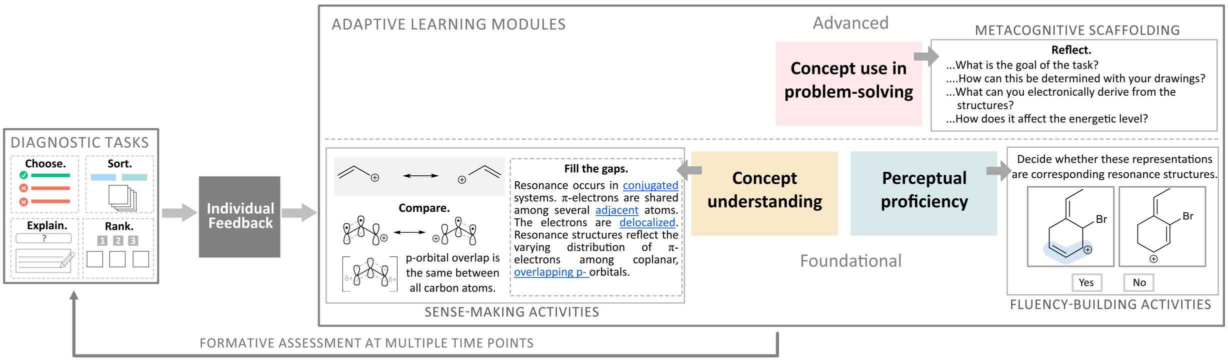
Using pre- and post-tests, the effectiveness of such a chunking intervention could be examined from different perspectives. On the one hand, eye-tracking could be employed to investigate how students' perception changes through visual chunking, *i.e.*, whether students adopt a broader and more holistic consideration of structural features when decoding molecular structures to recognize emergent properties in more complex structures. Additionally, qualitative interviews could serve as a means to explore the impact of different highlighting techniques on students' concept use. As our studies have shown, students who perceive structures more flexibly tend to be more successful in using resonance across different tasks (Section 1.5.3), so it could be examined whether chunking facilitates a deeper conceptual understanding of the emergent nature of resonance (*i.e.*, exploring the impact of perceptual processes on conceptual considerations). Building on studies showing that students encounter different structural features but do not use them in problem-solving (*e.g.*, Rotich *et al.*, 2024), it could be explored whether chunking fosters a more reflective consideration of features during problem-solving, or alters students' strategies in approaching resonance tasks (*e.g.*, due to indicating the electron density gradient in chunks). Finally, the influence of visual chunking on students' developing perceptual fluency could be explored (Kellman and Massey, 2013), *e.g.*, via fluency-efficiency measures (Rau *et al.*, 2019). Specifically, it could be compared whether students in the visual chunking groups (*i.e.*, highlighting groups) show a greater improvement in resonance recognition than students who solve similar fluency-building tasks but do not encounter highlighting of structural features. Depending on the effectiveness of such visual chunking strategies, this approach could offer a promising avenue for the design of fluency-building activities in general, and serve as a model for fostering students' recognition of other emergent properties in Organic Chemistry (Bhattacharyya, 2014).

1.7.2 Investigating the Development of Students' Concept Understanding

Although our studies highlight the diversity in students' concept use and related challenges (*e.g.*, the perceived cognitive load in recognizing resonance), our findings are limited to a one-time snapshot. However, since concept understanding is dynamic and evolves through exposure to varying contexts (Hammer *et al.*, 2005; DiSessa *et al.*, 2016), investigating the development of students' concept understanding longitudinally (*e.g.*, over two semesters) is critical to comprehend students' concept use and developing expertise in more depth. Similar to the task designs in our studies, students could engage in problem-solving tasks requiring resonance considerations and varying in complexity, and explain their reasoning at multiple time points during their courses. Fine-grained analyses of students' reasoning could address pending questions about students' perceptual and conceptual processes underlying resonance use this dissertation could not resolve, *e.g.*, *When and how does the interconnectedness of resources across different levels of granularity emerge? When do students develop perceptual fluency? Does students' use of resonance structures become more flexible with practice? How do students integrate resonance with other concepts? How does structure variation impact students' certainty in deciding about resonance stabilization?* Similarly, our study on students' drawing processes is limited to rather simple structures and a limited number of resonance structures. As such, including more complex drawing tasks (*e.g.*, involving aromatic compounds) would allow to shed light on students' perceptual processes when dealing with visually more demanding structures. Addressing these open questions could enlighten the dynamic nature of students' resonance understanding in more depth and provide further insights into the progression, interplay, and achievement of the resonance-related learning outcomes proposed by Carle and Flynn (2020). Likewise, capturing how students' understanding of resonance evolves over time could inform the design of interventions that support their conceptual and perceptual processes.

1.7.3 Adaptive Scaffolding of Students’ Concept Use

Our studies also highlighted the diverse challenges students might face when considering resonance. While some students struggled to recognize resonance, impacting their drawing processes and reasoning, others could successfully construct resonance structures but still encountered difficulties deriving meaning from them. These findings emphasize the need for adaptive support tailored to students’ individual needs (Aleven *et al.*, 2017; Plass and Pawar, 2020). Based on our analysis and aligning with Carle and Flynn’s (2020) interconnected learning outcomes, different broader areas of potential difficulties emerged pertaining to foundational issues underlying resonance use (*i.e.*, recognition of electron delocalization, conceptual underpinnings of resonance), and more advanced challenges regarding successful concept use in context (*e.g.*, the connection of resonance-related resources in problem-solving) (Figure 20). These insights could guide the design of adaptive learning modules within intelligent tutoring systems (Kulik and Fletcher, 2016).



...What is the goal of the task?
....How can this be determined with your drawings?
...What can you electronically derive from the structures?
...How does it affect the energetic level?

p-orbital overlap is the same between all carbon atoms.

Resonance occurs in conjugated systems. π-electrons are shared among several adjacent atoms. The electrons are delocalized. Resonance structures reflect the varying distribution of π-electrons among coplanar, overlapping p- orbitals.

Decide whether these representations are corresponding resonance structures.

Figure 20. An adaptive learning environment addressing different areas of potential challenges in using resonance at a foundational and more advanced level with exemplary tasks to foster students’ understanding and use of resonance.

To develop such an intervention, Tetschner and Nedungadi’s (2023) Resonance Concept Inventory could be expanded as a diagnostic tool. Beyond existing tasks assessing students’ conceptual understanding of resonance (*e.g.*, determining the contribution of different resonance structures to the resonance hybrid), additional tasks could focus on perceptual aspects (*e.g.*, addressing different resonance patterns, drawing resonance structures) and open-ended problem-solving tasks eliciting concept-related reasoning (*e.g.*, justifying reaction pathways). Using automated feedback (*e.g.*, via machine learning) (Martin and Graulich, 2023), appropriate exercises aligning with identified areas of challenges could be assigned to the students, addressing different entry points in students’ resonance understanding and use.

Students with foundational conceptual gaps (*e.g.*, difficulties in making sense of resonance structures or interpreting them dynamically) could benefit from sense-making activities first (Rau, 2018), emphasizing the conceptual understanding of electron delocalization (Figure 20). Here, integrating multiple representations could make the referential connections between visual features and the conceptual underpinnings more accessible (Seufert, 2003; Ainsworth, 2006; Rau, 2017). For instance, given its potential to support students’ problem-solving in Organic Chemistry (Keller and Habig, 2022), augmented reality could be implemented in exercises to illustrate the dynamic nature of resonance by showing the delocalization of electrons and orbital interactions. This could facilitate students’ connection-making between structural and electronic considerations. Additionally, guided exercises similar to those proposed by Hunter *et al.* (2025) (*i.e.*, connecting inferred ideas to structural features in the form of empty resource graphs), could foster students’ connection-making between structural features and electronic or energetic considerations, broadening and strengthening students' network of resonance-related resources (Hammer *et al.*, 2005; DiSessa *et al.*, 2016). Students showing gaps in flexibly recognizing the potential of resonance stabilization, but showing a foundational conceptual understanding of resonance, could be assigned to fluency-building exercises (Rau, 2017) as outlined in Section 1.7.1 (Figure 20). Students mastering perceptual and conceptual basics but struggling to connect their activated ideas flexibly and across different granularity levels could, for instance, profit from metacognitive scaffolding in problem-solving tasks (Yuriev *et al.*, 2017). Aligning with our study results, prompts encouraging students to reflect on their reasoning (*e.g.*, *What steps did you follow to determine the most stable resonance structure?*) could slow down students' problem-solving and promote a more nuanced consideration of resonance structures. Lastly, students showing proficiency in using resonance across different task types could practice resonance across different contexts with varying difficulty levels aligned with the various resonance learning outcomes (Carle and Flynn, 2020).

Implementing the adaptive learning environment with formative assessments at multiple time points across a semester would allow for monitoring individual progress and dynamically adjusting training (*e.g.*, providing more complex tasks or offering additional support as needed). As such, fading could gradually decrease support as students develop proficiency in using resonance (Kang *et al.*, 2014). Future research could evaluate the effectiveness of such adaptive interventions compared to non-adaptive approaches, where all students work on a sequence of different task types (Rau *et al.*, 2021), and explore the impact of such interventions on students' learning gains and transfer of resonance considerations across different tasks. Additionally, it would be valuable to investigate which student groups benefit most from tailored support and under what conditions.

1.8 References

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2. Let's Draw Molecules: Students' Sequential Drawing Processes of Resonance Structures in Organic Chemistry

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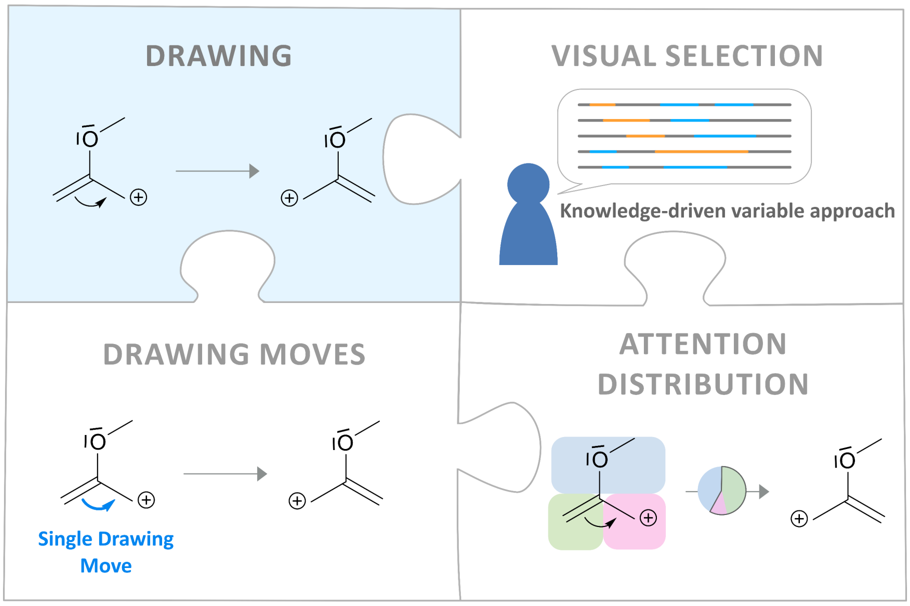

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Let's draw molecules: Students' sequential drawing processes of resonance structures in organic chemistry

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Drawing is a fundamental skill in science, technology, engineering, and mathematics (STEM) disciplines to express one's reasoning and externalize mental models in problem-solving. Although research has highlighted the effectiveness of drawing as a learning strategy and the importance of drawing accuracy for learning success, little is known about learners' actual drawing process. However, especially in organic chemistry, the investigation of drawing processes is of great importance as generating different representations, such as structural formulas, is inherent to problem-solving in this visual-laden discipline. Resonance structures, for example, are often used to estimate reactive sites in a molecule and to propose reaction pathways. However, this type of representation places a high cognitive demand on learners, which, besides conceptual difficulties, leads to drawing difficulties. To support learners in drawing and using resonance structures in problem-solving, it is necessary to characterize how they generate their drawings. To this end, a qualitative, exploratory study has been conducted to investigate undergraduate students' (N = 20) drawing processes of resonance structures while solving an organic case comparison task. Using eye-tracking, the characteristics regarding the construction of productive and unproductive drawings became visible. Results indicate that unproductive drawings often stem from integrating and connecting unrelated information during the drawing process. Further, the results show that the productivity of a drawing depends on learners' flexibility in information selection. Implications for supporting learners' drawing process and using eye-tracking for characterizing drawing processes in other STEM disciplines are discussed.

KEYWORDS

eye-tracking, organic chemistry, drawing, resonance, chemistry education research (CER), undergraduate, molecular structures

Introduction

In science, technology, engineering, and mathematics (STEM) disciplines, scientists and learners rely heavily on external representations to make sense of scientific concepts and phenomena (Fiorella and Zhang, 2018; Ainsworth and Scheiter, 2021). As representations constitute a fundamental means for the construction and transmission of knowledge, students need to be proficient in analyzing and using given representations (Nitz et al., 2014) and be fluent in generating them (Ainsworth et al., 2011). In fact, by expressing one's reasoning and externalizing mental models, drawings can help learning new concepts and support problem-solving (Cox, 1999; Ainsworth et al., 2011; Quillin and Thomas, 2015; Cooper et al., 2017; Wu and Rau, 2019). In recent years, much research has been conducted on drawing as a learning activity across different STEM contexts such as chemistry (Hellenbrand et al., 2019), physics (Maries and Singh, 2018), biology (Schmeck et al., 2014), and geography (Gobert and Clement, 1999) at school and college levels. Predominantly, it has been shown that prompting learners to visually depict content presented in text- or animation-based instructional materials is an effective learning strategy as students who draw not only build higher quality explanations and develop a more coherent mental model of a studied phenomenon, but also perform better in subsequent tasks and tests (Bobek and Tversky, 2016; Fiorella and Zhang, 2018; Cromley et al., 2019). Thus, drawing enhances learning outcomes related to retention, comprehension, and knowledge transfer (Van Meter and Garner, 2005; Leopold and Leutner, 2012; Schmeck et al., 2014; Fiorella and Zhang, 2018; Fiorella et al., 2020). However, drawing *per se* does not automatically enhance learning. By referring to the prognostic drawing principle, Schwamborn et al. (2010) point out that the quality of learners' drawings is predictive of their learning outcomes, i.e., the more accurately and correctly learners draw, the better their performance. This finding has been replicated in various studies (Mason et al., 2013; Schmeck et al., 2014; Rellensmann et al., 2016; Fiorella and Zhang, 2018; Hellenbrand et al., 2019; Schmidgall et al., 2020; Stieff and DeSutter, 2020).

Despite focusing on the quality of final drawing products and their relation to learning outcomes, the actual drawing process leading to these products has not received much attention in research so far (Lobato et al., 2014). However, drawing constitutes a core scientific practice itself and, consequently, necessitates a profound understanding of how a drawing is sequentially generated and which factors influence its quality. In organic chemistry, for instance, drawing is fundamental to scientific thinking and model-based reasoning as diagrams and structural formulas have a high explanatory power and make imperceptible entities and processes visible (Goodwin, 2008; Cooper et al., 2017; Graulich and Bhattacharyya, 2017). Whether in the laboratory or the lecture, chemists sketch and manipulate molecular structures to explain findings and communicate chemical content (Kozma et al., 2000). Besides this displaying function, drawings of molecular structures are crucial problem-solving tools. Since much chemical information (e.g., connectivity, polarity) is embedded within molecular structures, drawing enables the expression of assumptions or predictions about the properties of molecules or possible reaction processes (Cartrette and Bodner, 2009; Cooper et al., 2017). Constructing resonance structures of organic molecules, for instance, serves as a mean to estimate reactive sites in a molecule by representing multiple variants of the electronic delocalization in a molecule which cannot be adequately represented by a single structure. By considering the hypothetical electronic distribution in a molecular structure (i.e., the contribution of each resonance structure to the dynamic electron density distribution of a molecule), resonance structures enable the prediction of reaction pathways (Richardson, 1986). Therefore, constructing appropriate resonance structures constitutes the first critical step in a chain of steps of inferences to derive structural properties and chemical reactivities (Cooper et al., 2012). Thus, not succeeding in this step hinders students from using the resonance structures adequately in subsequent problem-solving (Strickland et al., 2010; Carle and Flynn, 2020). To support students in the adequate use of the resonance concept and the respective drawing process of resonance structures, it is crucial to understand how students are sequentially generating their drawings and which drawing behavior characterizes the generation of productive, thus valid and significant resonance structures, and unproductive drawings, i.e., wrong or insignificant resonance structures.

A more profound, process-oriented characterization of drawing processes can be achieved by using eye-tracking. Without interfering with the construction process, recording eye movements quantitatively captures students' visual processing of stimuli (e.g., by providing insights into learners' attention distribution on structural features or their search behavior in terms of gaze patterns). This can help to draw conclusions about learners' underlying cognitive processes and different strategic approaches when constructing representations such as molecular structures (Just and Carpenter, 1980; Cullipher et al., 2018). Therefore, using eye-tracking in the context of construction processes in STEM disciplines allows a deeper insight into students' drawing processes and offers a new perspective on obstacles students encounter when generating representations such as chemical structures.

Prior research on students' difficulties in the construction of organic molecular structures

Becoming proficient in using symbolic language in organic chemistry, such as drawing mechanisms or using the electron-pushing formalism, has been constantly shown to be difficult for students at various levels (Bodner and Domin, 2000; Graulich, 2015; Flynn and Featherstone, 2017; Dood and Watts, 2022). Several studies report that students depict mechanisms solely based on rote memorization, do not ascribe meaning to the electron-pushing formalism, place electron arrows as decoration instead, and exhibit difficulties in the construction of structural formulas (Bhattacharyya and Bodner, 2005; Cooper et al., 2010; Grove et al., 2012). Lewis structures are typically the first type of representations students encounter in organic chemistry to represent molecular structures as a variety of physical and chemical properties of molecular compounds can be inferred by constructing and inspecting Lewis structures (e.g., physical state, geometry, solubility) (Cooper et al., 2012; Tiettmeyer et al., 2017). In fact, drawing Lewis structures implies a high cognitive load on students, as students must consider various concepts (e.g., expanded octets, geometry) and sets of rules while coping with many exceptions to these very rules at the same time (Cooper et al., 2010; Kaufmann et al., 2017; Tiettmeyer et al., 2017; Karonen et al., 2021). Cooper et al. (2010) intensively investigated students' ability to construct and manipulate Lewis structures across different learning levels. As a main finding, they demonstrated that students' and even faculty members' competence in constructing valid Lewis structures is deficient. Most students struggled with creating valid Lewis structures involving two or more carbon atoms (Cooper et al., 2010). Moreover, it became apparent that the success rate depended on how the formulas were presented to students. While students struggled with drawing a Lewis structure of methanol in the form of CH_4O, more students could produce a correct structure if the functional group was depicted explicitly, i.e., as CH_3OH (Cooper et al., 2010). Other common errors that students exhibit when drawing Lewis structures encompass the inability to determine the correct number of bonds, the arbitrary assignment of (formal) charges in ions, or the overreliance on rules such as the octet rule (Cooper et al., 2010; Kaufmann et al., 2017; Karonen et al., 2021). Concerning the latter, students were either likely to apply the octet rule when it was not possible to show atoms with full octets or tended to violate the octet rule, e.g., by exceeding the octet or depicting atoms different from carbon (e.g., nitrogen or oxygen atoms) as electron-deficient (Cooper et al., 2010). Some students in Cooper et al.'s (2010) study even invented their own rules and invalid strategies (e.g., reaching the highest symmetry). All this suggests that students tend to rely on memorized, salient cues while drawing, use rules mechanically, or approach drawing tasks by unsystematic trial-and-error strategies (Ahmad and Omar, 1992; Cooper et al., 2010; Kaufmann et al., 2017; Sandi-Urena et al., 2020).

These problems reported for the generation of single Lewis structures also apply to the construction of resonance structures. Resonance structures provide a more accurate way of describing molecules that single Lewis structures cannot accurately display due to the delocalization of π-electron pairs over several atoms. As such, molecules can be best described by drawing multiple structural formulas (e.g., Lewis structures or skeletal formulas) of the same molecule with a varying electron distribution. The combination of these drawings, depending on their contribution to the overall stability of the molecule, ultimately forms the resonance hybrid of the given molecule. Consequently, the properties and reactivities (e.g., charge density and product distribution) of molecules that exhibit resonance lie between the different canonical structures. Although students are expected to have a thorough understanding of this core chemical concept after introductory courses in organic chemistry and should be able to use it fluently to depict the electronic structure of compounds, research in chemistry education has demonstrated that the resonance concept puts a high cognitive load on students, even at the university level (Duis, 2011; Brandfonbrener et al., 2021). This leads to various misconceptions, such as considering resonance structures as equilibrium or electron reservoirs (Taber, 2002; Kim et al., 2019; Xue and Stains, 2020). As the application of this concept requires the integration of different concepts and prior knowledge (e.g., electronegativity, hybridization, electron-pushing formalism), a fragmented conceptualization of these relationships may hinder subsequent problem-solving (Betancourt-Pérez et al., 2010). Besides studies focusing on students' conceptual understanding of resonance, little research has been conducted on how students draw resonance structures. For instance, Betancourt-Pérez et al. (2010), used different tasks to investigate students' competence in the construction of resonance structures across different learning levels in organic chemistry by prompting their participants to (a) draw curved arrows to show the electron movement in resonance structures, (b) draw alternative structures for a given ion or molecule, (c) identify the most stable resonance structure, and (d) draw the resonance hybrid. Their results show that students perform poorly in drawing resonance structures and exhibit different errors in both the first and second semester. The most prevalent errors encompass, for example, the violation of the octet rule, e.g., by moving π-bonds toward atoms with a full octet, irrespective of the atom's hybridization and number of bonds. Moreover, students tend to break σ-bonds between carbon and hydrogen atoms, put charges on atoms that are not charged or construct resonance structures with a different delocalized system, thus different connectivity, compared to the initial structure (Betancourt-Pérez et al., 2010). The authors concluded that students, especially at the beginning of their studies, do not pay much attention to details when drawing resonance structures (Betancourt-Pérez et al., 2010). In a recent study, Petterson et al. (2020) demonstrated that students struggled to identify the correct place to start the movement of electrons when deriving one resonance structure from another in the context of acid-base reaction mechanisms. Although these results may be explained as knowledge gaps related to the resonance concept, it remains unclear what actually characterizes students' drawing process, i.e., what structural features learners perceptually pay attention to when translating one resonance structure into another, eventually leading to invalid structures and therefore causing wrong or erroneous inferences. Thus, students' ability to decode and manipulate molecular structures requires a more profound analysis to determine the sources of students' success or difficulties while drawing.

Theoretical framework

Representational competence

Learning chemistry includes learning how to effectively use representations such as chemical symbols, diagrams, or ball-and-stick-models to make "sense of the invisible and untouchable" (Kozma and Russell, 1997, p. 949) and, consequently, connect the molecular level to the corresponding macroscopic phenomenon (Johnstone, 1991). Often, multiple representations are combined to facilitate learning and problem solving, as they can either complement each other by offering different perspectives of the given phenomenon, constraint the interpretation of the provided material, or help in constructing a more profound understanding (e.g., by facilitating abstraction) (Ainsworth, 2006). Depending on the coding system of the representations in the working memory channel (i.e., symbolic or analogous), one can differentiate between multiple heterogeneous (i.e., a combination of symbolic and analogous representations) and homogeneous (i.e., either exclusively symbolic or exclusively analogous representations) representations (Ott et al., 2018; Malone et al., 2020). While a heterogeneous representational system in chemistry could be, for example, the combination of a drawn Lewis structure and a ball-and-stick model, a homogeneous system could be the combination of a text and a reaction equation or, more specifically, the depiction of multiple resonance structures. Irrespective of the combination, to profit from (multiple) representations and their synergies for knowledge acquisition and problem-solving, learners need to develop representational literacy (Lesh et al., 1987; Gilbert, 2005; Cooper et al., 2017). This means not only becoming proficient in the use of each representation, but also being able to interrelate corresponding information within and across these different representations and, thus, construct a coherent mental representation of the phenomenon (i.e., local and global coherence formation) (Seufert, 2003; Seufert and Brünken, 2006). Concerning the construction and use of resonance structures, for instance, the relationship between different structures, i.e., how one structure can be transformed into another, and their specific contribution to the overall electronic distribution in a molecule, is crucial.

Based on the comparison of expert and novice representational practices, Kozma and Russell (1997, 2005) defined representational competence by deriving a set of cognitive skills and practices that enable a person to successfully use representations to reason about, express ideas, and create meaning for scientific phenomena. In particular, representational competence encompasses the abilities to (1) use representations to describe observable chemical phenomena and their underlying molecular entities and processes, (2) select or generate a representation and explain its appropriateness for a particular purpose, (3) identify, describe and interpret features of a particular representation, (4) make connections across different related representations by mapping features of one representation onto those of another, and explain the relationship between them, (5) take the epistemological position that representations are modeling but are distinct from the phenomenon observed, (6) evaluate representations by describing limitations and affordances of different representations, and (7) use representations in social situations to support claims, draw inferences, and make predictions about chemical phenomena (Kozma and Russell, 1997, 2005). These skills follow a developmental trajectory, i.e., they develop in sophistication over time. Different proficiency levels can be achieved in varying contexts with different types of representations. For instance, a learner may master most of the skills listed above regarding a particular representation (e.g., Newman projections) but achieve only a low level of representational competence for other representations (e.g., reaction coordinate diagrams) (Kozma and Russell, 2005).

To transform resonance structures into one another, multiple representational skills play a role. First, this transformational process involves analyzing the given starting structure by decoding structural features which have the capacity to delocalize electrons. This skill necessitates a global, holistic view of the structure since the delocalization of electrons can be spread over multiple parts of a molecule and is not limited to a single structural feature. Following this selection process, one structure is translated into another by delocalizing π-electrons and constantly evaluating the hypothetical, resulting structure regarding plausibility and the overall electronic distribution. This can subsequently serve as a basis for predictions of reactions. It becomes evident that the translation in this specific homogeneous representational system does not only require the careful mapping of structural features but crucially depends on the ability to interpret a given structure and possible sources for resonance.

In this regard, the ability to interpret representations further depends on different factors (Schönborn and Anderson, 2008, 2010). According to Schönborn and Anderson (2008, 2010), these factors consist of (1) the external features of the representation (Mode, M), (2) the use of underlying cognitive processes and skills to make sense of a representation (Reasoning, R), and (3) learners' (prior) knowledge of relevant concepts (Conceptual, C). Moreover, these three main factors are intertwined, resulting in four additional factors influencing students' ability to interpret representations. That is the

R-C factor which encompasses students' ability to employ appropriate conceptual knowledge necessary for interpreting the representation, the R-M factor that involves the deciphering and perception of the visual information embedded in the representation, and the C-M factor which describes the propositional scientific knowledge that is transmitted through the explicit features of a representation. This may concern, for example, the complexity and clarity of the representation. Finally, engaging all factors, the C-R-M factor embodies students' ability to successfully interpret a representation by linking their conceptual knowledge to the representational features when decoding information communicated by the representation (Schönborn and Anderson, 2008, 2010). It becomes evident that the interpretation and subsequent construction of resonance structures require a sound conceptual understanding of resonance and highly depend on students' ability to decipher and reason with relevant graphical features of a structural representation. Therefore, the perceptual mechanisms guiding the decoding of the representations and underlying the visuospatial operations when constructing resonance structures must be considered for a holistic characterization of students' approaches when constructing resonance structures.

Mechanisms of visual selection

In order to make sense of the visual information representations convey while organizing and integrating it with prior knowledge and making it subsequently available for higher-order cognitive processes such as reasoning, the visual input has to be filtered to select relevant stimuli (Mayer, 2005; Anderson, 2013). Research on visual search differentiates between three competing mechanisms of visual selection driving the allocation of attention: a stimulus-driven, a goal-driven, and history-driven selection (Awh et al., 2012; Anderson, 2013; Theeuwes, 2019). The stimulus-driven selection is considered a bottom-up process that depends on factors external to the observer, such as the visual salience of the stimulus (e.g., heteroatoms in molecules) that is responsible for the attraction of attention (Theeuwes, 2019). In contrast to that, the goal-driven selection proceeds in a top–down process. Here, the visual search goals and, therefore, the intentional, deliberate control of an observer (e.g., the active search for a specific feature due to rules or prompts) influences the attention to features of a stimulus (Theeuwes, 2019). As a domain-specific prompt or problem task requires where to look or what to attend to, the degree of sophisticated domain knowledge may influence how attention is directed to a given visual input and how it is perceived. In constructing resonance structures, this could be embodied, for example, by carefully examining the fulfillment of the octet rule. The history-driven selection applies when previous experiences drive attentional selection. Thus, information selected in the past affects the way information is selected in subsequent situations. That may encompass, for instance, the probability that features having been repeatedly attended to in the past are more often selected and identified in a given situation (e.g., considering double bonds in the context of resonance structures as they have been often delocalized in previous exercises) (Theeuwes, 2019).

Research questions and hypotheses

Although research indicates that students encounter numerous difficulties when constructing resonance structures and that the construction of resonance structures crucially depends on students' competence to deal with structural formulas in terms of decoding, selecting, and manipulating these representations (Kozma and Russell, 2005; Schönborn and Anderson, 2010), a profound analysis of their drawing processes is still lacking. Supporting students in drawing, therefore, requires a closer look at how students are sequentially generating their drawings. Recording and analyzing the eye-movement trajectories of students can help to characterize to what extent students use and perceive different drawing elements to generate resonance structures and to determine how different gaze patterns may relate to the productivity of the generated drawings. Specifically, by examining students' drawing processes quantitatively and qualitatively, we seek to answer the following research questions (RQ) in this exploratory study:

1. What drawing elements do students connect when constructing productive or unproductive resonance structures (i.e., in terms of transitions and relations of the Areas of Interest)?
2. What structural features do students attend to in terms of attention distribution when translating one resonance structure into another and how is it related to students' drawing moves?
3. How does a student's approach to visual selection to construct resonance structures relate to the productivity of the drawings?

With regard to the first research question, we assume that students with unproductive drawings might exhibit a more varied search behavior, thus, cognitively connect more drawing elements in the construction process, including the use of and the transition between unrelated drawing or task elements. This hypothesis is supported by previous eye-tracking research across different STEM education disciplines as it has been repeatedly shown that successful problem-solvers fixate more on relevant aspects of a representation and generally show a more focused behavior, whereas unsuccessful problem-solvers exhibit a more distributed visual behavior including more fixations on irrelevant aspects of a given representation (Tang and Pienta, 2012; Hejnová and Kekule, 2018; Havelková and Gołębiowska, 2019). In accordance to that, it has been demonstrated that inexperienced individuals more often attend to salient information (i.e., stimulus-driven information selection) that may be irrelevant for task performance. Experienced individuals, on the other hand, efficiently attend to information knowing which information is important for task performance (goal-driven selection) (Jarodzka et al., 2010). Based on the consideration of visual search mechanisms, we assume for the second research question that the construction of unproductive drawings may stem from difficulties to select more specific task-relevant information, such as identifying interacting structural features in a resonance structure, and may result in an overreliance on single, salient structural features. Finally, we assume for the third research question that students who explicitly apply conceptual knowledge to the construction of resonance structures, such as the application of rules or the inference of implicit structural properties, more often construct productive drawings than students whose drawing approach is characterized by a mere rearrangement of surface structural features (Graulich et al., 2019).

Materials and methods

Context and participants

This research study was conducted at a German university in summer 2021. Students were recruited on a voluntary basis via e-mail and in-class announcements in the Organic Chemistry 1 (OC1) course and were given 20 euros as compensation for their time. A total of 21 students agreed to participate in this study. The participants' ages ranged from 19 to 34; nine of them identified as male and twelve as female. One student was excluded from the analysis due to measurement errors, so the number of further analyzed participants was reduced to 20. All students were majoring in chemistry (i.e., they were chemistry, food chemistry, and chemistry teacher students) and were beginners in organic chemistry, i.e., all of them had taken OC1 as the first lecture in organic chemistry either in the second or fourth semester of their studies. Normally, this course consists of a weekly lecture (3 h) and weekly tutorial sections (1.5 h). Due to the pandemic situation, in summer 2021, a flipped format was adopted in which students watched tutorial videos and read material (e.g., book chapters) prior to solving content-related tasks and discussing questions in online tutorial sections. The OC1 course provides basic knowledge of organic chemistry, covers the reactivities of functional groups, deals with structure-property relationships and discusses typical reaction mechanisms (e.g., radical substitution, electrophilic addition, nucleophilic substitution, and carbonyl reactions). The study took place near the end of the course to assure that the students were familiar with the reactions used in this study, the resonance concept, and the construction of resonance structures.

All students who volunteered were informed about their rights and data handling beforehand; informed consent was obtained from all participants. Institutional Review Board approval was not required for this study. Nevertheless, the study followed ethical guidelines and it was clarified to the students that they had the opportunity to opt out at any time. All students gave their written consent for the collected data (i.e., their recordings and scans of their worksheets) being analyzed and published by the research team. In this study, participants were assigned pseudonyms and no identifying information was recorded or scanned to allow participants to re-identify. As the interviews were conducted in German, students' interview excerpts were translated into English for this publication.

Data collection

Study design

The study followed a qualitative approach and used a semi-structured interview to explore both students' reasoning with drawings and students' drawing processes of structural formulas in organic chemistry (**Figure 1**). Before starting the interview, the interviewer explained the interview procedure and briefed the students that the topic of the study would be the resonance concept. In the first section, general questions about the resonance concept (e.g., "When does resonance occur?") have been asked to refresh the students' minds and to gather information on students' abilities to draw resonance structures as well as to infer chemical information from the structural formulas (e.g., "What impact does resonance have on the energy of a structure?"). In the subsequent main section, the students were prompted to solve three organic case comparison tasks (Graulich and Schween, 2018) requiring resonance structures. We used case comparisons to elicit students' drawing process as they necessitate drawing resonance structures in order to solve the given problems and estimate the differences between the two given reactions. All reactions were covered in the OC1 lecture. In the last section, problems with regard to the completion of the tasks as well as students' needs for these types of tasks were addressed in a general reflection.

The subsequent analysis focuses on the third case comparison task as it allows the direct comparison of students' drawings. It describes the mechanistic leaving group departure step of a nucleophilic substitution reaction and asks the students to determine which of the two reactions would form the most stable product. As shown in **Figure 1**, bromide leaves as leaving group under the formation of a carbocation in both reactions. In each case, the substrate is a primary alkyl substrate which

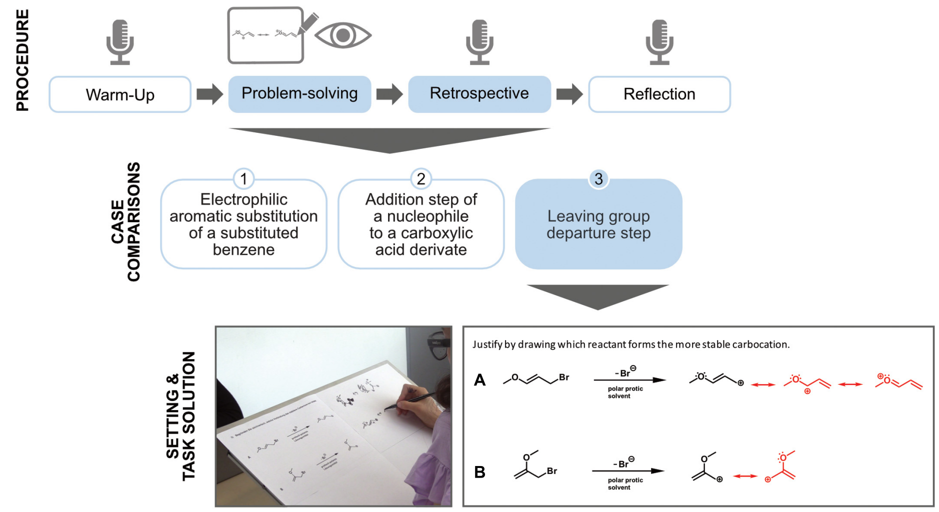


FIGURE 1
Study design and task solution for the utilized case comparison. Blue boxes indicate the results highlighted in this report.

enables stabilization via resonance. Only the position of the methoxy group differentiates the substrates. To determine the most stable carbocation, one has to draw and evaluate the electron density distribution in the resonance structures of both products. While there are two (productive) resonance structures in B, there are three in A. It follows that the positive charge can be better distributed across the whole molecule in A. This is responsible for the lower potential energy and, consequently, for the higher stability of product A.

Qualitative interview

A qualitative semi-structured interview guided the investigation of students' drawing and reasoning process. The interviews were conducted face-to-face between one participant and the interviewer, lasted between 83 and 140 min and were audio- and video-recorded. All materials were administered in a pencil-paper setting and the participants were encouraged to solve all the tasks freely, thus, they could write or draw as much as they considered necessary. To capture students' eye movements in their natural problem-solving behavior, they were not disturbed or had to explain their approach during the completion of the case comparison tasks. However, they were allowed to think aloud if they wanted. After completing each case comparison task, a subsequent retrospective interview focused on students' rationale for their drawings and their task specific problem-solving process. For instance, the students were asked to justify their final choice and to describe their drawing strategies (e.g., "How did you get to this structure?").

Eye-tracking

A mobile eye-tracker (Tobii Pro glasses 3, 50 Hz) served as a tool to capture the participants' eye-movements while drawing during the problem-solving process. To optimize the collection of the eye-tracking data, a drafting table was used and each task was presented on the upper left side of a 42.0 × 59.4 cm (DIN A2) sheet of paper (**Figure 1**). The eye-tracking glasses were calibrated and validated individually for each participant prior to solving the tasks. In case of nearsightedness and farsightedness, suitable corrective lenses were used. A vision test also validated their fit. All gaze samples ranged above 79% (average 91.7%).

Data analysis

Eye-tracking data

Data preparation

First, the gaze data of all participants' recordings during the problem-solving phase, i.e., until the students gave their answers prior to subsequent possible refinements of the drawings, were manually mapped by a trained student research assistant using the software *Tobii Pro Lab*. The first author double-checked the mapped gaze points to check accuracy. Second, for every participant, the Times of Interest (TOI) were defined for each drawing event (i.e., the time sequence until completion of a single student-generated resonance structure). The duration of the overall drawing process for the task varied for each participant ranging from 1.02 to 12.25 min (average 4.06 min). The construction of the single resonance structures took the participants from 6 s to 5.26 min (average 51 s).

Third, the Areas of Interest (AOI) were defined for each drawing event (i.e., every constructed resonance structure until the final decision of the student) for each student. For the subsequent analysis, the AOIs were set on different grain sizes. An AOI was defined for every complete drawing and for smaller parts of the respective molecules, always maintaining the main features of the structures (i.e., the methoxy group, the double bond, and the positive charge) (Figure 2A). All eye-tracking analyses were conducted with the software *Tobii Pro Lab* and *RStudio*.

Furthermore, the students' drawings were classified as productive, unproductive, and auxiliary drawings. While productive drawings encompass all correct resonance structures that help answer the given task, unproductive drawings are either incorrect resonance structures (e.g., violating the octet rule) or drawings that are technically correct, respecting the octet rule, but are, nevertheless, insignificant for this task due to the number of formal charges. The auxiliary drawings are either structures that the students copied from the given task or structures or texts that the students wrote for themselves and were, thus, not directly related to the construction of the resonance structures. They were thus not taken into consideration in the following analysis. Figure 3 provides an overview of the different drawing categories. Next, the data were analyzed in several steps using a combination of quantitative and qualitative approaches.

Examining the connection of drawing elements during the drawing process

To determine how students used the different drawing elements to construct subsequent resonance structures, the analysis of students' gaze behavior was twofold, looking at the structures' co-occurrence during the entire drawing process and the transitions between these structures (RQ 1). In doing so, we grouped all AOIs for each drawing event at a broader grain size into four categories to enable the comparison of the

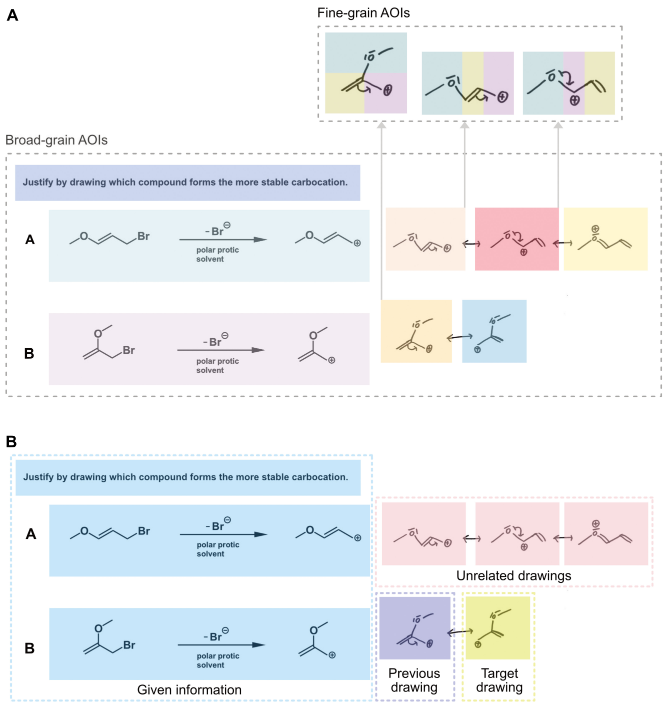


FIGURE 2
(A) Definition of the AOIs of the drawing elements at a broader and finer grain size exemplified by a student solution and **(B)** exemplary categorization of the AOIs in dependence of their function (target drawing, previous drawing, given information, unrelated drawings).

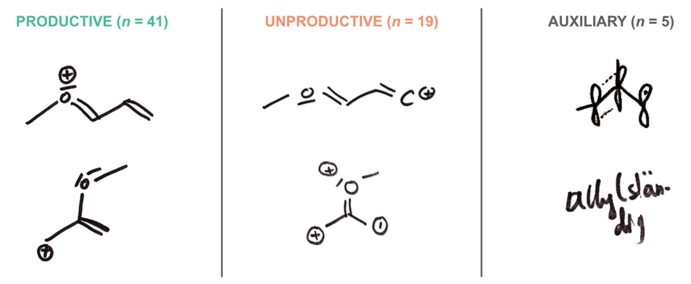


FIGURE 3
Classification categories for the resulting drawings with student examples.

various construction processes of every student: target drawing (T), previous drawing (P), unrelated drawings (U), and given information (G) (cf. **Figure 2B**). While the target drawing is the resonance structure of interest, the previous drawing represents the drawing from which the target drawing results. The given information consists of all the structures and text available to the students in the task prompt. The transformation of one structure into another is carried out at the local structure, i.e., apart from the previous drawing, no other information is necessary in order to construct the target drawing. Therefore, we labeled all the structures and texts that the students might have noted but that are *per se* not necessary for constructing the target drawing (e.g., resonance structures of the product in A when the participant is constructing the resonance structures in B as well as additional explanatory text) as unrelated drawings. Although the given information is neither required for the construction of resonance structures and thus also represents unrelated information, we maintained this category to investigate whether there are tendencies of revisits as anchors when constructing a productive or unproductive drawing.

First, we conducted an Epistemic network analysis (ENA) to examine the co-occurrence of the various drawing elements during the construction of resonance structures and, thus, to explore different gaze patterns depending on the resulting productivity of the drawing. The ENA is an analytical method from the field of learning analytics, which has been used in numerous contexts, including eye-tracking analyses (Andrist et al., 2015; Shaffer et al., 2016; Bruckner et al., 2020). This method can be used to identify and quantify the structure of connections among coded data elements in any system by representing their associations in networks, i.e., the mere presence of isolated elements is not as important as their interrelations (Shaffer et al., 2016). Thus, the ENA allows the characterization of even complex and dynamic relationships (e.g., patterns of association within discourse or gaze behavior) by illustrating both the structure and the strength of connections in both single networks (e.g., in terms of their plotted point position) and network difference graphs which illustrate the differences between two networks by subtraction (Shaffer et al., 2016; Shaffer and Ruis, 2017). While the nodes in the network correspond to the analyzed codes and appear in every modeled network in exactly the same position, the edge width between the nodes reflects the relative frequency of co-occurrences between two codes. In order to model the connections, ENA uses a singular-value decomposition which performs dimensional reduction on a high-dimensional space, producing fewer dimensions that capture the maximum variance in the data (Shaffer et al., 2016).

In our analysis, we used the *ENA Web Tool* (version 1.7.0) to compare the weighted epistemic networks of the construction processes of productive and unproductive drawings on the basis of students' collapsed AOI hit sequences during the construction of resonance structures. To this end, each drawing served as a *unit*, i.e., the piece of data for which the ENA constructs networks. *Conversations* indicate how to segment the data for analysis in terms of their relation to one another, i.e., *units* not in the same *conversation* are not related to one another in the network model. As we aimed at characterizing the drawing process of each resonance structure individually, again, we chose as *conversation* every drawing and chose the mode *whole conversation* so that the ENA modeled connections across the entire *conversation*. In the ENA, the nodes of the network represent the *codes*. In order to be able to compare the various drawing processes, our *codes* comprised the previously defined categories "given information," "unrelated drawings," "previous drawing," and "target drawing" for every drawing event. Finally, as *comparison* served the productivity of the drawings, i.e., we differentiated between productive and unproductive drawings.

In a second step, the same AOI hit sequences used in the ENA beforehand were analyzed to determine the transitions between individual pairs of AOIs that the students made to construct resonance structures in order to reveal how students integrated the various drawing elements (i.e., the defined four drawing categories) when constructing structural formulas

(Schmidt-Weigand et al., 2010; Johnson and Mayer, 2012). For that purpose, we used the *GrpString R package* (Tang et al., 2018) to calculate the transition matrix, the transition entropy and the total amount of transitions across the groups of unproductive and productive drawings, regardless of whether the drawings resulted from a previously productive or unproductive drawing as no discriminating differences could be found in a finer division. The transition entropy indicates the diversity of the transitions within a string or different string groups. While a higher entropy reflects more evenly distributed transitions, a lower entropy measure indicates a more biased distribution of transitions, mainly reflecting transitions between fewer AOIs (Tang et al., 2018). The transition matrices were also explored for statistical significance using the Mann-Whitney *U* test. A non-parametric test was chosen because a Shapiro-Wilk test ($p < 0.05$) indicated that not all of the data to be used for comparison are normally distributed (Shapiro and Wilk, 1965).

Analyzing the attention distribution while constructing resonance structures

To gain deeper insight into the translation process of single resonance structures, the analysis further concentrated on the connection of each drawing pair, i.e., the previous and target resonance structure (RQ 2). As the attention distribution may indicate the ascribed importance of a representation (Cullipher and VandenPlas, 2018), we examined the total fixation duration of the AOIs of the previous drawing to which students attended when constructing the target resonance structure. In doing this, we used the AOIs at the smaller grain size encompassing the different structural features of the respective previous resonance structure (cf. **Figure 2A**). With this data, we then calculated the ratio of attention distribution on each structural feature of the previous resonance structure. Again, we differentiated between productive and unproductive drawings for all drawings to examine possible differences in attention distribution.

Qualitative data

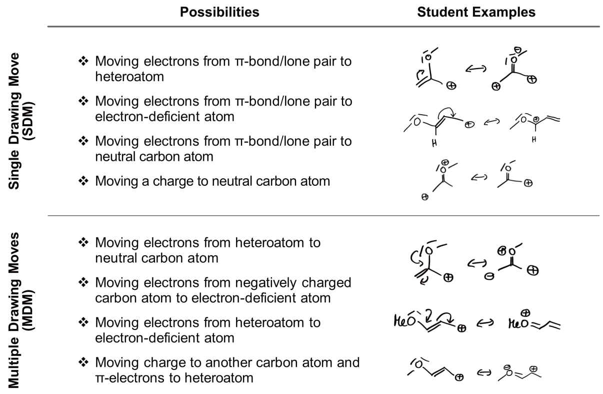
Determining the relationship between drawing moves and attention distribution while constructing resonance structures

To relate and compare the attention distribution to students' drawing moves for possible relationships (RQ 2), students' drawing moves made to get from one structure to the next one were inductively analyzed (i.e., the delocalization of electrons and change of the structural features). Different drawing moves could be identified which can be subsumed either as single drawing move (e.g., delocalizing one electron pair or charge) or as multiple drawing moves (e.g., delocalizing several electron pairs) (**Figure 4**).

The first author coded all drawings. Additionally, a trained student research assistant coded the entire data independently with the code book. A kappa coefficient κ_n of 0.87 (Brennan and Prediger, 1981) was calculated, showing high agreement and reliability for the coding rubrics (Kuckartz and Rädiker, 2019). Any ambiguities were discussed and resolved to reach a final agreement of 100%.

Characterizing students' approaches of visual selection

All audio recordings of the interviews were transcribed verbatim and implemented into the coding software *MAXQDA* for subsequent qualitative content analysis (Saldaña, 2016). To examine students' approaches of visual selection when constructing resonance structures and, consequently, triangulate the eye-tracking data findings, our qualitative

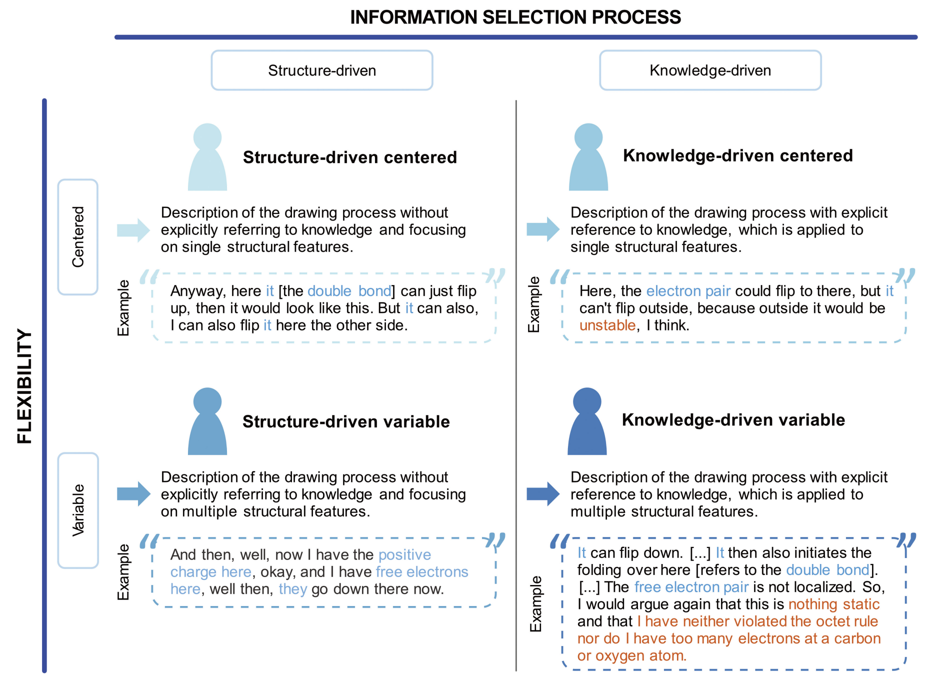


	Possibilities	Student Examples
Single Drawing Move (SDM)	❖ Moving electrons from π-bond/lone pair to heteroatom ❖ Moving electrons from π-bond/lone pair to electron-deficient atom ❖ Moving electrons from π-bond/lone pair to neutral carbon atom ❖ Moving a charge to neutral carbon atom	
Multiple Drawing Moves (MDM)	❖ Moving electrons from heteroatom to neutral carbon atom ❖ Moving electrons from negatively charged carbon atom to electron-deficient atom ❖ Moving electrons from heteroatom to electron-deficient atom ❖ Moving charge to another carbon atom and π-electrons to heteroatom	

FIGURE 4
Coding scheme for drawing moves with student examples.

analysis centered on how students verbally described their drawing process (RQ 3). The analysis was informed by the theory of visual selection described in section "Mechanisms of visual selection" (Theeuwes, 2019). However, we could not adopt the three different mechanisms of visual selection as codes due to different reasons. First, the problem-solving process in this study, as a whole, is clearly a top–down process because the participants knew that they had to use the resonance concept to solve the task and, consequently, to draw resonance structures by moving electrons within structural formulas. Therefore, the task demands by definition a goal-driven approach to construct the resonance structures. Second, it is not possible to properly distinguish between a stimulus-driven, history-driven, and goal-driven approach in many chemistry contexts, because reasoning and sense-making often depend on the interplay of deriving and perceiving explicit and implicit structural features and properties (Graulich et al., 2019). Students can exhibit both a bottom–up and top–down approach. Therefore, we adapted the aforementioned mechanisms into two categories which we applied as a lens to analyze students' descriptions of their drawing approach: a knowledge-driven approach and a structure-driven approach. The code "structure-driven" was ascribed whenever the students described their drawing process by only referring to and mentioning the explicitly drawn structural features. Thus, it can be considered a bottom–up process resembling the stimulus-driven approach. The code "knowledge-driven" was given when the students explicitly used and verbalized their knowledge to construct the respective resonance structure. This may include different kinds of knowledge, e.g., experiences or concept knowledge such as the reference to (implicit) chemical concepts (e.g., stability), or rules (e.g., the octet rule). Therefore, this approach can be considered a top-down process that resembles the goal-driven and history-driven approach.

Moreover, we characterized the flexibility of students' approaches. While a "centered" approach applies when students were focusing on one structural feature (e.g., the methoxy group of the molecule), students with a "variable" approach described their drawing process by taking into account the entire structure or at least several interacting structural sections of the starting



Structure-driven centered: Description of the drawing process without explicitly referring to knowledge and focusing on single structural features.

"Anyway, here it [the double bond] can just flip up, then it would look like this. But it can also, I can also flip it here the other side."

Knowledge-driven centered: Description of the drawing process with explicit reference to knowledge, which is applied to single structural features.

"Here, the electron pair could flip to there, but it can't flip outside, because outside it would be unstable, I think."

Structure-driven variable: Description of the drawing process without explicitly referring to knowledge and focusing on multiple structural features.

"And then, well, now I have the positive charge here, okay, and I have free electrons here, well then, they go down there now."

Knowledge-driven variable: Description of the drawing process with explicit reference to knowledge, which is applied to multiple structural features.

"It can flip down. [...] It then also initiates the folding over here [refers to the double bond]. [...] The free electron pair is not localized. So, I would argue again that this is nothing static and that I have neither violated the octet rule nor do I have too many electrons at a carbon or oxygen atom."

FIGURE 5
Coding scheme for students' visual selection approaches with definitions and student examples. The highlighted blue text in the quotes indicates the structural features the students referred to, while the orange text highlights the verbalized knowledge (e.g., rules and chemical concepts).

molecule. **Figure 5** provides the definitions of the resulting four codes and illustrates them by giving student examples for each coding category.

The first author coded the entire data set. During the data analysis, the authors regularly discussed and optimized the coding scheme to ensure that coding decisions faithfully represented the data. For interrater reliability, the second author coded a random sample of 20% of the data independently. A kappa coefficient κ_n of 0.94 (Brennan and Prediger, 1981) was calculated, indicating high agreement and reliability for the coding rubrics (Kuckartz and Rädiker, 2019). Any ambiguities were discussed and resolved. In the end, a 100% agreement between the two authors was reached.

Results and discussion

Of all 60 student-generated resonance structures, 41 drawings were productive, whereas 19 were unproductive, often resulting from previously productive drawings or building a sequence of unproductive resonance structures. Therefore, it is of interest to characterize what distinguishes the construction process of productive from unproductive drawings. Using a Mann–Whitney *U* test, we compared the construction of productive and unproductive drawings on the basis of different eye-tracking data (**Table 1**). Addressing our research questions, the subsequent sections present and discuss the main findings.

RQ 1: What drawing elements do students connect when constructing productive or unproductive resonance structures?

On a global level, students exhibit a similar gaze behavior when using information from different drawing elements to construct productive or unproductive resonance structures. In fact, as the mean epistemic networks of productive and unproductive drawings illustrate (**Figures 6A,B**), the co-occurrences of the different drawing categories (i.e., target drawing, previous drawing, unrelated drawings, and given information) appear with a similar density and show, in general, no considerable differences concerning the type and frequency of connections.

Consistent with this observation, a Mann–Whitney *U* test showed that neither along the *x*-axis (MR1) nor the *y*-axis (SVD2) productive drawings differ significantly from unproductive drawings (**Table 1**). From a qualitative perspective, the association between the previous drawing and the target drawing dominates in both groups. Comparing the different networks for productive and unproductive drawings, represented by the position of the respective network graph node (**Figure 6C**), no distinctive tendency concerning the patterns of co-occurrence of the drawing elements can be inferred. This result indicates that the construction of an (un-)productive resonance structure does, thus, not globally depend on the resulting network, i.e., the amount and density of associations of the different drawing elements. Hence, our hypothesis of unproductive drawings resulting from the connection of more drawing elements cannot be confirmed. However, the subtracted mean network (**Figure 6C**) shows that there exist differences concerning single connections. Students with productive drawings (green color) exhibit a stronger association of the previous and target drawing, whereas students with unproductive drawings (orange color) show more associations of the unrelated drawings with both the target drawing and the previous drawing. This indicates that using unrelated information seems to play a bigger role when constructing unproductive structural formulas. The subtracted mean network also illustrates that in both groups, the associations between the other drawing elements are altogether

TABLE 1 Results of the Mann–Whitney *U* test for different eye-tracking data comparing the construction of productive and unproductive drawings.

Variable	$Mdn_{pr.}$	$Mdn_{unpr.}$	U	z	p^a	r^b
Connection of AOIs (ENA)						
x-axis/MR1	-0.12	0.13	497.50	2.169	0.09	0.28
y-axis/SVD2	-0.32	-0.37	359.20	−0.620	0.64	0.08
Transitions						
Absolute number	15	17	378.5	−0.175	0.861	0.02
Entropy	1.96	2	342.5	−0.747	0.455	0.10
Transition types						
GU	0	0	384	−0.141	0.888	0.02
GP	0.053	0.067	363.5	−0.439	0.661	0.06
GT	0	0	359	−0.78	0.435	0.10
UG	0	0	386.5	−0.066	0.947	0.01
UP	0	0.029	367	−0.388	0.698	0.05
UT	0	0	252.5	−2.797	**0.005**	0.36
PG	0	0	367.5	−0.377	0.706	0.05
PU	0	0	371.5	−0.377	0.706	0.05
PT	0.33	0.24	262	−2.028	**0.043**	0.26
TG	0	0	378	−0.328	0.743	0.04
TU	0	0	266.5	−2.637	**0.008**	0.34
TP	0.29	0.16	249	−2.236	**0.025**	0.29
Fixation duration rate						
Relevant features	0.78	0.50	188	−3.212	**0.001**	0.41
Unrelated features	0.22	0.50	591	3.212	**0.001**	0.41

Significance level of 0.05 and confidence interval of 95%; pr., productive; unpr., unproductive; $N = 60$; ^{a}Significant *p*-values (<0.05) are displayed in bold. ^{b}Calculated as indicated by Rosenthal (1984).

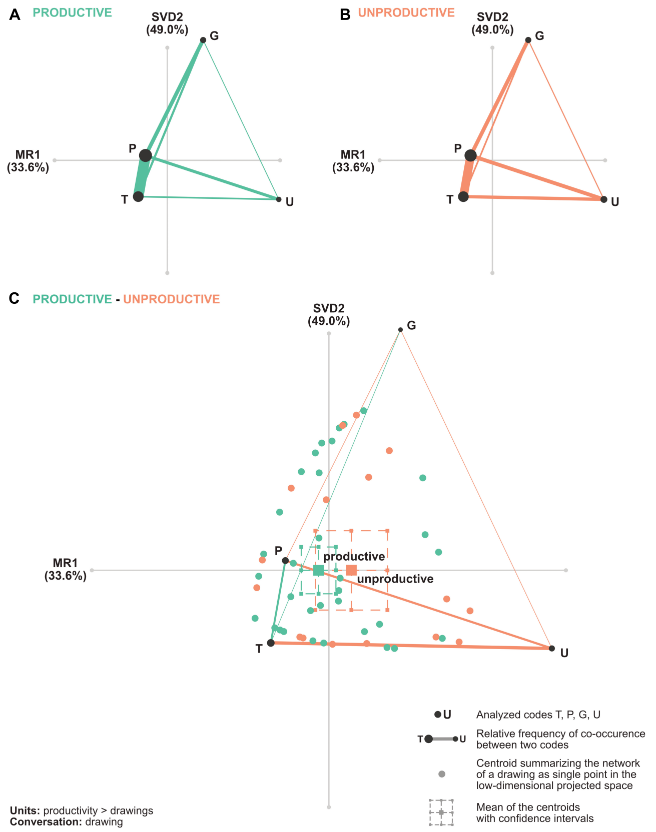


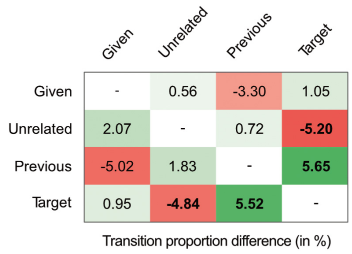
FIGURE 6
Epistemic network for **(A)** productive drawings, **(B)** unproductive drawings, and **(C)** the subtracted epistemic network of productive and unproductive drawings using the collapsed AOI hit sequences during the construction process of every drawing (*N* = 60). The drawing categories (T, target drawing; P, previous drawing; G, given information; U, unrelated drawings) serve as codes.

scarce and that the given information rarely co-occurs with the other drawing elements.

Although the ENA models the gaze-pattern networks of the different construction processes of (un-)productive drawings by depicting the weighted frequency of co-occurrences of the different drawing elements, it provides no insight into the direction of linkage, i.e., transitions, between those elements (e.g., in terms of backtracking). The ENA only depicts how often drawing elements co-occur altogether. However, transitions play a crucial role when processing information (Schmidt-Weigand et al., 2010). Thus, analyzing the linkage direction may also reveal differences regarding the direct connection of drawing elements, such as integrating information to construct productive and unproductive drawings.

A look at the different transitions during the drawing process of the resonance structures reveals that in general, in accordance with the ENA, the transition entropy for productive or unproductive resonance structures does not differ significantly (**Table 1**), thus, the gaze transition distribution is similar for both groups. Neither does the absolute number of transitions differ significantly. However, as listed in **Table 1**, there are significant differences between the types of transitions during the drawing process of a productive and unproductive drawing regarding the transitions to the target drawing.

Figure 7 depicts the subtracted transition matrix of productive and unproductive drawings with green cells indicating transitions more characteristic for productive drawings. In contrast, red cells show transitions rather occurring



	Given	Unrelated	Previous	Target
Given	-	0.56	-3.30	1.05
Unrelated	2.07	-	0.72	**-5.20**
Previous	-5.02	1.83	-	**5.65**
Target	0.95	**-4.84**	**5.52**	-

Transition proportion difference (in %)

FIGURE 7
Subtracted transition matrix indicating characteristic transitions regarding the construction of productive (green cells) and unproductive drawings (red cells); significant differences in transition types are displayed in bold (*p*-value of < 0.05).

with unproductive drawings. According to **Table 1**, it becomes evident that the drawing process of productive resonance structures encompasses significantly more transitions between the previous drawing and the target drawing ($p = 0.043$, $r = 0.26$) and vice versa ($p = 0.025$, $r = 0.29$). In comparison, the drawing process of unproductive drawings comprises more transitions between the target drawing and unrelated drawings ($p = 0.008$, $r = 0.34$) and vice versa ($p = 0.005$, $r = 0.36$). **Figure 7** shows as well that students with unproductive drawings connect the given information with the previous drawings more often than students who construct productive drawings. However, the difference of this transition type is statistically not significant. Given that transitions play a crucial role in the integration and processing of information (Schmidt-Weigand et al., 2010; Johnson and Mayer, 2012), an increased integration of unrelated information can impede the construction of valid resonance structures. In fact, integrating more information in the target drawing by focusing on diverse, less relevant, drawing elements, can indicate searching processes and uncertainty. That said, it is possible that learners try to align and transfer information from previous drawing processes or search for anchor points. This assumption is in line with previous research on problem-solving and the comprehension of visualizations (e.g., Gegenfurtner et al., 2011; Tang et al., 2014). For instance, Holmqvist et al. (2011) showed in the context of a mathematical problem-solving task that participants with low ability tended to scan all AOIs in the tasks while high-ability participants exhibited a more focused behavior. Existing research in STEM education also supports the finding that students' drawing process of productive drawings is characterized by more direct transitions from previous to target drawing. Therefore, multiple studies show that high-performing participants (e.g., experts) more effectively process information, e.g., by transitioning between relevant parts of tasks (Baluyut and Holme, 2019; Connor et al., 2021), by efficiently attending to task-relevant features (Jarodzka et al., 2010; Tang and Pienta, 2012; Topczewski et al., 2016; Hejnová and Kekule, 2018; Havelková and Gołębiowska, 2019), or by exhibiting a more focused searching behavior when problem-solving (Holmqvist et al., 2011; Rodemer et al., 2020).

However, despite the group-specific differences in transitions, the connection between the previous drawing and the target drawing overall plays a major role in students' construction process of resonance structures. This suggests that the students in this study already possess a distinct representational fluency concerning the direct translation from one representation into another. With regard to representational competence, as described by Kozma and Russell, students with productive and unproductive representations show similar abilities to identify and select structures necessary to transform a resonance structure into another (Lesh et al., 1987; Kozma and Russell, 1997, 2005).

RQ 2: What structural features do students attend to in terms of attention distribution when translating one resonance structure into another and how is it related to students' drawing moves?

Since all students mainly connected the previous and the target drawing when constructing productive and unproductive resonance structures, it is of interest to investigate students' attention distribution when translating one structure into another, and thus, to consider their fixation duration on the different parts of the starting molecule, the previous drawing, in order to characterize their decoding behavior (R-M factor) (Schönborn and Anderson, 2008, 2010).

Figure 8 illustrates the fixation duration rate for the construction of productive and unproductive resonance structures on the basis of productive, initial drawings (57 of 60 drawings). Due to their very specific and individual character, **Figure 8** does not comprise the remaining three structures resulting from unproductive drawings. The frames of the respective pie charts indicate the adjacent parts of the molecular structure which are relevant for translating this structure into the corresponding productive structure. As **Figure 8** illustrates, the fixation duration rate differs with regard to the constructed structures, showing an emerging attention distribution difference on different parts of the molecules when constructing productive or unproductive drawings. As indicated in **Table 1**, the fixation duration rate of relevant and unrelated structural features for productive and unproductive drawings differ significantly with medium effect size (relevant features: $p = 0.001$, $r = 0.41$; unrelated features: $p = 0.001$, $r = 0.41$). For the productive resonance structures, a slight trend emerges toward an increased attention to the relevant structural features for the resulting resonance structure. If we consider the productive subsequent resonance structures A1

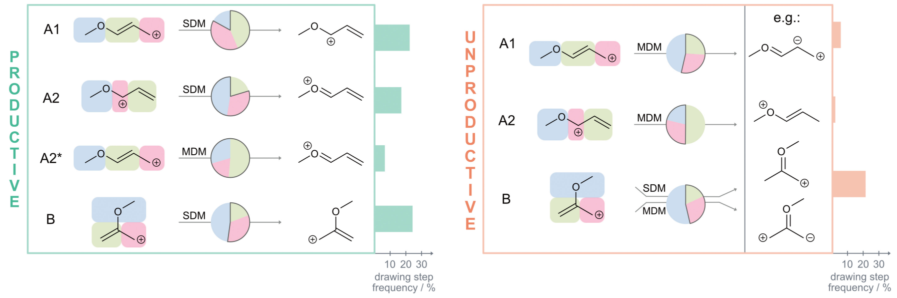


FIGURE 8
Relative drawing step frequency (*N* = 57) and fixation duration rates (pie charts) on the structural features of the initial structures (blue = methoxy group, green = double bond, pink = positive charge) when constructing a subsequent productive (green frame) or unproductive (orange frame) structure. The relevant, necessary structural features for the construction of the following structure are highlighted by framing. Drawing moves are indicated as single drawing move (SDM) and multiple drawing moves (MDM).

and A2, students who construct these structural formulas on average focused more on the interrelated structural features necessary for the construction of the respective structure, i.e., on the positive charge and the double bond in the first structure (83% of the attention distribution), and the positive charge and the methoxy group in the second structure (80% of the overall attention distribution). To draw the productive structure A2* on the basis of the given, initial product in A, thus, skipping the second structure, students have to consider every part of the structural formula as electrons are delocalized throughout the whole molecule. However, it becomes apparent that students' attention was guided by the double bond and the methoxy group (altogether 81%) and less by the positive charge (19%) that, however, represents a productive starting point for the drawing process.

Figure 8 further illustrates that few students constructed unproductive drawings in reaction A, while most unproductive drawings resulted when constructing resonance structures in reaction B. In general, it can be derived from **Figure 8** that unproductive drawings stem from a higher attention to unrelated structural features. For example, consider the attention distribution of the unproductive structure A1. In contrast to the productive structures A1 and A2, students shifted their attention more to the methoxy group (46%). In the unproductive structure A2, students payed their attention twice as often to the unrelated double bond (50%) whereas the structural features that are relevant for the construction of a productive structure (i.e., the methoxy group and the positive charge), were considered less (50%) compared to when students constructed a productive structure based on the same initial drawing. This trend of overly considering unrelated structural features while paying less attention to relevant, interacting structural features also applies to the unproductive resonance structures in B as students paid much attention to the methoxy group. However, here, the fixation durations rates do not differ as much from those that students exhibit when generating productive resonance structures in B. Regarding representational competence, it can be derived from these findings that although students are able to identify and connect relevant structures in order to construct subsequent resonance structures (Kozma and Russell, 2005), they differ in the decoding and interpretation of the representations by paying attention to different structural features. Consequently, they may perceive the external features of a structure differently (R-M factor), eventually resulting in unproductive drawings (Schönborn and Anderson, 2008, 2010).

Besides the attention distributions, **Figure 8** depicts the drawing moves the students made to construct their drawings. In this task, productive drawings often stem from a single drawing move where electrons are delocalized toward an electron-deficient atom. As **Figure 8** shows, students predominantly focus thereby on two adjacent, interrelated structural features, that is, the positive charge and the adjacent double bond or methoxy group. In contrast to that, students who perform multiple drawing moves construct either unproductive resonance structures, or draw a productive resonance structure but tend to skip a structure, which, however, would be necessary to answer the given task. Altogether, 13 of the 19 unproductive drawings are based on multiple drawing moves which may either involve arbitrarily moving charges, moving the lone pairs of the heteroatom throughout the whole molecule or moving electrons to an electron-rich atom (cf. **Figure 4** for examples).

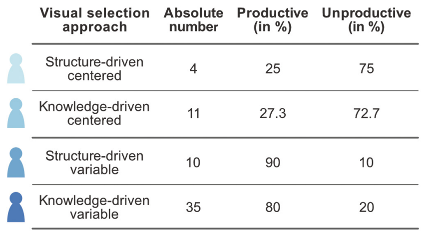
While there is a clear difference with respect to the fixation duration rate in the structures of reaction A, the gaze proportion on structures in reaction B does not differ much. Hence, our hypothesis for the second research question, that the construction of unproductive drawings results from difficulties in the selection of relevant information and, eventually, an overreliance on single, salient structural features, can only be partly confirmed. This lack of difference for reaction B may be due to different reasons. First, the different geometries of the molecules can be responsible for a different decoding behavior. While the molecules in reaction A are linear, the molecule in B is more branched, thus, spatially more complex. Following this, the decoding of the molecule and the identification of interacting structural features could have been cognitively more demanding and may have led to longer fixations of the methoxy group in order to decide upon its possible influence in the structure. In fact, a longer fixation on a structural feature correlates with longer mental processing of this information (Just and Carpenter, 1980), which may result from difficulties in interpretation or due to the perceived importance of the feature because of its salience (Cullipher et al., 2018). As students in both groups fixated much on the methoxy group, it may be that this structural feature was more difficult to interpret than the double bond, since a functional group containing an oxygen atom can have an electron-donating or electron-withdrawing function depending on its connectivity. Therefore, students may have tried to connect this feature with prior knowledge such as rules concerning its electronic effects (R-C factor) (Schönborn and Anderson, 2008, 2010). Our findings of students' varying decoding and use of structural features when constructing resonance structures align with existing research on representational competence in chemistry. While it has been shown that students often exhibit difficulties regarding the comprehension and interpretation of representations (e.g., Keig and Rubba, 1993; Kozma and Russell, 1997; DeFever et al., 2015), more specifically, Olimpo et al. (2015) have shown that the translation of Newman projections and Dash-Wedge representations is easier for students when dealing with less complex molecules. Moreover, using eye-tracking, in Baluyut and Holme's (2019) study it became evident that the visual complexity of particulate nature of matter diagrams impacted students' viewing behavior as low-performing students fixated on more features of a task when working with such representations. Rodemer et al. (2020), on the other hand, showed that visual characteristics seem to influence students' visual processing and problem-solving in organic chemistry, with more factors embedded in a case comparison leading to more transitions between representations.

Besides the higher spatial complexity, familiarity may also play a crucial role regarding students' gaze behavior in case of the linear structures in reaction A. Both the allylic position of the carbocation and the linearity of the molecule are familiar to the students from the lecture. Therefore, it is possible that students felt more confident in decoding the structures and, consequently, could determine relevant, interacting structural features more easily, narrowing their gaze distribution on specific parts of the whole structure.

Finally, focusing on several, interacting structural features instead of statically attending to singular structural features is in accordance with the concept of resonance, requiring a global, dynamic view on the static structural formulas with keeping different structural features in mind in order to construct valid resonance structures (Nakhleh, 1992). Therefore, a predominant focus on singular (salient) structural features often leads to drawing mistakes (Cooper et al., 2010). Although familiarity and geometry may explain differences in the gaze distribution, fixations on structural features alone do not suffice to characterize productive and unproductive approaches when dealing with spatial complex molecules. For this reason, students' explanations of their drawing approach need to be taken into account.

RQ 3: How does a student's approach to visual selection to construct resonance structures relate to the productivity of the drawings?

Different visual selection approaches for the construction of resonance structures could be identified through students' verbal explanations for their drawings, which differ regarding the information selection approach (knowledge-driven or structure-driven) and the flexibility of these approaches (centered or variable). Thus, four categories can be distinguished: structure-driven centered, structure-driven variable, knowledge-driven centered, and knowledge-driven variable (**Figure 5**). **Figure 9** provides an overview of the absolute number of these approaches used for structure construction and the success rate for constructing a productive drawing. It can be derived from this table that about half of the drawings were constructed via a knowledge-driven variable approach, while only four drawings result from a structure-driven centered approach. Moreover, it can be seen that, contrary to our initial hypothesis, not a structure-driven or knowledge-driven approach, i.e., the explicit application of conceptual knowledge (Graulich et al., 2019), decides upon the productivity of the resulting drawing, but rather the



Visual selection approach	Absolute number	Productive (in %)	Unproductive (in %)
Structure-driven centered	4	25	75
Knowledge-driven centered	11	27.3	72.7
Structure-driven variable	10	90	10
Knowledge-driven variable	35	80	20

FIGURE 9
Absolute distribution and success rate of the different visual selection approaches.

flexibility of this approach, i.e., whether students focus on single structural features or take multiple structural features into account. At least 80% of the drawings with a variable approach are productive, whereas the amount of productive drawings reduces to under 30% if a centered approach has been used. In accordance with the results in the previous section, this shows that, besides being able to use resonance-related knowledge in the construction process (R-C factor), the success of constructing resonance structures heavily relies on students' overall ability to decode the structural formulas (R-M factor) (Schönborn and Anderson, 2008, 2010). How these four approaches influence the construction of resonance structures and how they are related to the drawing moves, can be illustrated by taking a closer, exemplary look at descriptions of students' drawing processes.

Nina, for instance, generated all her drawings for reaction A and B following a knowledge-driven centered approach (**Figure 10**), eventually resulting in unproductive structures, as the oxygen atom does not fulfill the octet rule, missing a positive charge on the oxygen atom in both cases. While expressing cluelessness about how to construct the resonance structures at first, Nina describes both her drawings by referring to experiences of delocalizing electrons of the oxygen atom as done in previous tasks. Therefore, the oxygen atom serves as an anchor guiding the drawing process and leading to multiple drawing moves, each starting from the oxygen atom and initiating the subsequent delocalization of the π-electrons of the double bond. As for the resonance structure in reaction A, she consequently misses a structure, which is, however, crucial for answering the task. Interestingly, while the initial positive charge remains unchanged in both structures, she creates a new, negative charge in each structure. The anchoring function of the oxygen atom at the extent of neglecting the other, more relevant structural features of the positive charge and double bond is also reflected in her attention distribution concerning the different structural features of the starting molecules in reaction A and B. **Figure 10** shows that Nina spends about 70% of the fixation time on the methoxy group in reaction A. In reaction B, she almost exclusively (95%) focuses on the methoxy group, not paying attention to the double bond.

A similar knowledge-driven centered approach can be seen in Catherine's drawing process of the resonance structure in reaction A as she centers the drawing process description solely on the function of the oxygen atom (**Figure 11**). As Nina, Catherine explains her drawing approach by emphasizing that the oxygen atom must participate in generating resonance structures due to the lone pairs that could be delocalized. This utterance shows that Catherine employs an overgeneralized rule (McClary and Talanquer, 2011) guiding her drawing process and making the oxygen atom her starting point for the construction. Therefore, her prior knowledge, i.e., the R-C factor, mainly drives the interpretation of the structural formula and the constructing of the resulting resonance structure (Schönborn and Anderson, 2008). Similar to Nina, this results in multiple drawing moves involving the delocalization of electrons of the oxygen atom across the double bond to form another double bond. While the positive charge remains unchanged at the carbon atom, the oxygen atom does not carry a charge, thus, resulting in an unproductive drawing. However, Catherine's fixation duration rate does not clearly reflect her drawing strategy (**Figure 11**). Despite spending much time on the methoxy group, Catherine also takes the double bond

I'll just do something now [...]. *Yes, so theoretically it could be like that, I don't know if that's logical somehow, but okay, just before, I also flipped something over from the oxygen, and if I would do that just like that now, then I would theoretically have something like that* [draws the resonance structure in A]. *And in the other case* [refers to reaction B], *if I did it the same way, then it would look something like this* [points to resonance structure in B]. *I don't know if that's right and if that helps me at all, but it's somehow the only thing I can think of doing right now. [...] But yes, with what has somehow stuck in my mind from the previous tasks, it should actually theoretically work like this.*

FIGURE 10
Nina's drawing moves, fixation duration rates on the structural features and drawing description for her drawings in reaction A and B. The orange frame indicates the unproductivity of the resulting drawings.

If oxygen has two lone pairs, then it can be assumed that it does something with them, or that resonance structures can be formed.

FIGURE 11
Catherine's drawing move, fixation duration rate on the structural features and drawing description for her drawing in reaction A. The orange frame indicates the unproductivity of the resulting drawing.

and positive charge into account, showing that she somewhat considered the whole molecule for the construction process.

In contrast to these examples, Elizabeth has a structure-driven centered approach to the construction of the resonance structure in reaction B (**Figure 12**). Similar to the other students, she centers her drawing description only on the double bond as single structural feature after having tried to form a carbon–oxygen π-bond. Elizabeth's approach illustrates a trial-and-error strategy (Ahmad and Omar, 1992), as she decides to delocalize the π-electrons of the double bond to the oxygen atom after struggling to move the electrons in the inverse direction. Although it becomes clear that she considers both structural features, as reflected in the fixation duration rates (**Figure 12**), she does not consider them in an interrelated manner but rather focuses on these structural features successively as singular entities. In Elizabeth's case, this approach results in a single drawing move through which additional charges are generated, and the oxygen atoms clearly breaks the octet rule. Interestingly, neither in her description nor in the fixation duration rate, the positive charge gets much attention. Therefore, she does not see the positive charge as a prerequisite for resonance in this task, but rather approaches such drawing tasks by considering electron-rich features, as she stated: *I guess lone pairs are also an indication for me that you can apply resonance*, *not only double bonds*, *but also lone pairs.*

So far, the centered approach shows that students justify their drawing processes by only referring to single structural features at the extent of neglecting other features within a molecule and considering single structural features as an anchor leading the entire drawing process. Many studies in STEM education research support our finding, that this anchoring function may be due to overgeneralized rules and heuristics, eventually causing algorithmic or arbitrary unproductive drawing steps and hindering the analysis of the given structure as a whole. In chemistry education, it has been shown that students are prone to focus on familiar and surface features, which eventually negatively impacts their problem solving (Kozma and Russell, 1997; Kraft et al., 2010; Anzovino and Bretz, 2015; Graulich and Bhattacharyya, 2017; Graulich et al., 2019) and supports their reliance on heuristics (McClary and Talanquer, 2011; Weinrich and Talanquer, 2015). Similarly, Inglis and Alcock (2012) have shown in the context of reading mathematical proofs that compared to mathematicians, undergraduate students spend more time focusing on surface features of an argument, i.e., they attend less to its logical structure.

In addition, these results may complement existing findings concerning the construction of structural formulas. As Ahmad and Omar (1992) and Cooper et al. (2010) stated, students often exhibit a trial-and-error approach or rely on memorized cues in drawing, which may result from the overreliance on singular structural features. Such a structural overreliance in the interpretation of structural representations (Schönborn and Anderson, 2008) may also offer a possible reason for the observed drawing difficulties of resonance structures reported by Betancourt-Pérez et al. (2010) and Petterson et al. (2020).

In contrast to the centered approach, the variable approach is characterized by a more holistic approach to the drawing process of different resonance structures. Students showing this approach take multiple, interrelated drawing features into account. For instance, consider Paula's approach in reaction A (**Figure 13**).

Paula exhibits a structure-driven approach by merely referring to interacting structural features, i.e., the positive charge in both resonance structures and the electron-rich double bond or the lone pairs of the oxygen atom. However, in

Okay, if that does not work, I flip the double bond up [refers to the oxygen atom] *so that there is a negative charge here* [refers to the oxygen atom] *and a positive charge here* [refers to the carbon atom].

FIGURE 12
Elizabeth's drawing move, fixation duration rate on the structural features and drawing description for her drawing in reaction B. The orange frame indicates the unproductivity of the resulting drawing.

So here, I have the positive charge [points to the provided product in reaction A]*, then I flipped* [the double bond] *over here* [points to the positive charge] *so that the positive charge is created here* [refers to the newly created carbocation]. [...] *Then, here are the two* [free electron pairs of the oxygen atom] *and then one of them flips over again to the positive charge and makes the next double bond, and thus, the positive charge is at the oxygen atom* [refers to the second structure in reaction A].

FIGURE 13
Paula's drawing moves, fixation duration rates on the structural features and drawing description for her drawings in reaction A. The green frame indicates the productivity of the resulting drawings.

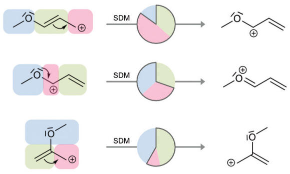
contrast to Elizabeth's approach, she does not just focus on one feature, but sequentially considers smaller, interacting parts of the molecule which may aid in the delocalization of the positive charge. Therefore, as **Figure 13** illustrates, this approach leads to single drawing moves delocalizing electron density toward an electron-deficient atom. This sequential approach is also reflected in Paula's fixation duration rate, as she focuses most of the time on the positive charge and the double bond in the first resonance structure, and then, on the newly created positive charge and the methoxy group in the second structure.

Figure 9 illustrates that 35 of 60 drawings stem from a knowledge-driven variable approach, in which rules and concepts, such as stability or electronic effects, guided students' drawing process. Phil's sequential drawing process in reaction A and B exemplifies this approach. As **Figure 14** depicts, each productive resonance structure results from a single drawing move, which shows the movement of electrons from an electron-rich source to an electron-deficient atom. In his verbalization of the drawing process, Phil repeatedly refers to the delocalization of the positive charge and stability as the driving force for the generation of each structure.

It can be inferred from Phil's drawing approach that he centers his drawing moves around the positive charge. He takes a rather analytic, holistic approach by considering adjacent structural features and analyzing their contribution to the delocalization of the positive charge. Consider therefore the fixation duration rate during the construction process of the different resonance structures, exhibiting an attention distribution trend for the structures in reaction A (**Figure 14**). While Phil mainly fixates the double bond and the positive charge in the first resonance structure, his attention is drawn to the methoxy group and the positive charge in the second structure. In contrast to that, he centers his attention on the methoxy group and the double bond in the resonance structure in reaction B. Given that he verbalizes stability as the driving force for the construction of the structures, this gaze distribution may be a result of the analysis and weighing of the structural features and their influences on resonance. Therefore, Phil's knowledge-driven variable approach shows that he reflects upon his drawing moves. This illustrates the need for the successful intertwined application of the different factors (R, C, M) in order to interpret a structural representation and subsequently construct another resonance structure (Schönborn and Anderson, 2008). This reflective drawing approach becomes even more apparent for Luke, another student who has a knowledge-driven variable approach. Concerning a resonance structure in A, he describes in detail the electronic effect of the oxygen atom and thereafter weighs the overall stability of the resulting resonance structure:

> *Then I thought, what does the oxygen atom do? The oxygen atom has a negative inductive effect, which is why the positive charge is intensified. But I thought that it can be neglected given the positive resonance effect, because the electron pair can be pushed toward the positive charge, and then, the positive charge would be here. I would say that is energetically not so favorable here with the positive charge on the oxygen, but it shows that the positive charge can be distributed relatively well.*

Given that the gaze proportion of productive and unproductive drawings does not differ much in reaction B (cf. section "RQ 2: What structural features do students attend to in terms of attention distribution when translating one resonance structure into another and how is it related to students' drawing moves?"), it may be inferred from these examples that students process the structural information differently by applying their related knowledge in different ways. While students with an unproductive drawing may tend to look at the given structure statically and apply thereon rules, for productive drawings, it may be the case that a higher gaze proportion indicates a more thorough weighing and



I know that the more delocalized the positive charge is, the more stable the [molecule] *is. And then I just looked, so in the first one, of course, the double bond can flip over here, so I have the positive charge two carbon atoms further* [refers to the first resonance structure in A]*. And then the oxygen atom is also involved and can give another pair of electrons* [refers to the second resonance structure in A]*. This means that I have basically distributed the positive charge over these three atoms* [...] *In the second resonance structure, the positive charge is on a carbon atom neighboring the oxygen atom. And this leads to the fact that one pair of electrons of the oxygen can simply flip over and form this bond.*

Here now [the double bond] *could also flip over* [refers to the resonance structure in B] [...] *I have the oxygen atom here, too, but it can't give its electron pairs to delocalize the positive charge. This is not possible in B because the positive charge is only at these two carbon atoms, which are basically two carbon atoms further from the oxygen, thus not at a directly neighboring atom. That's why it won't do any good for the further delocalization if another pair of electrons of the oxygen flips over. And it would not work at all because then, this carbon would be five-bonded.*

FIGURE 14
Phil's drawing moves, fixation duration rates on the structural features and drawing description for his drawings in reaction A and B. The green frame indicates the productivity of the resulting drawings.

reflection of its contribution to the drawing move. Hence, this inference strengthens Keig and Rubba's (1993) finding that solving information-processing tasks (e.g., translations between structures) requires a thorough understanding (and thus application) of the underlying concept.

Altogether, it can be derived from these examples that students with a variable approach demonstrate more flexibility when constructing resonance structures by showing a more sequential, distributed attention to structural features, often resulting in productive single drawing moves. By being analytic in nature, they exhibit a more expert-like task approach (Stieff and Raje, 2008). By successively analyzing structural features and their relationship in terms of constructing a subsequent resonance structure, students consequently demonstrate both a local and global coherence formation (Seufert, 2003), altogether resulting in a holistic approach.

Conclusion and implications

This study is the first to explore in-depth students' drawing processes in organic chemistry with the help of eye-tracking. It aimed at providing process-oriented insights into how students connect drawing-related information during the construction of resonance structures given students' struggle with these representations. To this end, we analyzed in detail students' transition patterns, the co-occurrence of fixated drawing elements during the construction process, students' gaze proportion on structural features, and shed light on their visual selection approaches to navigating the drawing processes.

As the main results, we found that on a global level, students exhibit a similar gaze behavior concerning information retrieval and integration, irrespective of the productivity of their drawing, i.e., the same amount of information was used for the construction of resonance structures. However, the transition types distinguished a productive drawing from an unproductive drawing. While productive drawings result from more transitions between previous and target drawings, the construction of unproductive drawings is characterized by more transitions between target and unrelated drawings (RQ 1). Due to a predominant connection of previous and target drawings across all resonance structures, the analysis of the gaze proportion on structural features of the previous drawing revealed that productive structures are characterized by a higher sequential fixation on interrelated structural features. In contrast, a tendency of focusing single (unrelated) structural features emerged for unproductive drawings. However, this difference did not apply to resonance structures that were spatially more complex (i.e., a non-linear, branched molecule) (RQ 2). Finally, a qualitative look at students' visual selection approaches, as reflected by students' descriptions of drawing processes, showed that a variable approach underlies many productive drawings, i.e., an analytical approach, in which students attended to interrelated, relevant structural features. This is contrary to a centered approach, resulting in more unproductive drawings; here, students focused on singular structural features in a static manner (RQ 3). These findings bear different implications for both instruction and research.

Given that students with unproductive drawings often connect and focus on unrelated drawing elements, when, however, a holistic, analytical approach is required, instructional interventions should aim more at directing students' attention, thus, supporting them to assess given information such as structural features, their relevance and their role within the construction of resonance structures (e.g., as possible starting points), therefore foster students' ability to decode given representations (R-M factor) (Schönborn and Anderson, 2008, 2010). In this regard, possible instructional interventions could use process-oriented highlighting of interacting structural features, e.g., via tutorial videos (e.g., Rodemer et al., 2021). In this way, the learners' attention could be better directed, as they can see and follow the actual drawing process instead of only seeing the static resonance structures as the final result on paper. As a possible intervention to externalize the viewing process, eye-movement-modeling examples could be used as worked examples (van Gog et al., 2009; Jarodzka et al., 2013). In addition, the results indicate that students' conceptual knowledge of the resonance concept, specifically its flexible application, seems to be of great importance with respect to drawing productive resonance structures, thus, besides the R-M factor, emphasis should also be placed on the R-C factor (Schönborn and Anderson, 2008). Consequently, teaching algorithms *how* to draw such structures is not enough for building sustainable drawing skills. Instead, more effort should be put into addressing *why* certain drawing steps occur, e.g., what chemical concepts the drawing steps build upon. Creating such interventions would make students more reflective in assessing drawing moves. In turn, this could help students' ability to flexibly decide when resonance applies and reduce their overreliance on heuristics and rules, such as searching for familiar or salient surface features.

As this study is explorative, more research in other contexts, with different task designs, and with more participants is needed to complement our findings and test whether our results can be confirmed. By finding little differences in eye movements while dealing with the more complex structure in reaction B, the construction of more complex structures deserves more attention. Due to their complexity and relevance, aromatic compounds are suitable for this purpose. However, more complex structures complicate the comparative analysis because, depending on the complexity, the number of differing drawing products increases. At the same time, the use of simpler aromatic compounds may lead students to proceed algorithmically. For instance, to investigate the differences in the information retrieval of drawing-related structural features, multiple choice tasks could be used, in which learners are asked to decide on a resulting structure based on an initial compound. As such, the comparative investigation of differing fixation distributions when choosing a productive or unproductive structure would be possible. Likewise, in such a setting, a stationary eye-tracker could be used, which provides more precise results regarding the fixation of single bonds and structural features.

By inferring underlying processes for previously documented drawing difficulties, this study adds to existing research by focusing on the context of the resonance concept. Furthermore, given its process-oriented character, this study adds to existing STEM-related drawing research in general. Despite previous research on the effects of drawing activities and the drawing products' quality on learning outcomes, few research focused on the construction process underlying learners' drawing products so far (Lobato et al., 2014). However, a process-oriented perspective can provide additional diagnostic insights into representation-related difficulties as the drawing processes can reveal learners' scientific thoughts and conceptions (Lobato et al., 2014) as well as their unconscious actions when generating representations. As this study exemplified, the use of eye-tracking showed that, besides conceptual knowledge, students' ability to construct productive scientific representations crucially depends on their competence to decode and manipulate such representations. As such, this methodology could be also applied in other contexts and STEM disciplines to reveal cognitive processes underlying the generation of representations, e.g., what features learners (unconsciously) use and integrate to depict submicroscopic processes in biology or to construct diagrams in physics, and whether the use of specific features or drawing elements influences the overall drawing quality. Eye-tracking could also be used in other contexts in organic chemistry, such as observing learners' stepwise construction of mechanisms and the use of the electron-pushing formalism (e.g., Bhattacharyya and Bodner, 2005; Grove et al., 2012; Flynn and Featherstone, 2017), or observing the order and linearity of the diagram construction depending on the learners' expertise. Although our work yields first process-oriented insights, further research across different scientific disciplines is needed to provide a comprehensive picture of students' drawing approaches and difficulties for scientific representations.

Limitations

This study was meant to be exploratory in nature and aimed at offering insights into students' drawing processes in organic chemistry. Therefore, some limitations with respect to the analysis and results must be considered. First, the small number of students ($N = 20$) and the focus on one task might limit the generalizability of the findings. Additionally, students were required to construct only two additional resonance structures in the first, and one structure in the second reaction, both dealing with rather simple structural formulas. Unlike in the first reaction, the construction of resonance structures did not build upon each other in the second reaction. Given these constraints, it remains unclear to which extent our findings apply to drawing processes of more complex structures. Furthermore, case comparisons might have motivated students to include and compare information of both reactions in their drawing process, since the given structures only differ in their connectivity. Thus, this variable may also have influenced students' drawing processes, specifically on the integration of unrelated information. Concerning the interviews, the participants were prompted to describe their drawing process. However, it is possible that they used knowledge that they did not verbalize and which, thus, remained implicit.

Finally, technical limitations with respect to the mobile eye-tracker must be considered. The eye-tracker exhibits technical measurement inaccuracies due to, among others, a variable field of view, movement of the head, and the slippage of the glasses as a result of a longer measurement period. These inaccuracies can affect the results and the data analysis (e.g., requiring the correction of systematic gaze point offset by adjusting the AOIs).

Data availability statement

The datasets presented in this article cannot be made openly available because of the privacy policy stated in the participants' consent form. Requests to access the datasets should be directed to the corresponding author NG, Nicole.Graulich@didaktik.chemie.uni-giessen.de.

Ethics statement

Ethical review and approval was not required for the study on human participants in accordance with the local legislation and institutional requirements. The participants provided their written informed consent to participate in this study. Written informed consent was obtained from the individual(s) for the publication of any potentially identifiable images or data included in this article.

Author contributions

IB designed the study with the help of NG, collected the data, and wrote the manuscript. IB and AL analyzed the data. IB, AL, and NG reviewed, edited, and discussed the manuscript and the analyses. All authors contributed to the article and approved the submitted version.

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Conflict 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.

Publisher's note

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3. Exploring Diversity: Student's (Un-)productive Use of Resonance in Organic Chemistry Tasks through the Lens of the Coordination Class Theory

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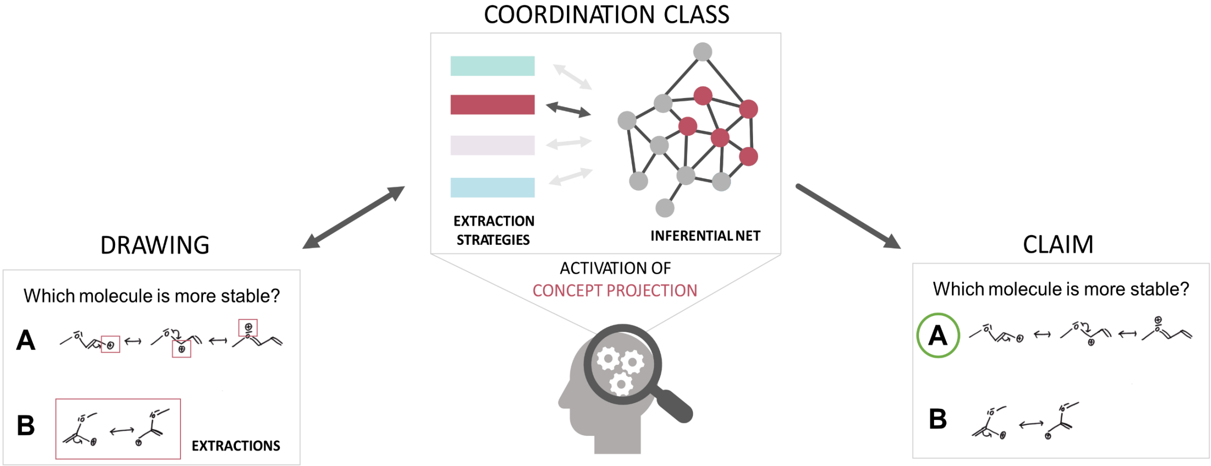

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Exploring diversity: student's (un-)productive use of resonance in organic chemistry tasks through the lens of the coordination class theory

Irina Braun and Nicole Graulich *

Resonance is a crucial concept in Organic Chemistry that enables both deriving chemical properties from molecular structures and predicting reactions by considering electron density distribution. Despite its importance for problem-solving and learning success, learners encounter various difficulties with this concept. Although prior research suggests that learners struggle to reason about resonance in problem-solving tasks, existing studies are often limited to singular contexts. Given that task approaches and reasoning are context-dependent, little is known about how learners use resonance across task contexts and which characteristics underlie productive concept use. To this end, a qualitative interview study was conducted, in which undergraduate chemistry students (N = 21), all beginners of Organic Chemistry, solved three organic case comparison tasks requiring the consideration of resonance. Through the analytical lens of the coordination class theory, we analysed the extent to which students used their representations of resonance structures, their task approaches, and the variety of resonance-related resource activation and connection in problem-solving across three different contexts. The results show that students' use of resonance is diverse across the contexts. It can be characterized by a complex interplay of multiple factors reflecting the multifold processes when considering resonance. However, some essential characteristics of productive concept use in problem-solving (*e.g.*, the activation of resources across different granularity levels) could be deduced. Implications for supporting learners' use of resonance in problem-solving are discussed.

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Introduction

Due to its visual nature, external representations play a key role in making sense of chemical phenomena and processes in Organic Chemistry. They carry the explanatory weight of the discipline and make imperceptible entities and processes visible since much implicit and explicit information (*e.g.*, connectivity, polarity, geometry) is embedded within external representations (Hoffmann and Laszlo, 1991; Goodwin, 2008; Cooper *et al.*, 2017; Graulich and Bhattacharyya, 2017). Representations such as molecular structures and mechanistic representations not only fulfil a displaying function but constitute a fundamental means for transmitting and constructing knowledge. They also serve as indispensable problem-solving tools. For instance, inferring molecular properties from representations can help to predict and weigh possible reaction pathways (Goodwin, 2008; Cartrette and Bodner, 2009; Cooper *et al.*, 2017). Proficiency in the sensemaking of representations is crucial for successful reasoning in Organic Chemistry. Successfully engaging with representations, however, is not limited to interpreting given representations. In terms of representational competence, it is also important that learners are able to generate representations and use them in problem-solving (Kozma and Russell, 1997; Kozma and Russell, 2005). Constructing representations (*e.g.*, drawing structural formulas) may provide diagnostic insights into one's mental models by externalizing ideas and may enhance one's chemical thinking (Gilbert, 2005; Van Meter and Garner, 2005; Cooper *et al.*, 2017). Within these sensemaking processes, engaging with representations is always linked to considering and weighing different chemical concepts (Talanquer, 2022). For instance, to assess the acid strength of a compound, one maps and connects the visual features (*e.g.*, functional groups) in a representation to relevant ideas such as pK_a values or solvent effects. In turn, these ideas are derived by linking given structural features at a finer grain size (*e.g.*, single atoms) to inductive effects, electronegativity, hybridization, hyperconjugation, or the size of the basic atom. It becomes evident that both the visual features in a representation and the related concepts mutually influence one another in the reasoning process *via* bottom-up (*i.e.*, infer from the structure) and top-down (*i.e.*, apply knowledge and concepts) processes (Kintsch, 1988; Kriz and Hegarty, 2007).

The resonance concept is closely related to generating and interpreting different representations (*e.g.*, electron potential maps, structural formulas). It describes the delocalization of π

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electrons between multiple atoms in a conjugated system of a molecule. Usually, this is depicted by several Lewis structures that differ in the spatial arrangement of electrons among overlapping p-orbitals on adjacent atoms (*i.e.*, resonance structures). The hybrid of all possible resonance structures can adequately describe the actual electronic structure of and bonding in a molecule. This is related to energetic considerations as the delocalization of π electrons contributes to the molecule's stabilization (*i.e.*, resonance energy): the more electrons can be reasonably delocalized in a molecule, the lower the potential energy, and the more stable the molecule (Anslyn and Dougherty, 2006; Ogilvie *et al.*, 2018). By constructing resonance structures, the hypothetical electron density distribution in molecules can be visualized, which helps to reason about preferred molecular structures or geometry, to derive chemical properties (*e.g.*, acidity or stability), and to predict or justify reaction pathways (Richardson, 1986; Carle and Flynn, 2020). Moreover, other concepts, such as aromaticity or conjugation, build upon the resonance concept. Given that the resonance concept is pivotal for problem-solving and successful learning in Organic Chemistry, it is critical to understand how students understand and reason about resonance across contexts.

Students' understanding and use of the resonance concept

Students' conceptions of resonance. Although students are expected to have a thorough understanding of resonance after introductory courses in Organic Chemistry and should be able to use this core concept fluently to depict the electronic structure of compounds, research in chemistry education has shown that the resonance concept puts a high cognitive load on learners (Duis, 2011; Brandfonbrener *et al.*, 2021; Tetschner and Nedungadi, 2023). For instance, students have varied perspectives on resonance. Studies show that many students effortlessly recognize resonance structures and explain resonance by describing *how* to construct resonance structures (Brandfonbrener *et al.*, 2021). Students also sometimes perceive resonance as a rapid exchange of electrons, and interpret resonance structures as equilibrium or as a structural change over time (Taber, 2002; Xue and Stains, 2020; Tetschner and Nedungadi, 2023). Additionally, students may consider resonance structures as distinct species or different perspectives of a molecule through picture analogies (Kim *et al.*, 2019; Brandfonbrener *et al.*, 2021). These findings indicate that learners have varying ways of understanding resonance, *i.e.*, to interpret the static representations on paper as a dynamic electron distribution. Even though some of these ideas represent alternative conceptions, in parts, they touch upon aspects of the scientifically correct explanation of resonance. For instance, although the picture analogy does not reflect the idea that individual resonance structures do not exist as distinct structures, this conception indicates that students understand that single resonance structures do not provide a complete structural representation of a molecule (Brandfonbrener *et al.*, 2021).

Connection with other concepts. Understanding and using resonance necessitates that learners connect this concept with their prior knowledge (*e.g.*, hybridization, charge separation) and other concepts (Betancourt-Pérez *et al.*, 2010). Studies investigating students' conceptual understanding of resonance show that students associate resonance with concepts such as stability or reactivity but often cannot appropriately link these concepts. As such, students often use these relationships as general statements or rules (Xue and Stains, 2020; Brandfonbrener *et al.*, 2021). For instance, in a recent study eliciting students' mental models on acid and base strength in Organic Chemistry (Demirdöğen *et al.*, 2023), it became evident that the relationship between resonance and basicity remained unclear for some students. While they recognized the importance of resonance in assessing the base strength of molecules, their problem-solving often relied on broad, memorized statements (*e.g.*, "the more resonance, the more stable", p. 1134) (Demirdöğen *et al.*, 2023). Brandfonbrener *et al.* (2021) furthermore showed that students describe the influence of resonance on reactivity in a more general sense, or establish the relationship between these two concepts by referring to common applications such as acid–base chemistry. While the latter shows that students can establish appropriate conceptual relationships, at least in some contexts, a restricted or overgeneralized view on these intertwined concepts may hinder subsequent problem-solving.

Construction of resonance structures. Besides the necessary link to other concepts, students' competence in constructing resonance structures is an indispensable prerequisite to correctly make assumptions about resonance and use it in various situations (Betancourt-Pérez *et al.*, 2010; Carle and Flynn, 2020). A few studies targeting students' drawing processes of resonance structures point out that students' main challenges in drawing resonance structures are situated in identifying the correct place to start the movement of electrons, or arise from conceptual difficulties (*e.g.*, adhering to the octet rule) (Betancourt-Pérez *et al.*, 2010; Petterson *et al.*, 2020). Related to these struggles, students with productive resonance structures show a more straightforward drawing process with more direct transitions between the previous and target drawing. In doing so, students with successful drawings adopt an analytical approach by focusing on and carefully assessing relevant, interrelated structural features (Braun *et al.*, 2022).

Use of resonance in problem-solving. Although studies emphasize resonance as an important concept to determine reaction pathways and to assess properties of molecules (*e.g.*, Ferguson and Bodner, 2008), using this concept in practice (*i.e.*, moving beyond the definition), might be difficult for students (Cartrette and Mayo, 2011). A recent investigation by Carle and colleagues (2020) on students' achievement of resonance-related learning outcomes revealed that only a few students spontaneously consider resonance in mechanistic tasks when they are not explicitly prompted to do so (Carle *et al.*, 2020). Similar insights are given in studies by Shultz and colleagues in the context of addition and acid–base reactions (Finkenstaedt-Quinn *et al.*, 2020; Petterson *et al.*, 2020). They document that students seldom utilized resonance to determine reaction pathways or assess stability. In particular, students in this study seem to have difficulty identifying which entities (*i.e.*, reactants or products) should be considered for determining stabilization through electron delocalization. This indicates the necessity of explicit prompting (Finkenstaedt-Quinn *et al.*, 2020; Petterson *et al.*, 2020).

In summary, students have diverse perspectives on resonance and may face challenges in fully grasping its dynamic nature and interconnectedness with other concepts. Still, it remains unclear how learners use constructed (or given) representations to deduce information to *use* the resonance concept in problem-solving tasks. Little is known about the various resources (*i.e.*, ideas) related to resonance students activate when engaging with organic chemical tasks. Such insights, however, could inform instructional approaches to support students in learning and considering aspects of resonance in Organic Chemistry.

Theoretical framework

Resource-based model of cognition

According to the *resources framework* informed by Hammer and colleagues, knowledge cannot be considered as an "intact unit of cognitive structure" (p. 92) (Hammer *et al.*, 2005) acquired in one context and transferred as a whole to another context. Instead, following a fine-grained constructivist view (Elby, 2000), this framework conceives the mind as a dynamic, complex system with a manifold view of the cognitive structure: the activation of fine-grained resources or knowledge elements characterizes one's knowledge and reasoning (Hammer *et al.*, 2005). This framework considers the dynamic nature of students' reasoning and takes both their in-the-moment thinking and existing knowledge in terms of cognitive structure organization into account (Louca *et al.*, 2004; Hammer *et al.*, 2005; Conlin *et al.*, 2010). As such, resources are cognitive elements at varying grain sizes ranging from small, basic elements like phenomenological primitives, p-prims (*i.e.*, intuitive ideas that constitute one's sense of mechanism without any further justification, such as "closer means stronger" (DiSessa, 1993; DiSessa, 2018)), to more complex structures like coherent theories (Hammer *et al.*, 2005; Richards *et al.*, 2018). The resources are at different states of activation, which can be used across contexts (Hammer *et al.*, 2005; Richards *et al.*, 2018). In this regard, resources can be activated alone or simultaneously within a set with other resources, in which one resource builds onto another, altogether forming chains of successive inferences. A network of resources that is repetitively activated over time may become a cognitive unit, *i.e.*, act as a resource, itself (Hammer *et al.*, 2005). Resources are neither right nor wrong and can only be activated (in-)appropriately in a certain context (Hammer *et al.*, 2005; Richards *et al.*, 2018). In general, resource activation is highly sensitive to the constraints of contexts, as differing contextual features cue the activation of different resources (Hammer *et al.*, 2005; Conlin *et al.*, 2010). Consequently, as resources are not robust in their activation, knowledge cannot be considered *stable* (Hammer, 2000; Richards *et al.*, 2018). Which resources are activated and to what extent depends on one's framing (*i.e.*, (implicit) expectations) of a given situation, guided by prior knowledge, experiences, and understanding. Framing shapes how a particular situation is perceived, thereby activating a locally coherent set of resources (Tannen, 1993; Hammer *et al.*, 2005; Hutchison and Hammer, 2010). Consequently, task and context variation and prompting impact resource activation and influence one's task approaches and reasoning (Hammer *et al.*, 2005).

Concept understanding through the lens of the coordination class theory

Conceptualization of coordination classes. In line with the *resources framework*, the coordination class theory conceptualizes concept understanding (*i.e.*, having a *coordination class*) as a profound and intertwined knowledge system. It comprises a complex network of fine-grained knowledge elements (*i.e.*, resources in the realm of a concept) activated by perceptual cueing (DiSessa and Wagner, 2005). Consequently, this knowledge system allows us to flexibly "see" a concept in different contexts by reading concept-relevant information from various situations in the world (DiSessa and Sherin, 1998; DiSessa and Wagner, 2005; DiSessa, 2018). Given this core function of coordination classes, not all concepts can be considered coordination classes. DiSessa and Sherin (1998) distinguish coordination classes from category-like concepts. For instance, compare the concept of "cat" and "velocity". For the first category-like concept, knowing a cat's defining attributes is core, making it possible to decide whether an animal belongs to this species. However, it is impossible to learn *how* to see these characteristics across varying situations – whether the animal is a cat or not. In contrast, one has to deal with the concept of "velocity" differently to get concept-relevant information. For instance, one might determine the amount of velocity by comparing the movement of two cars in one situation. At the same time, it is necessary to calculate with numbers presented in tables in other situations. As a result, the coordination class theory considers those concepts, which necessitate learning *how* to see them in a wide range of situations in which they can be applied and recognized (DiSessa and Sherin, 1998; DiSessa and Wagner, 2005). This can be done, for instance, by using different strategies or activating various resources. According to DiSessa and Sherin (1998), coordination classes help to understand how (especially complex, abstract scientific) concepts function in explanation and problem-solving. As such, prior research across the STEM disciplines focusing on learners' concept understanding has used the coordination class theory to shed light on numerous concepts like energy (Barth-Cohen and Wittmann, 2017), velocity and frequency (Parnafes, 2007; Parnafes and DiSessa, 2013), the law of large numbers (Wagner, 2006), or, in chemistry, reaction rate (Rodriguez *et al.*, 2020a), light- and light-matter interactions (Balabanoff *et al.*, 2020), and the varied population schema (Rodriguez *et al.*, 2020b). In line with the requirements for a coordination class, we argue that the concept of resonance can also be modeled as a coordination class. By reasoning about the electron density distribution in various molecules, thus, touching in its core upon molecules' properties, resonance can help to describe a molecule's (electronic) state. While this is often done by considering and weighing the stability of resonance structures in a system, one must also be able to perceive resonance in other representations, such as resonance hybrids or electron potential maps. Given that resonance applies in various reaction contexts, one must be able to deal with this wide range of contexts (Carle and Flynn, 2020), thereby using resonance flexibly to reach task-specific conclusions (*e.g.*, assessing molecules' stabilities or deducing possible reaction pathways).

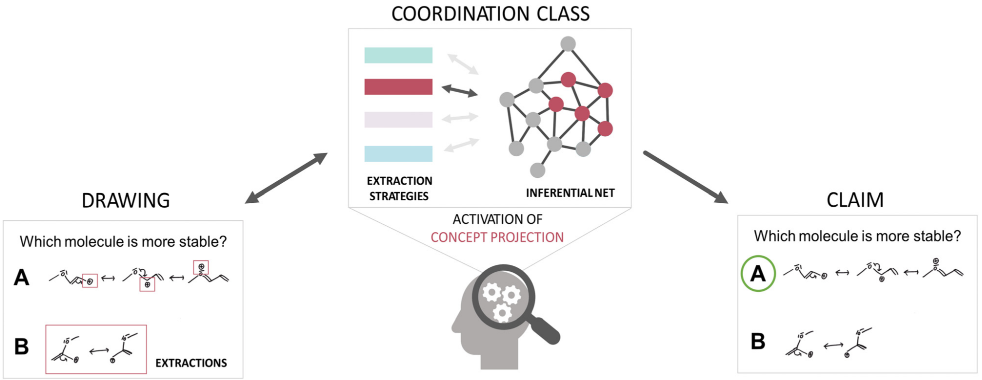


Fig. 1 Illustration of the different components of a coordination class.

Architecture of coordination classes. Given this perspective on what counts as a coordination class, it is consequently impossible to decide whether one has a concept or not. Instead, following the coordination class theory, concept understanding is complex and context-dependent. For educational purposes, it is important to understand how a learner ''sees'' these concepts in different situations (DiSessa and Sherin, 1998; DiSessa and Wagner, 2005; Rodriguez *et al.*, 2020b). Consequently, it is crucial to characterize the processes involved within the knowledge system of a coordination class. The architecture of coordination classes is conceptualized as an internal structure characterized by two interdependent structural components: *extraction strategies* and the *inferential net* (*cf.* Fig. 1). In early literature, the coordination class components have been referred to as *readout strategies* and *causal nets*. As these terms appeared counterintuitive and caused confusion, DiSessa *et al.* (2016) suggested a revised terminology by replacing *readout strategies* with *extraction strategies* and the *causal net* with *inferential net*. These terms also will be used in this publication.

Extraction strategies capture the individuals' overarching approaches for obtaining information and organizing sensory information (*cf.* framing) and thus describe how individuals focus on specific information (*i.e.*, problem-solving approaches) (Wittmann, 2006; Rodriguez *et al.*, 2020b). *Extractions* are the specific perceptual components attended to by an individual (DiSessa *et al.*, 2016). These might be, for example, structural features of constructed resonance structures (*e.g.*, a conjugated system, the absolute number of resonance structures, charges) (DiSessa and Sherin, 1998; Wittmann, 2002; DiSessa and Wagner, 2005; DiSessa *et al.*, 2016; Rodriguez *et al.*, 2020b). The extractions, in turn, cue the activation and combination of a cluster of concept-related resources, forming an inferential net and helping to reason through a given situation (DiSessa and Sherin, 1998; DiSessa and Wagner, 2005; DiSessa, 2018). As such, resources (often also referred to as *knowledge elements*) may encode a variety of ideas (*e.g.*, p-prims, if-then statements, heuristics) (Buteler and Coleoni, 2016; Rodriguez *et al.*, 2020b). Therefore, the coordination class of a learner functions as a filter for one's problem-solving (Rodriguez *et al.*, 2020b). To illustrate, consider problem-solving in Organic Chemistry, which is often based on reasoning with drawings of structural formulas. Usually, these drawings contain much chemical information (*i.e.*, connections, involved entities, and their interaction), so the focus of attention can vary depending on the problem. If, for instance, a learner is asked to compare the stability of two carbocations (Fig. 1), they might focus their attention on factors enhancing the stability of the respective structures and employ a task approach driven by stability considerations (*extraction strategy*). A learner might focus in detail on features in the structure that influence the stability, *e.g.*, hetero atoms, the location of the positive charge, or, if resonance applies, the overall number of valid resonance structures (*extractions*). These structural features attended to then cue different resources, which result in an *inferential net*. The activated resources might be, for instance, electronic effects of the hetero atoms (*i.e.*, implicit properties), the overall electron density distribution, or energetic aspects that are combined and lead to the answer to the task. In general, extraction strategies and inferential nets are closely related and influence one another, as new extractions might lead to the activation of new resources. The activation of resources might lead to or hinder the learning and activation of new extraction strategies (DiSessa and Sherin, 1998). As described in the example, given information, such as the prompt to consider stability or the type of representations, might as well cue the activation of specific extraction strategies.

Performance characteristics of coordination class use. A coordination class allows the perception of certain information using different extraction strategies dependent on the situation. As such, a well-formed coordination class works with a broad set of sophisticated strategies and understandings. They can be applied across contexts and task types with certainty, proving a great extent of *span* and *alignment* (DiSessa and Sherin, 1998). *Span* describes the stability with which knowledge elements can be activated across various contexts and whether a coordination class can be broadly operated across various problem-solving contexts to activate resources and draw conclusions. According to DiSessa and Wagner (2005), this is also the defining feature of robustly transferable knowledge. *Alignment*, on the other hand, targets the inner consistency of a coordination class. Although different tasks and contexts might necessitate different approaches and might activate various resources, they must yield the same information, *i.e.*, the same conclusion in problem-solving tasks (DiSessa and Wagner, 2005; Buteler and Coleoni, 2016; Rodriguez *et al.*, 2020a). When reasoning about resonance, a high span would mean that students have enough conceptual resources to reason about resonance in a wide range of contexts (*e.g.*, in aromatic and non-aromatic contexts). A high alignment would suggest that students can determine the perceived information reliably by displaying the electron density distribution in a molecule in combination with its thermodynamic consequences (and, for instance, not as distinct structures in certain situations). Otherwise, the coordination class would be ill-formed. Considering these two characteristics, mastery of a coordination class means coordinating resources in various ways depending on the context's requirements (DiSessa and Sherin, 1998). Due to the different relations between these components, it is noteworthy that a learner's coordination class can never be fully captured. One can also show competent task performance even though some relations within the coordination class might be incorrect (Buteler and Coleoni, 2016).

Given that students' extraction strategies and inferential nets usually remain tacit in problem-solving, using interviews or other qualitative methods helps to shed light on these coordination class components. Singular contexts, however, do not require the activation of the whole coordination class but only a subgroup of activated extraction strategies and resources for that particular context (referred to as *concept projections*) (DiSessa and Wagner, 2005; DiSessa *et al.*, 2016). Therefore, combining different task contexts offers a more in-depth insight into the nature of one's coordination class and helps to seize the richness of students' concept understanding and consideration at different scales (Wittmann, 2002; DiSessa, 2018; Rodriguez *et al.*, 2020b).

Research questions

Concept understanding cannot be modeled as an intact cognitive unit being transferred from one context to another. Hence, the coordination class theory can help to explore and grasp the richness of students' use of resonance in problem-solving by considering it as an interplay of representation-based reasoning and resource activation on different levels across various contexts. It allows us to characterize how students use resonance across different contexts and helps to gain insight into which factors underlie a productive consideration of this concept. Specifically, this qualitative study aims at addressing the following research questions:

(1) How diverse are students' concept projections of resonance across different problem-solving contexts?

(2) How do the coordination class components contribute to the productivity of students' concept projections of resonance?

Methods

Context and participants

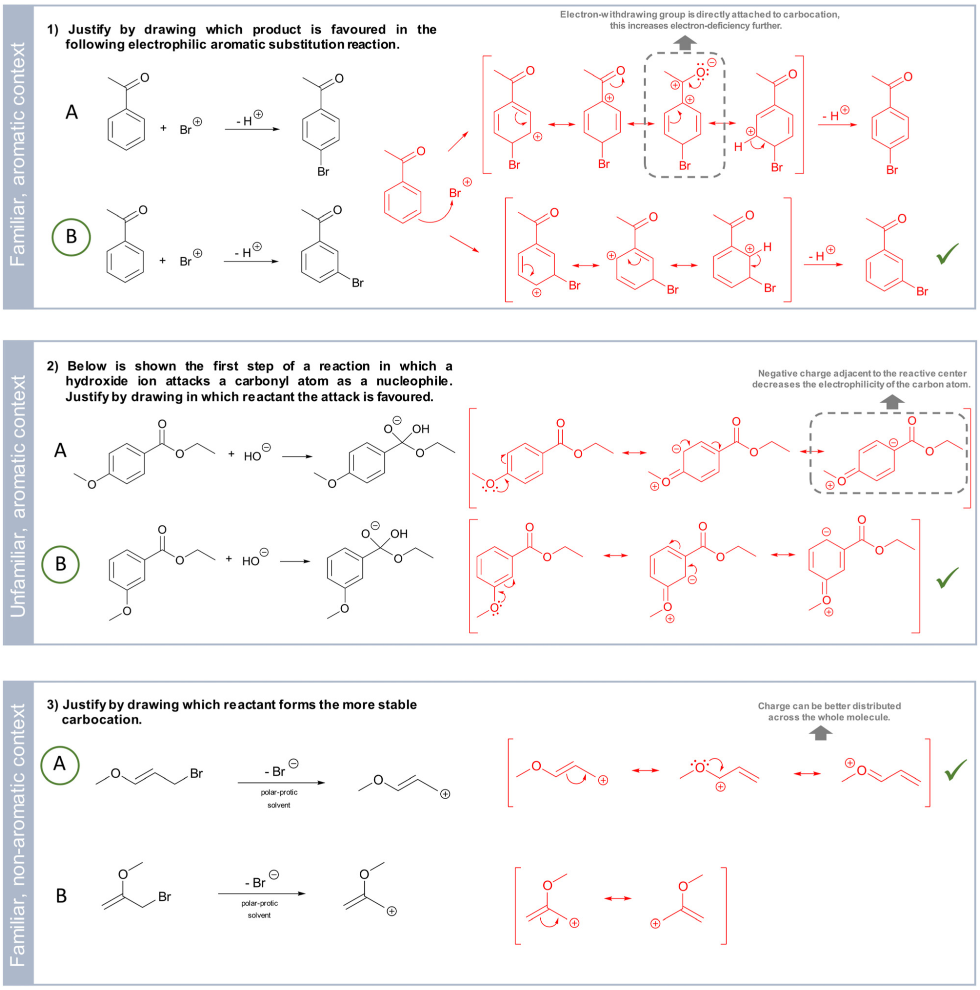
This research study was conducted at a German university in summer 2021. 21 students majoring in chemistry (*i.e.*, chemistry and food chemistry bachelors, and chemistry student teachers) participated in this study. They were recruited on a voluntary basis *via* e-mail and in-class announcements in the Organic Chemistry 1 (OC1) course. As compensation for their time, the students received 20 euros. The participants' ages ranged from 19 to 34. Nine of them identified as male, twelve identified as female. Given that the OC1 course is the first lecture in Organic Chemistry at this university, students typically take it in the second or fourth semester of their study programs. The OC1 course has a weekly lecture (3 hours) and tutorial sections (1.5 hours). However, due to the pandemic, during the summer semester 2021, a flipped format was adopted in which students watched tutorial videos and read material (*e.g.*, book chapters), before solving content-related tasks and discussing questions in online tutorial sections. The OC1 course follows a traditional curriculum to convey introductory knowledge of Organic Chemistry by first focusing on structure–property relationships and reactivities of functional groups. It covers typical reaction mechanisms such as electrophilic addition reactions, eliminations, nucleophilic substitutions, and carbonyl reactions. As the study took place near the end of the course, the students were familiar with the reactions addressed in the interview and the resonance concept. The resonance concept and the construction of resonance structures were introduced to the students during the first two weeks of the course and have been applied continuously during the semester with various topics (*e.g.*, to discuss aromaticity).

All participants were informed about their rights and data handling beforehand; informed consent was obtained from all study participants. No further approval by an Institutional Review Board is required at the German university where the study was conducted. Nevertheless, the study followed ethical guidelines, and it was clarified to the students that they could withdraw from the study at any time. All students gave their written consent for the collected data (*i.e.*, their recordings and scans of their worksheets) to be analysed and published by the research team. In this study, participants were given pseudonyms. No identifying information was recorded or scanned to allow participants to re-identify. Since the interviews were conducted in German, students' interview excerpts were translated into English for this publication.

Data collection

This qualitative study is part of a project that explores students' reasoning with drawings in problem-solving, and their drawing processes of structural formulas in Organic Chemistry in relation to the resonance concept. Semi-structured interviews have been combined with a paper-pencil setting to investigate students' use of resonance in problem-solving tasks. They were audio- and video-recorded and lasted between 83 and 140 minutes. Since this study also focused on exploring students' drawing processes, a mobile eye-tracker (Tobii Pro glasses 3, 50 Hz) was used to capture students' eye movements during task completion. However, this analysis is not part of this publication. A thorough description of the methodical approach and respective results of this part of the project are reported elsewhere (Braun *et al.*, 2022).

The interviews consisted of three parts. In the first part, the students were asked general questions about resonance (*e.g.*, "When does resonance apply?", "What is resonance?", "How do you draw resonance structures?") as a warm-up. This also served to gain first insights into the participants' understanding and ability to construct and infer information from their resonance structures. In the second part, students were prompted to solve three organic case comparison tasks that required the application of the resonance concept. First, they were encouraged to solve the tasks freely, *i.e.*, they could write and draw as much as they considered necessary without being disturbed. If they wished, they could also think aloud. After each task, a subsequent retrospective interview focused on their problem-solving. The students were asked to justify their answers, and to explain their problem-solving approach and thought process for the respective tasks. Furthermore, they were asked to describe their drawing strategies and the rationale behind their constructed resonance structures. The interview protocol for the retrospective can be found in


1) Justify by drawing which product is favoured in the following electrophilic aromatic substitution reaction.

Electron-withdrawing group is directly attached to carbocation, this increases electron-deficiency further.

2) Below is shown the first step of a reaction in which a hydroxide ion attacks a carbonyl atom as a nucleophile. Justify by drawing in which reactant the attack is favoured.

Negative charge adjacent to the reactive center decreases the electrophilicity of the carbon atom.

3) Justify by drawing which reactant forms the more stable carbocation.

Charge can be better distributed across the whole molecule.

Fig. 2 Task solutions for the utilized case comparisons in the study.

Appendix 1. Finally, the last part of the interview comprised an overall reflection, in which general problems concerning the tasks and students' further needs for these types of tasks were discussed. The study was piloted with five students in spring 2021. The analysis of pilot data led to slight changes of the drawing setting and the interview protocol, with the addition of more follow-up questions to gain deeper insights into students' problem-solving and drawing processes.

Task design

In the second part of the interview, three case comparison tasks were used to elicit students' use of and reasoning about resonance in problem-solving. They required the construction of resonance structures to solve the given problems and estimate the differences between the contrasting reactions. Case comparisons support a deeper engagement with a problem. By considering and weighing influential factors when comparing reaction pathways, this task type enhances closely analysing the representations, inferring reactivities and properties, and reflecting on the underlying reaction process (Alfieri *et al.*, 2013; Graulich and Schween, 2018). Therefore, case comparisons represent a suitable instrument for characterizing students' concept projection of resonance in problem-solving. The utilized case comparisons show varying degrees of familiarity for the students and are situated in aromatic and non-aromatic contexts (Fig. 2).

The first task addresses an electrophilic aromatic substitution reaction of acetophenone with a bromine ion, either resulting in a *para*-substituted (A) or *meta*-substituted product (B) (task 1, Fig. 2). In this task, the two possible reaction pathways need to be contrasted. Given the electron-withdrawing property of the carbonyl substituent of acetophenone, a substitution is favoured in the *meta*-position. This is due to the instability of the *Wheland*-intermediate when substituting at the *para*-position. More precisely, when the bromine is added as a *para*-substituent, the resulting resonance structures show a low electron density adjacent to the carbonyl substituent. Given its electron-withdrawing property, the electron deficiency would increase even more. This would be energetically unfavourable. In contrast to that, the resulting resonance structures for the attack of the bromine in the *meta*-position show that a lower electron density can be found at the *ortho*- and *para*-positions. This does not lead to energetically unfavourable electronic interactions. Besides this scientifically correct approach to the task, the influence of the electron-withdrawing property of the carbonyl group is often considered to decide on its directing effect as a substituent (Klein, 2012). Similar to the previous approach, here, the corresponding resonance structures of acetophenone illustrate that the electron density is low at the *ortho*- and *para*-position. An electrophilic attack necessitates electron density, so the substitution occurs at the *meta*-position. Since the electrophilic aromatic substitution has been covered in detail during the OC1 course, this task represents a familiar context for the participants.

The second task shows the first step of the alkaline hydrolysis of substituted ethyl benzoates in which a hydroxide ion is added as a nucleophile to the substituted ethyl benzoates (task 2, Fig. 2). Consequently, students have to compare in which of the two compounds the nucleophilic attack is favoured (Trabert and Schween, 2020). Here, one has to compare the influence of the methoxy substituent on the reactive centre and the electrophilicity of the attacked carbon atom. By doing so, one can infer that in the case of the methoxy substituent in the *para*-position (A), more electron density can be distributed *via* electron-donating effects (resonance and inductive effects) to the reactive centre. This lowers the electrophilicity of the carbon atom. Consequently, the nucleophilic attack is favoured at the 3-methoxy ethyl benzoate (B) (Trabert and Schween, 2020). Although this task is seemingly embedded in an aromatic substitution context, the actual mechanism, alkaline hydrolysis, plays a role in this case. This combination is considered an unfamiliar case for the students.

Unlike the first two tasks, the third is situated in a non-aromatic context (task 3, Fig. 2). It addresses the first step of a nucleophilic substitution reaction, in which a bromide ion leaves as a leaving group under the formation of primary carbocations. Here, the students are asked to decide which product is more stable. This can be determined by considering the electron density distribution of the cations reflected by the number of plausible resonance structures of both products. The positive charge can be better distributed in task solution A. Given that during the OC1 course students were regularly asked to assess the stability of carbocations by considering electronic effects, this task is considered familiar to the students.

Data analysis

The interview recordings were transcribed verbatim and implemented into the coding software *MAXQDA* for subsequent qualitative analysis. Given that a coordination class includes different structural components, the analysis involved several rounds of iterative coding (steps 1–7) to elicit students' extraction strategies, extractions, and their activated resources (*i.e.*, inferential nets) (Fig. 3).

Initial coding of extractions and resources. In the first coding cycle, the participants' interview transcripts were coded in an open process using *in-vivo* coding (Saldaña, 2016) to derive students' extractions and every activated resource concerning the resonance concept for each task. The resulting codes were then summarized by creating 31 higher-level codes for activated resources and 17 codes for extractions (*i.e.*, structural features) focused on (Fig. 3, step 1). Examples of student utterances for a resource and the entire lists of inferred extractions and resources can be found in Appendix 2 and 3. In a subsequent coding cycle, students' transcripts were reanalysed by hierarchically coding their resources in dependence of the extraction, as depicted in Fig. 3 (step 2). Both authors discussed and regularly optimized the coding scheme during this process to represent the data faithfully.

Construction and characterization of resource graphs. Resource graphs were constructed in a third step to further characterize students' activated resources within the inferential net (Fig. 3). As developed by Wittmann (2006), resource graphs represent networks of activated, observation-driven resources using a circle and line model. While circles illustrate resources, the lines (or arrows) demonstrate their linkage. This type of diagram sheds light on the activation of resources in a particular

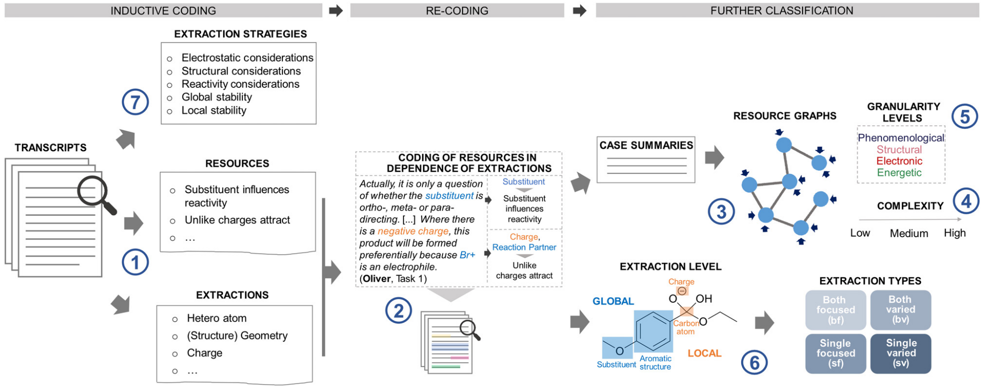


Fig. 3 Illustration of the different steps in data analysis.

setting and emphasizes the students' task-specific inferential nets. This type of representation has recently been used in chemistry education research to visualize students' ideas of buffers, varied population schema and reaction rate (Rodriguez *et al.*, 2020a; Rodriguez *et al.*, 2020b; Sheppard and Bauer, 2022). In the following, we refer to inferential nets and resource graphs interchangeably, as both describe the types and combinations of activated resources. To elicit the relationships between the resources, we described students' problem-solving for each task in case summaries (Kuckartz, 2013) before constructing individual resource graphs for each student. While the first author constructed the resource graphs, both authors engaged in regular discussions and reflection to ensure faithful data representation. Given that resource graphs are individual in nature, we characterized the diagrams further by their complexity to compare the resource graphs across the participants (Fig. 3, step 4). We adapted Yin's *et al.* (2005) classes of structure complexity in concept maps to differentiate students' resource graphs as low, medium, and high complexity. If students' resource graphs mainly demonstrated a loose, linear, or circular structure, they were associated with low complexity. If the resource graphs showed few interconnections illustrated by star and tree structures, they were considered medium complexity. Lastly, a network structure of the activated resource graph demonstrates high complexity and is characterized by many interconnections. Examples of the varying complexity of the resource graphs can be found in the results section and in Appendices 4 and 7. Moreover, we classified the deduced 31 resources by adopting Deng and Flynn's (2021) analytical framework of granularity levels to differentiate them. As such, the resources were either phenomenological, structural, electronic, or energetic in nature (Fig. 3, step 5). A detailed explanation of the granularity levels and an overview of the granularity of the resources can be found in Appendix 3. The first author coded the entire data set. A trained student research assistant independently coded a random sample of 20% of the resource graphs for interrater reliability. A Cohen's kappa coefficient of 0.87 was calculated, which indicates almost perfect reliability and agreement (Landis and Koch, 1977). Any ambiguities were discussed and resolved. In the end, a 100% agreement was reached.

Classification of extractions. Students' extractions were further characterized by the level and variety of the respective extractions (Fig. 3, step 6). For this, the extractions were first categorized into local and global extractions. While local extractions are single structural features such as hetero atoms, charges, or mere bonds, global extractions refer to features as a whole (*e.g.*, substituents comprising several atoms, the number of resonance structures). After this, the total number of mentioned extractions within a task and the absolute number of extractions on local and global levels were counted. The degree of local/global extractions in dependence of the total number of extractions was calculated to characterize the level of encountered extractions. If the degree made up less than 1/3 (or, respectively, more than 2/3), students were given the code ''single'', as the ratio indicates a predominant use of structural features on one level only, either global or local. If the degree ranged between 1/3 and 2/3, they were ascribed the code ''both'' as the proportions of both levels were more balanced. For the variety of encountered extractions, the absolute number of different extractions was divided by the total number of mentioned extractions. If more than half of all mentioned extractions differed, students were assigned the code ''varied''. Otherwise, they got the code ''focused'' if they tended to refer to the same extractions when reasoning about the given task. The codes and an exemplary calculation are illustrated in Fig. 4.

Induction of extraction strategies. To examine students' extraction strategies, the interview transcripts were coded inductively for general trends in students' described problem-solving approaches by constant comparison (Fig. 3, step 7) (Strauss and Corbin, 1990). As such, five general extraction strategies to the tasks could be identified: (1) *electrostatic considerations*, (2) *structural considerations*, (3) *reactivity*

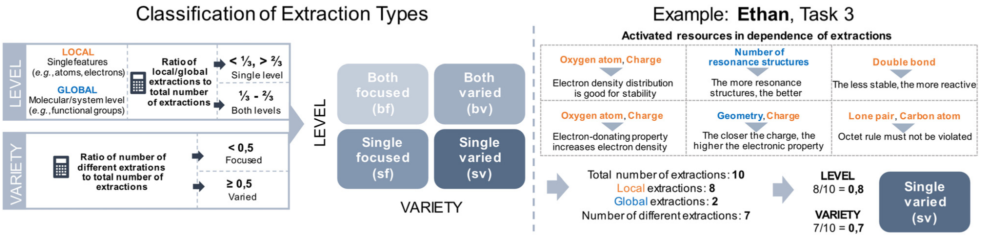


Fig. 4 Classification of the extraction types with a student example to illustrate the calculation.

considerations, (4) *consideration of global stability*, and (5) *consideration of local stability*. Table 1 provides the definitions of the resulting codes and illustrates them by giving student examples for each code.

Table 1 Coding scheme for students' extraction strategies with definitions and student example

Extraction strategy	Definition	Student example
Electrostatic considerations (E)	The focus is placed on the interaction of charges (*i.e.*, mainly charge attraction/repulsion).	*And then I thought, I'll go back to the topic, resonance. And I just drew, ok, what kind of resonance structures are there for this molecule. I think that this was somehow correct. Later, I drew in the arrows again* [referring to electron arrows in a structure] *just to see, where a positive charge in the ring is possible, because I know, the substitution will take place at the ring. So, the idea was to dock the Br minus there.* (Charlotte, Task 1)
Structural considerations (S)	The focus is placed on the structure itself, *i.e.*, on the structural composition of the compound and static electron distribution (*e.g.*, steric hindrance, type of substituent, product similarity).	Tiffany: *It would be the geometry. I know that lone pairs take up a lot of space* [. . .] *They are just closer, it would be logical to say that it reacts here* [refers to reaction B], *because here* [refers to reaction A], *the electron density is already very high and when such an addition takes place, it would perhaps be more unrealistic compared to here, where it is a bit further apart.* I: *Is that related to sterics, then?* Tiffany: *I, yes, I would say so, because the lone pairs take up a lot of space. There* [refers to oxygen atom in reaction A] *are also lone pairs again. I would imagine that might have something to do with that as well.* (Tiffany, Task 2)
Reactivity considerations (R)	The focus is placed on differences in the molecules with regard to the given reaction pathway (*e.g.*, comparison of electrophilicity). This may also involve considerations of local or global stability with regard to the reaction course.	*Yes, there are certain unfavourable positions for positive charges, in which, for example, with electron-withdrawing groups (.) bromine has a minus I-effect, but a plus M-effect, because the plus M-effect actually always predominates. That is, if we now have, for example, a positive charge with bromine, which in this case actually cannot be the case, that would be an unfavourable situation, or if I have a negative charge here* [refers to the carbonyl group in a structure of the Wheland-intermediate], *that would also be quite unfavourable, because the minus M- and minus I-effect actually pull the electrons out here, that is, this partially positive charge would be increased.* [. . .] *The reason why it is B, is simply because the positive charge is farthest away from the group, and here, we have it just close to the group* [refers to carbonyl group], *which would be unfavourable regarding stability.* (Jack, Task 1)
Considerations of global stability (G)	The focus is placed on stability considerations related to the molecule as a whole; stability is the guiding (possibly over-generalized) principle (*e.g.*, involving considerations of electron density distribution, charge balance, number of resonance structures).	*I think I know what the task is getting at, if I am not mistaken, namely, we can push the negative charge around once in the ring completely and that means it is conjugated. Maybe, who knows.* [. . .] *That is, we have a stabilization here, yes. So, theoretically, that is actually the idea, that you can push this around here once* [refers to reaction A], *so that is probably the more stable one and the whole thing will not be the case with the other one* [refers to reaction B]. (Jack, Task 2)
Considerations of local stability (L)	The focus is placed on stability considerations focusing on singular parts of the molecule (*e.g.*, most stable position of a charge, thus, *local* interpretation of charges).	*I would say that A is more stable, because here, this resonance structure is stabilized* [refers to the second resonance structure in A] *by the plus I-effect of the alkyl substituent. And here, it is just at the end and there is nothing more* [refers to the resonance structures in B], *therefore, yes.* [. . .] *So here, it is obviously about the product, so I just looked how can I delocalize the positive charge, I drew the two/, so I drew the resonance structures of it and then I just briefly thought about it and came to the conclusion that this is the best possible distribution* [refers to the second resonance structure in A]. *The positive charge can then be best stabilized, because there are actually two resonance structures for each molecule. But up here, this one* [second resonance structure in A] *is, I don't know, the most valuable, because it can be stabilized best there.* [. . .] *Um, because then, I also have this positive charge on the O, but that's not necessarily stable and that's why I thought that it makes more sense if I have my positive charge on the C-atom.* (Nora, Task 3)

Some students changed their extraction strategy during problem-solving due to new activation of resources or dead-ends. To capture this, we coded multiple extraction strategies within a task whenever the change led to bigger changes in the problem-solving, *e.g.*, choosing a different answer or constructing new drawings. Again, the first author coded the entire data set, while a trained student research assistant coded a random sample size of 20% using the deduced coding scheme. The calculations permitted a Cohen's kappa value of 0.90, indicating almost perfect agreement (Landis and Koch, 1977). Any ambiguities and differences were resolved, leading to a total agreement of 100%.

The final stage of data analysis involved the comparison of students' problem-solving to find trends in concept projections across the different tasks, and characteristics of productive concept projections of resonance with respect to the different coordination class components. We considered a concept projection productive if the resulting problem-solving was successful, *i.e.*, if the answer resulting from the problem-solving was correct and if it moved the student closer to the final correct answer (Rodriguez *et al.*, 2019).

Results and discussion

In the following subsections, we present the results of our analysis of students' resonance consideration in problem-solving organized by our research questions (RQs), (1) the diversity of students' concept projections across different tasks, and, building on that, outline (2) characteristics underlying productive concept projections of resonance.

RQ 1: How diverse are students' concept projections of resonance across different problem-solving contexts?

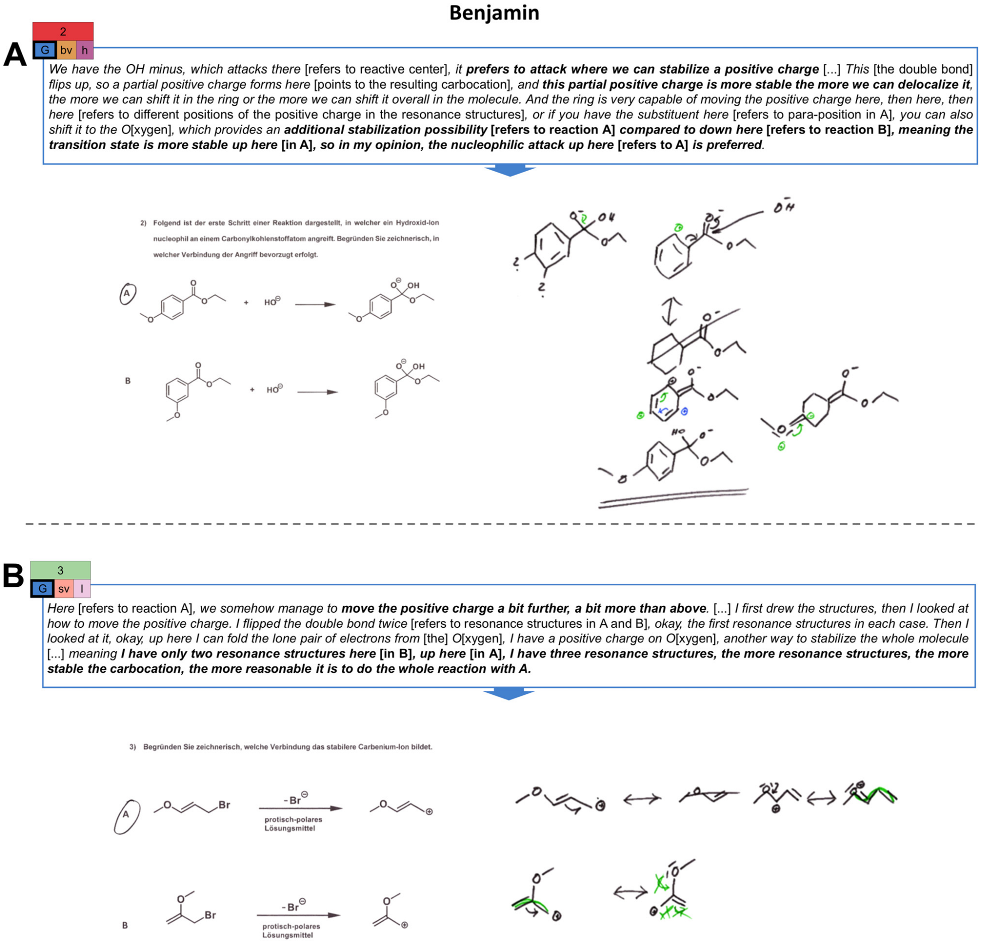
Across the three contexts, all students in our sample showed varying concept projections in terms of the extraction strategies, the types of extractions, the activated resources, and the complexity of the resulting inferential nets. This section outlines general findings on the diversity of students' concept projections and describes the general use of the coordination class components.

Multiplicity of extraction strategies within and across tasks. With regard to the extraction strategies, in general, the three tasks required different approaches. While for the first and second task (electrophilic aromatic substitution and nucleophilic addition step), the impact of the different substituents and their electron density distribution on the reactive centre needs to be closely examined, the third task (departure step of a leaving group) demands the comparison of the stability of the resulting products. This suggests that students ideally activate a *reactivity* extraction strategy for the first two tasks and a *global stability* extraction strategy for the third task. However, students' extraction strategies differed, as they employed various extraction strategies for the same task as well as inconsistently over all tasks. For instance, in the first task, two students employed a *global stability* extraction strategy, while 14 chose a *reactivity* approach. One student used a *structural considerations* strategy, and four used *electrostatic considerations* as an extraction strategy. While not all of these extraction strategies led to successful problem-solving in the first task, the same extraction strategies could be productive in other tasks. For instance, Benjamin's extraction strategy, *global stability*, did not contribute to a correct task solution in the second task as he evaluated the stability of the two given molecules in general (Fig. 5A). Yet, by framing the third task similarly and activating the same extraction strategy, he solved the task successfully (Fig. 5B). Altogether, across all three contexts, various extraction strategies led to productive concept use. This highlights that there are different ways of considering resonance for successful problem-solving, as suggested by the coordination class theory. The inconsistency of students' extraction strategies over all tasks aligns with this assumption. Students often changed their strategies, for instance, from considering the reactivity in the first task and focusing on global stability in the second task. This indicates that students, perhaps due to the higher structural complexity in the second task, framed the two tasks differently (Tannen, 1993; Hammer *et al.*, 2005; DeFever *et al.*, 2015).

Even when students applied the same extraction strategy for a task, it did not necessarily lead to the same claim. For instance, despite choosing the same *global stability* extraction strategy for the third task, Anna's and Liam's success differed (*cf.* Fig. 6). Given that the extraction strategy is only one component of a coordination class, the interplay between the different coordination class components might have caused these students' varying overall problem-solving success. As depicted in Fig. 6, Liam and Anna attended to different structural features as extractions (*single-focused vs. both-focused*). Although the subsequent connection of inferred resources results in inferential nets of similar complexity, the resources within the inferential net differ, so that the nature of the inferred resources might have heavily contributed to the overall problem-solving success. This example shows well that even though students seem to approach a task similarly, they can deal with it differently, focusing on other structural features and activating different ideas about resonance.

In many cases, students changed their extraction strategies within a task, sometimes multiple times (5 students in the first and third task, 10 students in the second task). This suggests that in the rather unfamiliar context, students needed more time to orient themselves. This might be possibly due to cognitive overload, *e.g.*, deciding and focusing on relevant aspects (Sweller, 1988). But generally, it shows that the unfamiliar context may have led them to adjust their reasoning, thus, activating more suitable extraction strategies to overcome dead-ends.

Variety of extraction types. According to the coordination class theory, extraction strategies guide students' attention to structural information which is extracted during problem-solving (DiSessa and Wagner, 2005). Similar to the extraction strategies, the types of extractions used in the three contexts varied and were not particularly related to unsuccessful or successful problem-solving. Across the contexts, students used



We have the OH minus, which attacks there [refers to reactive center], *it* ***prefers to attack where we can stabilize a positive charge*** [...] *This* [the double bond] *flips up, so a partial positive charge forms here* [points to the resulting carbocation], *and* ***this partial positive charge is more stable the more we can delocalize it****, the more we can shift it in the ring or the more we can shift it overall in the molecule. And the ring is very capable of moving the positive charge here, then here, then here* [refers to different positions of the positive charge in the resonance structures], *or if you have the substituent here* [refers to para-position in A], *you can also shift it to the O*[xygen], *which provides an* ***additional stabilization possibility* [refers to reaction A] *compared to down here* [refers to reaction B], *meaning the transition state is more stable up here* [in A], *so in my opinion, the nucleophilic attack up here* [refers to A] *is preferred***.

2) Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.

Here [refers to reaction A], *we somehow manage to* ***move the positive charge a bit further, a bit more than above****.* [...] *I first drew the structures, then I looked at how to move the positive charge. I flipped the double bond twice* [refers to resonance structures in A and B], *okay, the first resonance structures in each case. Then I looked at it, okay, up here I can fold the lone pair of electrons from* [the] *O*[xygen], *I have a positive charge on O*[xygen], *another way to stabilize the whole molecule* [...] *meaning* ***I have only two resonance structures here* [in B], *up here* [in A], *I have three resonance structures, the more resonance structures, the more stable the carbocation, the more reasonable it is to do the whole reaction with A.***

3) Begründen Sie zeichnerisch, welche Verbindung das stabilere Carbenium-Ion bildet.

- Br$^{\ominus}$

protisch-polares Lösungsmittel

Fig. 5 (A) Benjamin's activation of the global stability (G) extraction strategy in the second (unproductive concept projection) and (B) third task (productive concept projection) along with his constructed drawings as task solution. For the tasks, *cf.* Fig. 2. Extraction types (bv = *both-varied*, sv = *single-varied*) and the complexity of resource graphs (h = high, l = low) are also indicated. The resource graphs can be found in Appendix 7.

a *single-focused* extraction type in 21% of the concept projections (success rate of 69%). The *single-varied* extraction type was used in 17% of the concept projections (success rate of 91%). 33% of the concept projections involved a *both-focused* extraction type (success rate of 57%), while students used a *both-varied* extraction type in 29% of the concept projections (success rate of 72%). Although the extraction strategies highly influence the extraction of concept-related information, in our cohort, extraction strategies only evoked a certain extraction type in a few cases, underlining the complex interplay of coordination class components. For instance, students with a *reactivity* extraction strategy took during problem-solving more often structural information at a local and global level into account.

Frequency of activated resources. As addressed in Anna's and Liam's problem-solving for the third task, the productivity of a concept projection is highly influenced by the interplay and contribution of the different coordination class components, which impact one another. As such, based on the extraction strategies, students' extractions elicit multiple resources (*e.g.*, p-prims, rules, if-then statements), which are combined to reason and draw meaningful conclusions for the tasks at hand (DiSessa and Wagner, 2005). A closer look at the distribution of resources across the three contexts reveals some tendencies in resource activation. Fig. 7 shows that some resources are activated with a similar frequency across all tasks (*e.g.*, *stable is energetically favourable*, *the closer the charge, the higher the*

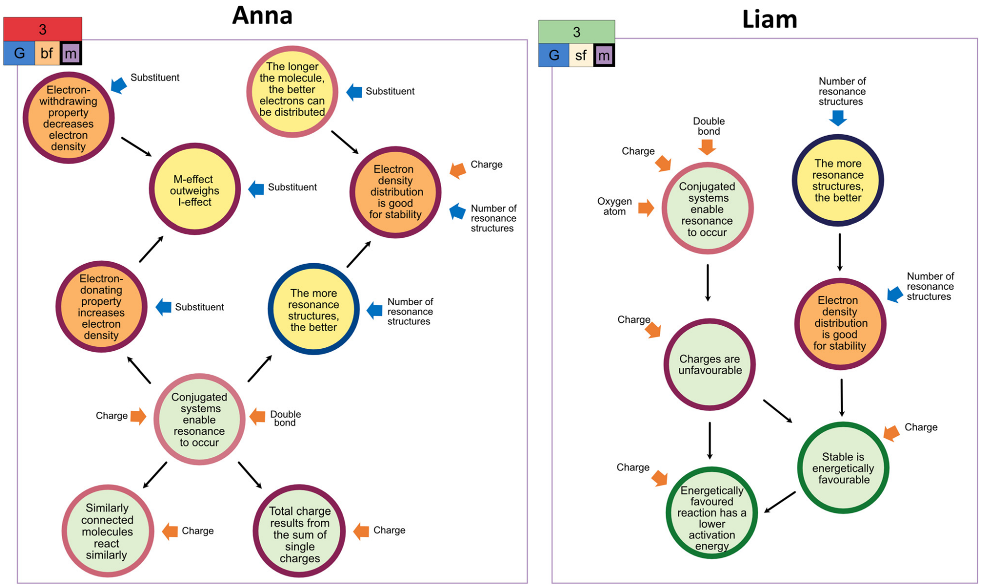
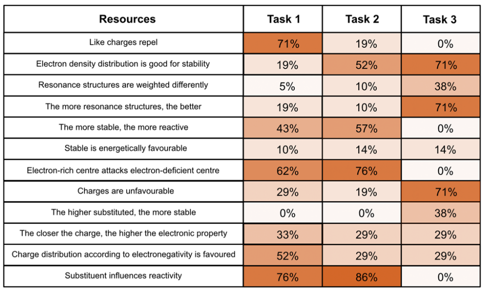


Fig. 6 Anna's and Liam's concept projections for the third task illustrating the respective resource graphs and indicating readout strategy (G = *global stability*), extraction types (bf = *both-focused*, sf = *single-focused*) and complexity of resulting resource graphs (m = medium). For a detailed explanation of the resource graphs, *cf.* section "Theme 5. The interconnectedness of resources across different levels of granularity enhances productive concept projections".



Resources	Task 1	Task 2	Task 3
Like charges repel	71%	19%	0%
Electron density distribution is good for stability	19%	52%	71%
Resonance structures are weighted differently	5%	10%	38%
The more resonance structures, the better	19%	10%	71%
The more stable, the more reactive	43%	57%	0%
Stable is energetically favourable	10%	14%	14%
Electron-rich centre attacks electron-deficient centre	62%	76%	0%
Charges are unfavourable	29%	19%	71%
The higher substituted, the more stable	0%	0%	38%
The closer the charge, the higher the electronic property	33%	29%	29%
Charge distribution according to electronegativity is favoured	52%	29%	29%
Substituent influences reactivity	76%	86%	0%

Fig. 7 Relative frequency of activation of selected resources across the different tasks. A full overview of the resource activations can be found in Appendix 5.

electronic property). Additionally, there exist some context-specific differences in resource activation. For instance, most students activated resources related to reaction processes in the first two tasks. This includes, among others, the activation of resources considering the impact of substituents on the reaction pathway, or the interaction between electron-rich and electron-deficient centres. Interestingly, students in the first task often activated ideas related to electronegativity and the repulsion of similar charges. However, they seldom activated the influence of electron density distribution on the molecule's stability as a resource. In contrast to that, in the third task, students seldom used the resource *the more stable, the more reactive* even though this task requires comparing the stability of the two compounds. Instead, the students activated the resource *the higher substituted, the more stable* and *charges are unfavourable* with higher frequency, indicating that the students activated more resources considering the molecules at a rather local level. Compared to the first two tasks, students more often weighed the resonance structures and used the overall number of resonance structures to determine the molecules' stability. It is noteworthy that some resources related to electron distribution (*e.g.*, *electron density distribution is good for stability, charge distribution according to electronegativity is favoured*) are not equally activated across the tasks, although considering electron density is inherent to the resonance concept (Richardson, 1986). Despite differences in students' activation of resources, the overall complexity of their activated inferential nets does not influence *per se* the productivity of their concept projections. In fact, students' resource activation and combination can be productive (*i.e.*, contribute to successful problem-solving), regardless of whether the resource graph is of a low or high complexity (*cf.* examples in Fig. 6, 13, 15, and Appendix 7). This indicates that an inferential net with suitable resources matching the task affordances seems more beneficial than the actual complexity of the resulting inferential net.

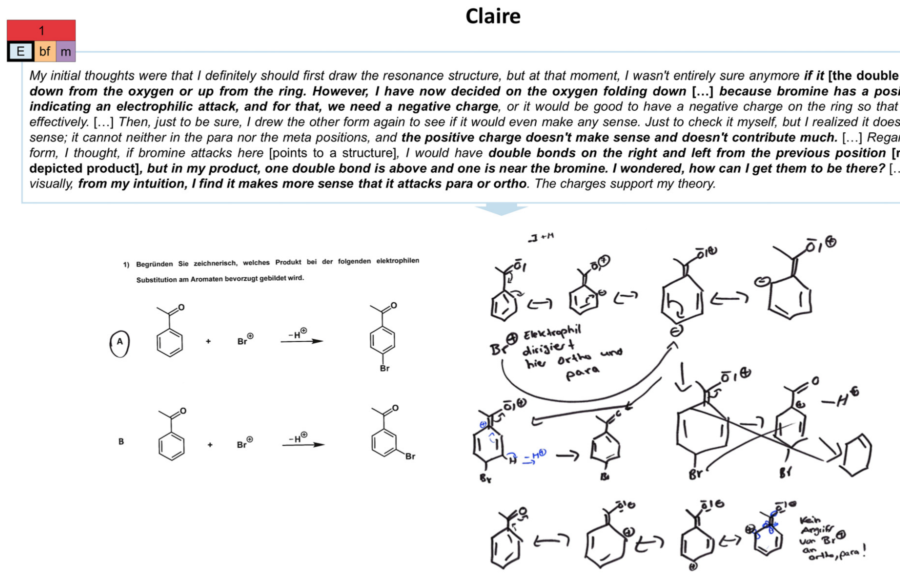
It can be concluded from these results that students' concept projections of resonance are diverse and individual across the tasks. They result as a product of the complex interplay of coordination class components, which impact one another and contribute as a whole to the (un-)productivity of a concept projection. As different extraction strategies, extraction types and resources can lead to successful problem-solving, there is not *one* way of using resonance productively. Given the variety of concept projections and the (un-)productive consideration of resonance in problem-solving, RQ 2 explores what differentiates students' productive concept projections of resonance from unproductive ones, and what characteristics within the coordination class components underlie the overall productivity of a concept projection.

RQ 2: How do the coordination class components contribute to the productivity of students' concept projections of resonance?

While acknowledging the diversity of concept projections, focusing in more detail on students' individual problem-solving processes (Hammer *et al.*, 2005) makes it possible to elicit underlying characteristics within the coordination class components and to show their contribution to the overall productivity of the concept projection. Therefore, multiple cases of productive and unproductive concept projections will be qualitatively contrasted to shed light on differences within the coordination class components, their impact on one another, and the aspects differentiating the various concept projections in terms of successful problem-solving.

Theme 1. Inductively and reflectively activated extraction strategies and the task affordances contribute to the productivity of concept projections

Fragmented use of drawings and uncertainty. Across the three tasks, students used various extraction strategies for dealing with resonance. However, comparing students' problem-solving revealed some reoccurring trends in their approaches. Irrespective of the concrete extraction strategy, these strategies affected the extractions, the activation of resources, and the overall productivity of the concept projections (*i.e.*, resulting in varying problem-solving success). Consider, for instance, Claire's reasoning in the electrophilic substitution reaction in which she activated *electrostatic considerations* as an extraction strategy to frame her subsequent problem-solving process (Fig. 8). The excerpt shows that Claire has a strong focus on structural features. Cued by the positive charge (*i.e.*, extraction), she decides to solve the task by forming a negative charge. Although Claire considers the interaction of entities as an important aspect of mechanisms (Russ *et al.*, 2008), her extraction strategy is unproductive. This is due to her focus on salient structural features (*i.e.*, charges) instead of analysing her constructed structures to infer properties enabling the reaction to occur. Consequently, Claire shows a narrowed structural focus when approaching the task. As in many other cases of unproductive concept projections, the extraction strategies were often paired with uncertainty about how to approach the task in general. In Claire's case, this led to the activation of resources, which were rather competing ideas (*cf.* her resource graph in Appendix 7). More precisely, Claire was unsure



My initial thoughts were that I definitely should first draw the resonance structure, but at that moment, I wasn't entirely sure anymore ***if it*** **[the double bond]** ***folds down from the oxygen or up from the ring. However, I have now decided on the oxygen folding down*** **[…]** ***because bromine has a positive charge, indicating an electrophilic attack, and for that, we need a negative charge****, or it would be good to have a negative charge on the ring so that it can attack effectively.* […] *Then, just to be sure, I drew the other form again to see if it would even make any sense. Just to check it myself, but I realized it doesn't make any sense; it cannot neither in the para nor the meta positions, and* ***the positive charge doesn't make sense and doesn't contribute much.*** […] *Regarding the ring form, I thought, if bromine attacks here* [points to a structure], *I would have* **double bonds on the right and left from the previous position [refers to the depicted product]*****, but in my product, one double bond is above and one is near the bromine. I wondered, how can I get them to be there?*** […] *In general, visually,* ***from my intuition, I find it makes more sense that it attacks para or ortho****. The charges support my theory.*

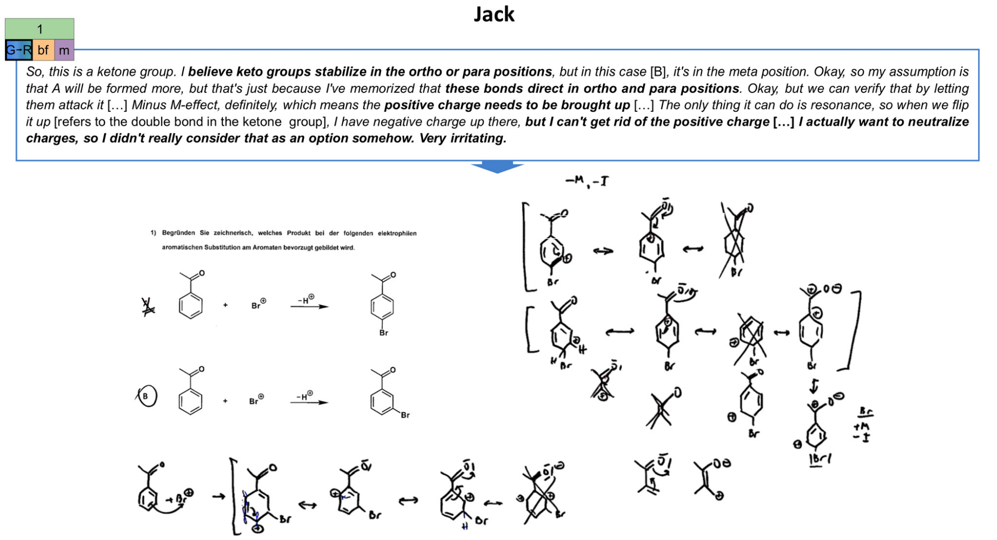
1) Begründen Sie zeichnerisch, welches Produkt bei der folgenden elektrophilen Substitution am Aromaten bevorzugt gebildet wird.

Fig. 8 Illustration of Claire's *electrostatic considerations* (E) extraction strategy in the first task (*cf.* Fig. 2) and her constructed drawings. As indicated, her unproductive concept projection also encompasses a *both-focused* (bf) extraction type and a resource graph of medium complexity (m). The resource graph can be found in Appendix 7.

how the ketone substituent impacts the electrophilic substitution and assumed that, depending on the situation, the ketone could have different electronic properties. Consequently, she constructed multiple resonance structures with the ketone being both electron-donating and electron-withdrawing (Fig. 8). She then decided on the electron-withdrawing property due to the positive charge of the bromine cation which "need[s] a negative charge". Claire's case aligns with a huge body of research in chemistry education, demonstrating that if learners struggle to activate relevant conceptual resources (*i.e.*, derive implicit properties), a reliance on explicit structural features occurs, often hindering successful problem-solving (*e.g.*, McClary and Talanquer, 2011; Anzovino and Bretz, 2015; Anzovino and Bretz, 2016; Graulich and Bhattacharyya, 2017; Galloway *et al.*, 2018; Popova and Bretz, 2018b; Graulich *et al.*, 2019). Claire's case exemplifies that students with unproductive extraction strategies do not or only partly use their drawings as a problem-solving tool (Cooper *et al.*, 2017). Instead, they tend to project their ideas into the structures. This approach might be supported by salient structural features or students' personal views (Hogan and Maglienti, 2001). Claire explored through her drawings the different possibilities for the electronic effect of the carbonyl group. She concluded that the *para*-position "looked" more plausible to her (Fig. 8). In fact, activating an unproductive extraction strategy might also be related to difficulties in dynamically interpreting electron distribution. As documented by Taber (2002), students' difficulties in conceptualizing resonance are related to the tendency to interpret structural diagrams *literally*, with resonance being the re-location of bonds instead of a dynamic delocalization of electrons. Aligning with that, Claire considered the resonance structures as static entities given that she got stuck with the double bond, which, in her opinion, must correspond to the depicted product.

Activation of overgeneralized rules. Generally, in unproductive concept projections, students' activation of extraction strategies is in line with many characteristics documented in research on students' problem-solving in Organic Chemistry (*e.g.*, Ferguson and Bodner, 2008). For instance, with the fact that students' activation of unproductive extraction strategies is often linked to a narrowed focus on single structural features or the activation of overgeneralized rules. In our study, this often led to problem-solving dead-ends. The excerpt from Jack's initial problem-solving process in the first task, in which he applied a *global stability* extraction strategy (before changing it later to the *reactivity* extraction strategy), illustrates that (Fig. 9). Jack struggles with the electron-withdrawing property of the ketone substituent and tries to make the positive charge disappear to gain a more stable system (*i.e.*, the extraction strategy *global stability*). He does recognize important aspects such as stability in a reaction, and pays attention to charges to consider the impact of varying electron density distribution. But in relation to the activation of ideas targeting the electron-withdrawing effects, the resource *electron-withdrawing property removes charges* strongly influenced how he used the extraction strategy *global stability* (*cf.* his resource graph in Appendix 7). As such, he ended up being puzzled by his approach, as he could not link the electronic effect to resonance, *i.e.*, he got stuck trying to remove the charge. He tried multiple variants to draw his resonance structures, as evident by the number of his drawings (Fig. 9).

Inductive and analytical approaches. Unlike Claire's extraction strategy for the first task, a closer look into her *reactivity*



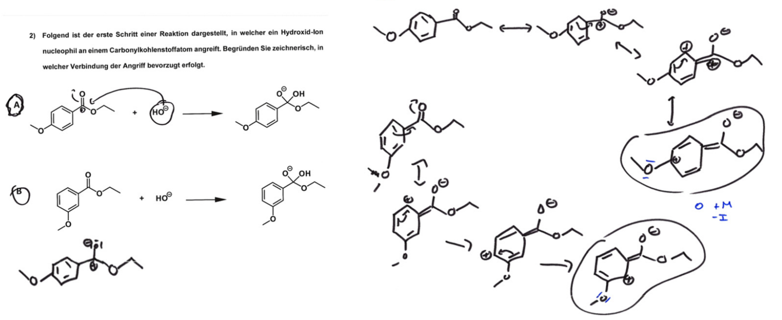
So, this is a ketone group. I ***believe keto groups stabilize in the ortho or para positions****, but in this case* [B], *it's in the meta position. Okay, so my assumption is that A will be formed more, but that's just because I've memorized that* ***these bonds direct in ortho and para positions****. Okay, but we can verify that by letting them attack it* […] *Minus M-effect, definitely, which means the* ***positive charge needs to be brought up*** […] *The only thing it can do is resonance, so when we flip it up* [refers to the double bond in the ketone group], *I have negative charge up there,* ***but I can't get rid of the positive charge*** **[…]** ***I actually want to neutralize charges, so I didn't really consider that as an option somehow. Very irritating.***

1) Begründen Sie zeichnerisch, welches Produkt bei der folgenden elektrophilen aromatischen Substitution am Aromaten bevorzugt gebildet wird.

Fig. 9 Illustration of Jack's initial *global stability* (G) extraction strategy in the first task (*cf.* Fig. 2) and his constructed drawings. As indicated, his (initially unproductive) concept projection also encompasses *a both-focused* (bf) extraction type and a resource graph of medium complexity (m). The resource graph can be found in Appendix 7.

Claire

I think that ***due to the plus M- and minus I-effects, the positive charge in the first reaction is better stabilized, and*** **[…]** ***the more unstable, the better; the more a compound is stabilized by resonance, the more stable and less reactive it is****. Because the better it's stabilized, the more the charge would distribute here* [pointing to the reactive center]*, and* ***we need the positive charge there so that the OH minus attacks****.* […] *So, the only difference between the two starting compounds is actually the ether. Therefore, I thought about that the difference in the reaction could be caused by the ether group. The position where our nucleophile attacks is the same, that doesn't change, which means the* ***attacking strength can only be influenced by the ether group, making it either decrease or increase****. That's why I thought it could be related to how well the group stabilizes the positive charge, depending on its location. So, I looked at the stabilities to figure out what happens to the charge* […] ***First, I checked where our hydroxide ion would attack.*** **[…]** ***Just to have an overview of where it attacks or what could happen there. What needs to happen for it to attack there?***

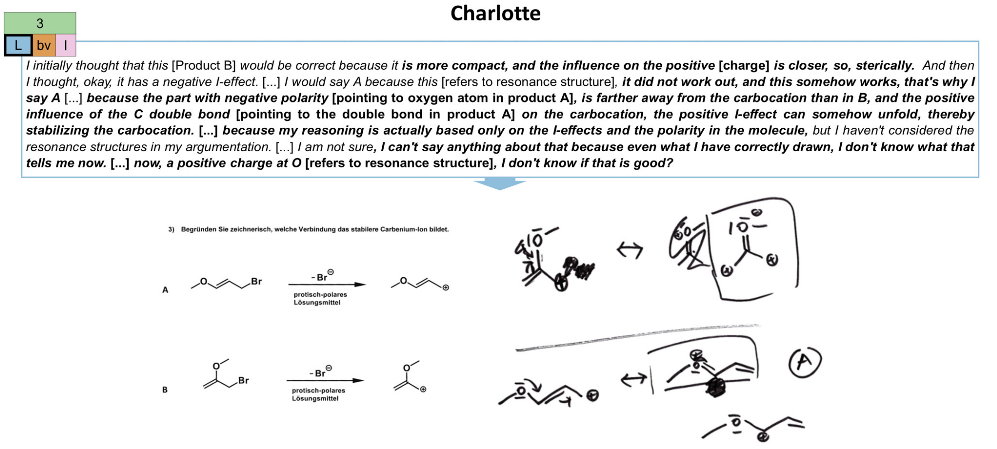


2) Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.

Fig. 10 Illustration of Claire's *reactivity* (R) extraction strategy in the second task (*cf.* Fig. 2) and her constructed drawings. As indicated, her productive concept projection also encompasses a *single-varied* (sv) extraction type and a resource graph of low complexity (l). The resource graph can be found in Appendix 7.

extraction strategy for the second task reveals various aspects that explain productive concept projections (*i.e.*, contributing to successful problem-solving) (Fig. 10). The excerpt shows that Claire approaches the second task inductively by making herself aware of the problem. Claire reconstructs the reaction step by closely examining the reaction conditions and prerequisites (*What is demanded in the task?*). She then points out the structural differences and their impact on the reaction (*i.e.*, the impact on the electrophilicity of the reactive centre). Hence, in contrast to the first task (Fig. 8), Claire has a differentiated process orientation and approaches the task more analytically. As a result, Claire interprets and reflects her derived findings regarding resonance (*i.e.*, the extent of charge stabilization) within the given reaction context. She activates resources targeting chemical concepts (*i.e.*, varying electrophilicity) to come to an answer (*cf.* her resource graph in Appendix 7). Her productive approach is in line with existing research on students' problem-solving and reasoning, indicating that a more thorough examination of reaction conditions and prerequisites seems beneficial for successful problem-solving (Yuriev *et al.*, 2017; Caspari and Graulich, 2019). As such, Chi *et al.* (1981) revealed in their early work on experts' and beginners' problem-solving that in comparison to beginners who base their approaches on the problems' literal features, experts approach tasks by initially abstracting underlying scientific principles to solve a problem. Taken together, productive concept projections often occur when extraction strategies match the task affordances (Airey and Linder, 2009), necessitating a more nuanced and analytical approach to a task.

Compensation of unsuitable extraction strategies through activation of relevant resources. Extraction strategies are not always a clear indicator of the productivity of the resulting concept projection. Instead, the different components in the coordination class may compensate for each other. Even if choosing an unsuitable extraction strategy, the components' interplay gives rise to a productive concept projection, resulting in successful problem-solving (Buteler and Coleoni, 2016). Consider, therefore, Charlotte's problem-solving in the third task as an example, in which she chooses *local stability* as an extraction strategy (Fig. 11). Here, Charlotte evaluates different factors contributing to the products' stability. Yet, she does not directly incorporate aspects of resonance concerning electron density distribution. Similar to using a mental rolodex (DeFever *et al.*, 2015), she adeptly navigates through other ideas, such as steric hindrance, inductive effects, and polarity, relative to the structures' geometry, indicating that she tried out several resources to solve the task. Thus, her focus was guided by singular fragments of the molecule. As a reason, she admits that her approach partly stems from her challenges in constructing the structures ("*it did not work out, and this somehow works*"). The cognitive overload to manage the information (Sweller, 1988) might be a reason why Charlotte incorporated resources targeting other (more familiar) concepts, as they might be easier to activate. For instance, Finkenstaedt-Quinn *et al.* (2020) showed in their study that students favoured the consideration of substitution over resonance when assessing the stability of molecules, as it allows the mere use of explicit chemical features instead of underlying, implicit electronic properties. Nevertheless, in Charlotte's overall task solution, she somewhat incorporated relevant resources, that enabled a successful task solution. As such, she considered the impact of electronic properties on stabilizing the positive charge (*cf.* her resource graph in Appendix 7). Even if she constructed valid resonance structures



I initially thought that this [Product B] *would be correct because it* ***is more compact, and the influence on the positive*** **[charge]** ***is closer, so, sterically.*** *And then I thought, okay, it has a negative I-effect.* [...] *I would say A because this* [refers to resonance structure], ***it did not work out, and this somehow works, that's why I say A*** [...] ***because the part with negative polarity*** **[pointing to oxygen atom in product A]**, ***is farther away from the carbocation than in B, and the positive influence of the C double bond*** **[pointing to the double bond in product A]** ***on the carbocation, the positive I-effect can somehow unfold, thereby stabilizing the carbocation.*** **[...]** ***because my reasoning is actually based only on the I-effects and the polarity in the molecule,*** *but I haven't considered the resonance structures in my argumentation.* [...] *I am not sure*, ***I can't say anything about that because even what I have correctly drawn, I don't know what that tells me now.*** **[...]** ***now, a positive charge at O*** **[refers to resonance structure]**, ***I don't know if that is good?***

Fig. 11 Illustration of Charlotte's *local stability* (L) extraction strategy in the third task (*cf.* Fig. 2) and her constructed drawings. As indicated, her productive concept projection also encompasses a *both-varied* (bv) extraction type and a resource graph of low complexity (l). The resource graph can be found in Appendix 7.

for the reaction in A (Fig. 11), she could not interpret these structures dynamically and did not consider the overall electron density distribution. Instead, due to her *local stability* approach, she assessed the quality of singular resonance structures by considering the resonance structures as discrete, static entities. Stated differently, she compared in which position the charge is most likely to be stabilized through substituents. Due to that, she struggled to evaluate the positive charge on the oxygen atom (Fig. 11). Although Charlotte's task approach does not match well with the task affordances, it leads to the activation of relevant electronic resources and a correct answer.

Theme 2. Analytically engaging with one's drawings induces productive changes in extraction strategies

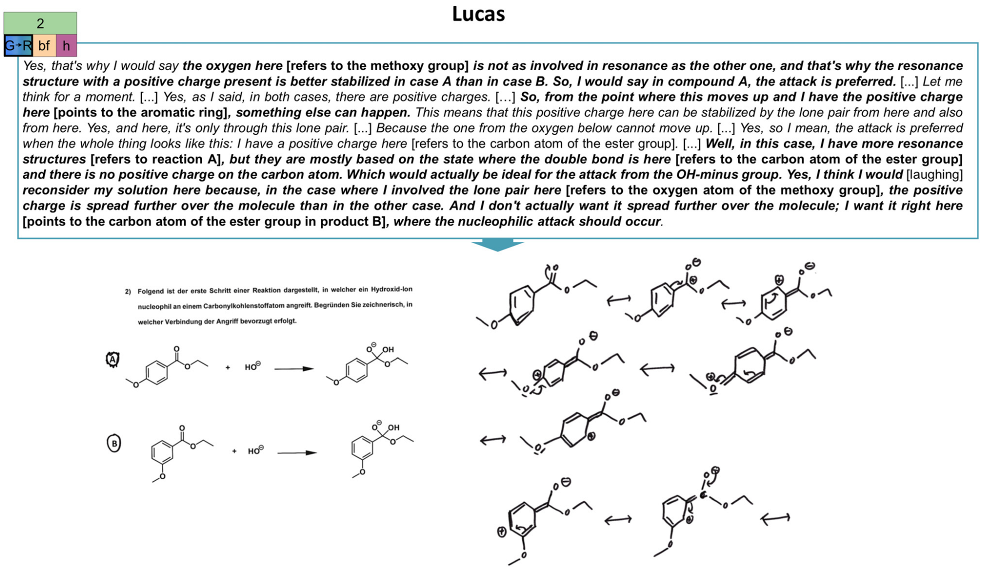
Some students changed their extraction strategies within a task due to new insights during their problem-solving process. Whether the changes in extraction strategies contributed to productive or unproductive concept projections often depended on students' engagement with their drawings. To illustrate, consider the excerpt from Lucas' retrospective for the second task (Fig. 12).

First, Lucas applied a *global stability* extraction strategy to assess the preferred reactivity in both reactions, which he changed to a *reactivity* approach. By doing this, he advanced his ideas. He developed them further by reconsidering and closely analysing his drawings in relation to the task affordances (*i.e.*, comparison of the electrophilicity in the two molecules). He was zooming in and out based on his drawings. Other students also changed their extraction strategies toward successful problem-solving after describing their approach and reasoning. This indicates that (self-)explanations for why one did something help students to refocus, reflect, and engage analytically with the task and their ideas (Chi *et al.*, 1994). Such a meta-level perspective gives rise to productive task approaches with extraction strategies matching the task affordances (Airey and Linder, 2009). In our cohort, students often realized while elaborating their task approach by referring to the respective drawings that something was missing or incongruent with the task requirements. They then started to re-examine their drawings critically. In some cases, the consecutive construction of resonance structures helped the students refocus and gain further insights (*e.g.*, Claire's problem-solving in task 2, *cf.* Fig. 10). Following that, the analytical engagement with and nuanced analysis of the structures in relation to the task affordances crucially influence the activation of suitable extraction strategies for the tasks. These extraction strategies affect the structural features encountered, as outlined in the following section.

Theme 3. Managing the variety of structural extractions makes the difference

The diversity of concept projections was not paired with clear trends in extraction types regarding productivity (*cf.* RQ1). Nevertheless, the analysis of students' problem-solving process indicates that considering structural features in their variety and across the global and local levels contributed to a productive concept projection. Students who encountered different structural features as extractions (sv, bv) were more likely to have a productive concept projection than those who narrowed their extractions to a few structural features (sf, bf) (*cf.* RQ 1). The reasons for this finding can be exemplified in more detail by contrasting excerpts of Emily's and Alina's problem-solving for the first task.

In both cases, the inferential nets do not show high complexity and are comparable as each has multiple linear connections (Fig. 13). However, different extraction types are underlying and have influenced the students' problem-solving success. Consider Emily's focus on single structural features. She predominantly uses extractions at a global level (*i.e.*, the number of resonance structures and the substituent). Even though she refers to the local level, she only focuses on the positive charge (Fig. 13). This indicates that she



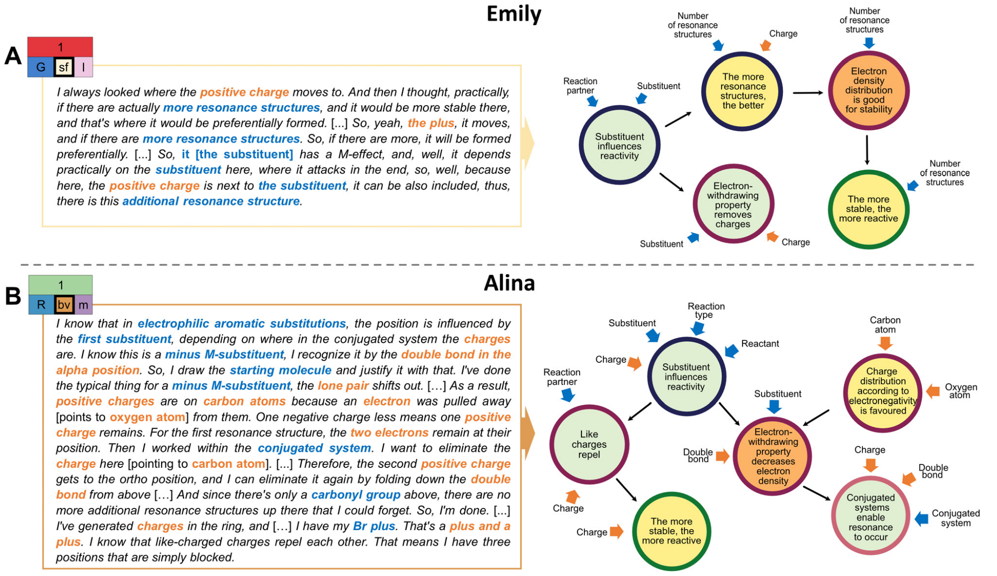
Yes, that's why I would say ***the oxygen here*** **[refers to the methoxy group]** ***is not as involved in resonance as the other one, and that's why the resonance structure with a positive charge present is better stabilized in case A than in case B. So, I would say in compound A, the attack is preferred.*** [...] *Let me think for a moment.* [...] *Yes, as I said, in both cases, there are positive charges.* [...] ***So, from the point where this moves up and I have the positive charge here*** **[points to the aromatic ring]*****, something else can happen.*** *This means that this positive charge here can be stabilized by the lone pair from here and also from here. Yes, and here, it's only through this lone pair.* [...] *Because the one from the oxygen below cannot move up.* [...] *Yes, so I mean, the attack is preferred when the whole thing looks like this: I have a positive charge here* [refers to the carbon atom of the ester group]. [...] ***Well, in this case, I have more resonance structures*** **[refers to reaction A]*****, but they are mostly based on the state where the double bond is here*** **[refers to the carbon atom of the ester group]** ***and there is no positive charge on the carbon atom. Which would actually be ideal for the attack from the OH-minus group. Yes, I think I would*** [laughing] ***reconsider my solution here because, in the case where I involved the lone pair here*** **[refers to the oxygen atom of the methoxy group]*****, the positive charge is spread further over the molecule than in the other case. And I don't actually want it spread further over the molecule; I want it right here*** **[points to the carbon atom of the ester group in product B]*****, where the nucleophilic attack should occur****.*

2) Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.

Fig. 12 Illustration of Lucas' change from the *global stability* (G) extraction strategy to the *reactivity* (R) extraction strategy in the second task (*cf.* Fig. 2) and his constructed drawings. As indicated, his productive concept projection also encompasses a *both-focused* (bf) extraction type and a resource graph of high (h) complexity. The resource graph can be found in Appendix 7.

looked at her drawings with a specific focus, *i.e.*, searching for cues that support stability considerations. As a result, though mentioning the mesomeric effect, she could not specify the carbonyl's electron-donating or -withdrawing property. Her focused attention to structural features in problem-solving is also a common observation in other studies. For instance, Anzovino and Bretz (2015) showed in the context of electrophiles and nucleophiles that students tend to rely primarily on charges when defining and identifying electrophiles and nucleophiles in general, and when dealing with specific chemical reactions. Our own recent findings on students' drawing processes of resonance structures also show that a focus on singular features such as charges or hetero atoms without a link to other structural features often results in invalid resonance structures (Braun *et al.*, 2022). As a result, Emily struggled to draw missing resonance structures and did not activate charge interactions in her problem-solving. The few extractions encountered in her problem-solving influenced how she approached the task (*i.e.*, she got stuck with the *global stability* extraction strategy). In fact, across the 19 unsuccessful task solutions, in 12 cases, students used *focused* extractions. Albeit possibly considering both the local and global levels within their drawings, they generally paid attention to a limited number of structural features and overemphasized certain structural components when activating resources. Consequently, this static focus on singular features might have contributed to activating unproductive resources (*e.g.*, immediately linking the extraction *aromatic compounds* with the resource *aromatic compounds are stable*).

In contrast to these focused extractions, a closer look into Alina's excerpt demonstrates that she takes a broad amount of structural information into account (Fig. 13), which underlines a more thorough structural analysis. As seen in both retrospectives (Fig. 13), Alina and Emily approach the task similarly by highlighting the substituents' function in determining the position of the electrophilic substitution. In doing so, unlike Emily, Alina approaches this differently. She includes more structural information by transitioning between various structural features at the local (*e.g.*, charges, double bond, atom types, lone pair) and global levels (*e.g.*, substituent, reaction partner, reactant, reaction type), and considering a variety of features on each level. As such, she uses an analytic, differentiated approach. She pays attention to the drawings as a coherent system. The interplay of various structural features gives rise to conclusions and resource activations that are relevant to the reaction at hand. This resonates with the *reactivity* extraction strategy, which is often paired with a more nuanced analysis of the task affordances, as reported in the previous section. Managing the granularity of extractions seems to be beneficial for problem-solving. This involves zooming in and out to analyse in detail the structures in their *entirety* across both local and global levels (*i.e.*, taking into account the multiplicity of structural features), and combining them to activate resources for problem-solving. Eventually, it allows one to widen the perspective on the given task and the conditions at hand and, consequently, guides one's thinking to



*I always looked where the **positive charge** moves to. And then I thought, practically, if there are actually **more resonance structures**, and it would be more stable there, and that's where it would be preferentially formed. [...] So, yeah, **the plus**, it moves, and if there are **more resonance structures**. So, if there are more, it will be formed preferentially. [...] So, **it [the substituent]** has a M-effect, and, well, it depends practically on the **substituent** here, where it attacks in the end, so, well, because here, the **positive charge** is next to **the substituent**, it can be also included, thus, there is this **additional resonance structure**.*

*I know that in **electrophilic aromatic substitutions**, the position is influenced by the **first substituent**, depending on where in the conjugated system the **charges** are. I know this is a **minus M-substituent**, I recognize it by the **double bond in the alpha position**. So, I draw the **starting molecule** and justify it with that. I've done the typical thing for a **minus M-substituent**, the **lone pair** shifts out. […] As a result, **positive charges** are on **carbon atoms** because an **electron** was pulled away* [points to ***oxygen atom***] *from them. One negative charge less means one **positive charge** remains. For the first resonance structure, the **two electrons** remain at their position. Then I worked within the **conjugated system**. I want to eliminate the **charge** here* [pointing to ***carbon atom***]. *[...] Therefore, the second **positive charge** gets to the ortho position, and I can eliminate it again by folding down the **double bond** from above […] And since there's only a **carbonyl group** above, there are no more additional resonance structures up there that I could forget. So, I'm done. [...] I've generated **charges** in the ring, and […] I have my **Br plus**. That's a **plus and a plus**. I know that like-charged charges repel each other. That means I have three positions that are simply blocked.*

Fig. 13 Comparison of Emily's and Alina's extraction types (*single-focused* [sf], *both-varied* [bv]) with an illustration of their overall resulting resource graphs (low [l] and medium [m] complexity) in the first task. While Emily's concept projection is unproductive and exhibits a *global stability* (G) extraction strategy, Alina's concept projection is productive and involves a *reactivity* (R) extraction strategy. The orange highlighting in the quotes indicates local extractions, the blue highlighting global extractions.

activate more productive, analytical resources (*e.g.*, derive electronic effects of the structural composition in a molecule).

Theme 4. Productive concept projections involve more analytical-comparative resources

In comparing the cases of productive and unproductive concept projections, differences in the types of activated resources become evident. Fig. 14 illustrates the activation frequency for a subset of resources used in (un-)productive concept projections.

When qualitatively contrasting the frequency of resource activation, it becomes evident that students with unproductive concept projections tended to infer more resources that do not touch upon the electron density distribution as the underlying idea of the resonance concept (*e.g.*, the resource *steric hindrance makes attack more difficult*) (Fig. 14). The students also included more often heuristic-like resources such as *similarly connected molecules react similarly* or *aromatic compounds are stable*, and activated other resources like *electron-withdrawing property removes charges*. The activation of resources that are not related to the actual meaning of resonance (or only consider it in a very simplified way) often does not allow one to make productive concept projections, as in line with former studies (Brandfonbrener *et al.*, 2021; Tetschner and Nedungadi, 2023). Some of these resources are reflections of students' *structural considerations* and *electrostatic considerations* extraction strategies. As such, these resources refer to the structure itself (*e.g.*, *steric hindrance makes attack more difficult*) and are rather static in nature (*e.g.*, *unlike charges attract*).

On the contrary, when showing productive concept projections, students more often elicited resources that are (structural-) analytic and weighing-comparative in nature. For instance, they included more often the electronegativity of the atoms in their reasoning and considered the prerequisites for resonance (*e.g.*, *conjugated systems enable resonance to occur*) during problem-solving. This indicates that students with productive resonance use activate more nuanced ideas. In contrast to unproductive concept projections, students also considered some energetic considerations more frequently (*e.g.*, the relationships between stability and reactivity and *energetically favoured reaction has a lower activation energy*) (Fig. 14).

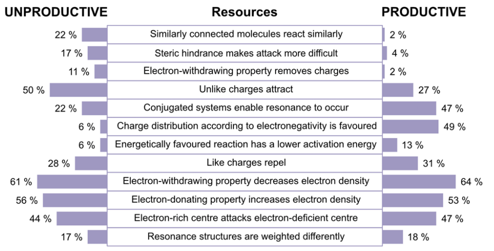


Fig. 14 Relative activation frequency of selected resources in (un-)productive concept projections.

Despite these slight differences in the activation of resources, Fig. 14 also shows that students, regardless of the productivity of their concept projection, activated many resources with comparable frequency (*cf.* also the complete list in Appendix 6). The activation of a specific resource is thus not a sufficient indicator of how resources contribute to the productivity of concept projections. Instead, in accordance with the coordination class theory, it is pivotal to further shed light on how students combine and organize the activated resources within their inferential nets (DiSessa and Sherin, 1998).

Theme 5. The interconnectedness of resources across levels of granularity enhances productive concept projections

When looking at students' combination of activated resources in their inferential nets, one can contrast Audrey's and Louis' resource graphs for the first task. Both students used similar types of extractions by referring to the local and global level, but focusing altogether on relatively few features (*i.e.*, *both-focused* extractions). However, their inferential nets differ in complexity, with a low complexity for Audrey's and a high complexity for Louis' reasoning (Fig. 15).

Audrey's resource graph reveals that in her reasoning, one resource consecutively activates another one, resulting in a rather linear structure. It depicts two branches of dualistic thoughts and shows different possibilities for reactivities. Similar to Claire (*cf.* Fig. 8), she assumed that the substituent can have, depending on the situation, an electron-withdrawing or electron-donating effect. Her activated set of resources targets different, singular (static) aspects, such as charge interactions and their influence on the reaction pathway in terms of electron density. Thus, they are analytic and distributive in nature. Her graph further reveals that her resources are mainly situated at the electronic level. She first activates a resource mapping the oxygen atom's reactivity with similar-looking structures from her experience (*i.e.*, a resource at a structural level). Subsequently, she focuses on aspects targeting electron density (*i.e.*, electron-withdrawing or -donating properties, low electron density attracting high electron density, and charge interactions). These are, in fact, crucial aspects when evaluating reaction pathways as they give insight into *why* a reaction happens (Cooper, 2015). However, Audrey fails to connect her resources with energetic considerations. Similar findings have been recently reported by Pölloth *et al.* (2023), showing that also high-school chemistry students seldom activate resources attributing energy to structural changes when reasoning about a chemical reaction.

In contrast to that, Fig. 15 shows that Louis' resource graph is characterized by a higher complexity with resources being (inter-)connected, building a complex net of inferences to solve the task at hand. His reasoning is grounded in considering aspects such as electronegativity and activation energy, which make his problem-solving more differentiated than Audrey's. This is supported by the fact that he activates and combines multiple resources

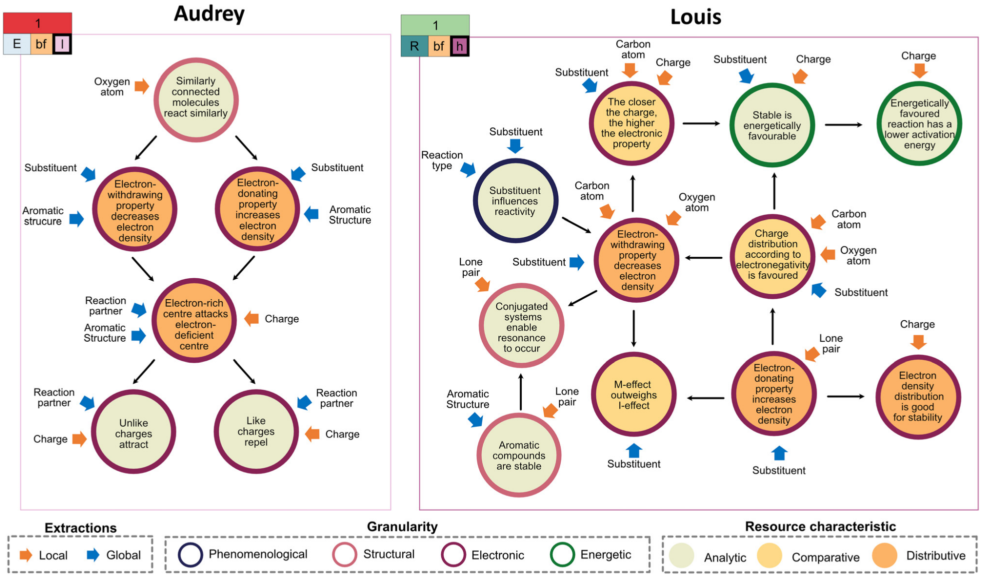


Fig. 15 Resource graphs for Audrey's and Louis' problem-solving in the first task with an indication of the resource granularity (color of outer circles) and resource characteristic (color of the inner circles). Louis exhibits a productive concept projection with a *reactivity* (R) extraction strategy, a *both-focused* (bf) extraction type and a resource graph of high (h) complexity. Audrey's concept projection is unproductive and encompasses an *electrostatic considerations* (E) extraction strategy, a *both-focused* (bf) extraction type and a resource graph of low (l) complexity.

that can be modeled with Deng and Flynn's (2021) analytical framework of granularity levels. As such, he transitions in his problem-solving between different levels. While he first states at a phenomenological level that the substituent influences the position of substitution, he proceeds by activating resources at a structural (*e.g.*, *conjugated systems enable resonance to occur*), electronic (*e.g.*, *electron-withdrawing property decreases electron density*), and energetic level (*e.g.*, *stable is energetically favourable*). Along with the intended learning outcomes of resonance formulated by Carle and Flynn (2020), the transition across granularity levels shows that the student adopts a dynamic, holistic perspective of resonance. By activating resources that target the affordances in this task, Louis activates resources with different characteristics, altogether helping him to draw correct conclusions to the task. His resources are not only analytic and distributive, but also weighing-comparative in nature (*i.e.*, assess the influence and extent of effects, such as electronic effects, by referring to chemical principles). Concretely, he decides on the electron-withdrawing effect of the substituent by combining this resource with electronegativity considerations. Although Audrey also activates the same resource (*i.e.*, electron-withdrawing properties), she does not activate other weighing-comparative resources. In light of the overall comparable frequency of resource activation for all students (*cf.* Fig. 14), these examples illustrate that the linkage between the different resources crucially decides whether the activated set of resources becomes productive for the concept projection. Irrespective of the overall complexity in their inferential nets, most students activated the electronic effects of substituents across the tasks. However, their joint activation and connection with weighing-comparative resources differentiated a productive from an unproductive resource activation, resulting in a more reflective use of resonance. Results in other disciplines and contexts also leverage this. For instance, Richards and colleagues (2018) found that students tend to activate combinations of different resource types when making conceptual breakthroughs in the context of photovoltaic cells. Similarly, a recent study focusing on students' conceptualization of buffers points out that emphasizing relations and connections between resources is valuable for conceptual understanding (Sheppard and Bauer, 2022).

Conclusions and implications

This paper aimed at delving into students' use of resonance in organic-chemical problem-solving across different contexts through the analytical lens of the coordination class theory. It sees a concept in its architecture as an interacting system of extraction strategies and activated resources based on extractions in a given situation. As such, we characterized students' engagement with constructed drawings of resonance structures, and qualitatively highlighted characteristics that distinguish productive from unproductive concept projections. In line with the assumptions of the *resource framework*, no apparent, general trend among the concept projections emerged. Instead, students' consideration of resonance varied for the different contexts (RQ 1). Given the variety of combined coordination class components, it became evident that a different focus in task approaches can lead to successful problem-solving. There is not only one valid way of considering resonance in problem-solving. The diversity is not only caused by different task affordances which lead to situation-specific framing, but also by the complex and individual interplay of extraction strategies, extractions, and activated resources. This detailed analysis also illustrated that a lot is going on when students are asked to consider the resonance concept in problem-solving, *i.e.*, constructing and drawing resonance structures, activating implicit properties of structural features, and linking these together to make a claim about the outcome. However, qualitatively contrasting these diverse concept projections revealed some characteristics underlying productive concept use (RQ 2). We could illustrate how the coordination class components mutually impact one another in a complex interplay. There are multiple ways to come to a correct conclusion. Still, unsurprisingly, a more reflected engagement with the structural drawings favoured a productive concept projection of resonance across all components of a coordination class. This is in line with former research (*e.g.*, Furió *et al.*, 2000; Domin *et al.*, 2008; Cooper *et al.*, 2013; Maeyer and Talanquer, 2013; Popova and Bretz, 2018a; Talanquer, 2022) and stresses the importance of representational competence in problem-solving. In our analysis, it became evident that the structures must be considered holistically for successful problem-solving, *i.e.*, considering and combining structural features across the global and local levels. Often, this was supported by a more inductive and reflective analysis of the task affordances, which resulted in the activation of more appropriate extraction strategies. Since the coordination class components inform one another, a thorough structural analysis of the structures also supports productive changes in extraction strategies during problem-solving.

In unproductive cases, extraction strategies focusing on overgeneralized approaches to the tasks often led to focused extractions, *i.e.*, only paying attention to a few (salient) structural features throughout the problem-solving. Besides being stuck with overgeneralized ideas (*e.g.*, overgeneralized application of global stability), uncertainty and drawing difficulties frequently caused unproductive task approaches. In terms of the resulting inferential nets, students often activated similar resources, whereby students with unproductive concept projections (*i.e.*, unsuccessful problem-solving) slightly tended to infer more often ideas unrelated to the idea of resonance (*e.g.*, steric hindrance), or heuristic-like ideas. What differentiated the activated resources' productivity was their connection and, thus, *how* students used the resources. As such, a productive concept projection of resonance often involved resources being activated and (inter-)connected across levels of granularity, ranging from phenomenological to energetic considerations. The overall complexity of inferential nets was not inherently related to productivity. Instead, students who successfully solved the problems tended to combine resonance-related ideas by jointly activating analytical and comparative resources. Such an interplay gave rise to a more reflective consideration of the resonance concept.

Implications for teaching and learning

Many intertwined aspects impact the consideration of resonance in problem-solving. This comprises constructing valid resonance structures, matching the task affordances, unpacking the representations (*e.g.*, recognizing and using relevant structural information), and interpreting and connecting inferred conceptual ideas (Talanquer, 2022). As a result, there is not just *one* way to use resonance in problem-solving, as shown in the complex and diverse interplay of extraction strategies, extractions, and resource activation. Concerning the coordination class components, it became apparent that students experience conceptual and procedural challenges when reasoning with their resonance structures, eventually hampering productive concept projections. Therefore, teaching should consider these different conceptual and procedural aspects of concept use more. Stated differently, we should encourage students to pay more attention to their drawings, as they are crucial for the dynamic conceptualization and comprehensive use of resonance in problem-solving. Since in our interviews, simple metacognitive follow-up questions (*e.g.*, "*How did you get to your solution?*") often helped the students to focus and refine their reasoning, the need for slowing down students' problem-solving process became apparent. To foster analytic thinking and a more reflective approach to the tasks, a suitable intervention could be scaffolding the use of resonance by sequencing the complex, multistep problem-solving process (*e.g.*, Wood *et al.*, 1976; Benson, 1997; Graulich and Caspari, 2020). One possibility could be the use of checking lists as well as metacognitive questions (*e.g.*, Yuriev *et al.*, 2017). They explicitly guide students to focus their attention on structural prerequisites for resonance, to incorporate those structural features, and to elicit and connect diverse ideas across levels of granularity. For instance, in our study, students activated many resources with a similar frequency, irrespective of the productivity of the concept projection. But they did not always *connect* their ideas. For example, they referred to aspects on a phenomenological level but did not always link the activated resources to the structural, electronic, or energetic level. Consequently, metacognitive questions could target more holistic reasoning across the levels of granularity. Fig. 16 depicts a possible scaffold by sequencing the problem-solving process into the steps "*Analyse*" (*i.e.*, become aware of the affordances of the task, but also the given structures and structural properties), "*Draw*" (*i.e.*, help students to assess and reflect on their drawings), and "*Conclude*" (*i.e.*, connect drawing-based inferences to the initially stated requirements of the tasks), altogether guiding the students through the steps in problem-solving and facilitating a more differentiated task approach.

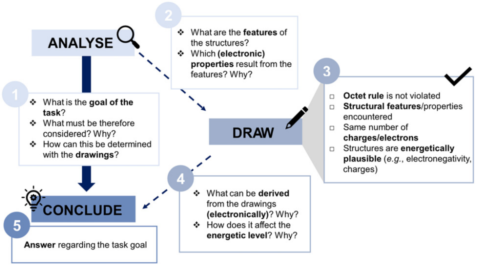


Fig. 16 Possible metacognitive scaffold for supporting students' concept use in problem-solving.

Taking different structural features into account is beneficial for successful problem-solving. However, being able to construct valid resonance structures is a crucial prerequisite for that. Our findings revealed that students who (partially) struggled with constructing resonance structures or were uncertain about their drawings' plausibility, often avoided the resonance concept or applied it arbitrarily. Consequently, this emphasizes that drawing valid resonance structures must be sufficiently trained before it can be used in problem-solving. Besides scaffolding reflective drawing by using, for instance, checking lists, the externalization of drawing processes could help students construct resonance structures by focusing learners' attention on relevant features (Braun *et al.*, 2022).

There is more to the successful use of resonance besides supporting students' reflective engagement with their constructed representations. To build a more integrative coordination class (DiSessa and Wagner, 2005), it is also crucial to use the concept in a variety of situations with differing task affordances to match resonance-related learning outcomes (*e.g.*, assess stability, acidity, predict reaction pathways) (Carle and Flynn, 2020). The exposure to multiple contexts is necessary for building a variety of extraction strategies, extending concept projections, and, thus, coordinating a sufficient range of resources (DiSessa and Wagner, 2005). This could support a more flexible and proficient use of resonance when approaching problem-solving tasks. Unproductive extraction strategies often resulted when students relied on a fixed sequence of steps, applied overgeneralized rules, or, irrespective of the task affordances, used static approaches equalizing resonance with global stability. This heavily affected the extractions and the subsequent activation of resources. To overcome students' static reference to stability whenever reasoning about resonance (*e.g.*, Brandfonbrener *et al.*, 2021), teaching should highlight more explicitly the link to the idea of electron density distribution and the energetic account. In doing so, the actual meaning of resonance would be taken more into account (Xue and Stains, 2020). Expanding tasks to the consideration of resonance beyond stability assessments can also help to overcome students' overreliance on stability, and to deal successfully with resonance in various contexts.

Implications for research

This paper focused on the qualitative characterization of students' use of resonance in problem-solving in three contexts at one time point during the semester. Therefore, future studies could consider how students' concept projections develop throughout the semester, what differentiates the conceptual use of experts in comparison to novices, or how effective interventions targeting the differentiated use of resonance in problem-solving are. Given some students' difficulties in constructing resonance structures and recognizing if resonance applies (for instance, in the non-aromatic context), more research is needed to elicit the underlying reasons for students' difficulties (*e.g.*, how the variation of structural features contributes to the activation of resonance related resources). Our study also showed that students, in line with the resonance concept, often focus on electronic effects in their reasoning. Yet, they sometimes express alternative conceptions and use electronic effects in an overgeneralized way. Thus, students' conceptualization of electronic effects necessitates more research.

Limitations

This qualitative study is explorative; thus, several limitations must be considered. We characterized students' concept use in a study setting that differed from their usual instructional environment. This might have influenced their overall concept projections as well. Furthermore, given the duration of the interview, the sophistication of the explanations might have also varied due to fatigue, students' motivation, or the prompts of the retrospective. Given that we relied in our analysis on students' utterances, students may have paid attention to other structural features as extractions and activated other resources, which were not verbalized. As such, the result is also an artifact of the interview process, in which follow-up questions might have cued students to different aspects of the task, albeit similar for all participants. Lastly, although we iteratively and carefully characterized students' resource activation, the constructed resource graphs represent a summary of the reasoning process, which heavily depended on students' verbal explaining and, thus, could not display the process in detail.

Author contributions

Irina Braun: conceptualization, investigation, methodology, formal analysis, visualization, writing – original draft. Nicole Graulich: conceptualization, supervision, methodology, visualization, writing – review and editing.

Conflicts of interest

There are no conflicts to declare.

Appendices

Appendix #1: interview protocol for the retrospective

1. Please justify your answer and explain in detail your thought process for solving this task.
    a. How did you know what to do? How did you get to your solution?
    b. Can you please describe chronologically your created drawings (*i.e.*, how do they develop over time?)
    c. If started anew, why?
    d. If problems were encountered, what were the difficulties?
2. Why did you construct the drawings, *i.e.*, how did they help you to solve the problem?
    a. What (and how) did you deduce from your single drawings?
    b. What do the different components of the drawings mean (*e.g.*, charges) with regard to the problem?
    c. Why did you skip/ignore certain drawings?
    d. If no drawings: Why did you solve the tasks mentally?
3. How did you construct your drawings (resonance structures)?
    a. What is the rationale behind your drawings? Based on what criteria did you move from one structure to another? How did you get to your structures?
    b. How do you determine that your drawings are valid?
4. On a scale of 1–5 (1 = easy, 5 = difficult), how difficult was the task completion for you?
    a. Why?
    b. Why was the task simpler/harder than the other tasks?

Appendix #2: codes for extractions and resources

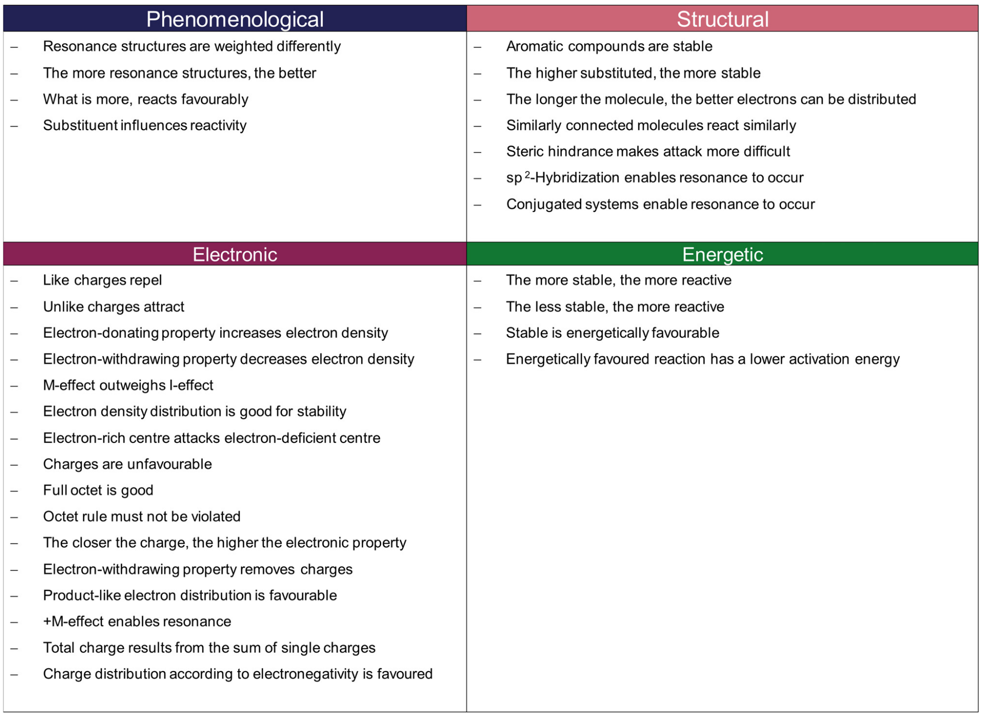
The codes for the extractions and resources were inductively derived from the interview transcripts using *in-vivo* coding in a first coding circle. Subsequently, broader categories for grasping underlying ideas concerning the extractions and resources were inferred. The following examples illustrate the coding process:
Example I: *Substituent influences reactivity*, exemplary student utterances:
- "Substituent influences positive charge"
- "Keto group directs meta"
- "First substituent stabilizes or destabilizes the resulting charge"
- "The substituent has a different impact, depending on its position"

Example II: *Unlike charges attract*, exemplary student utterances:
- "Adjacent positive and negative charges make no sense"
- "Positive and negative charges neutralize each other"
- "Different charges attract"
- "The plus attracts electrons"

Across the different interviews, 31 resources could be found (*cf.* Appendix #3), as well as 17 extractions. These are listed as follows as local/global extractions:

Local	Global
Charge	Number of resonance structures
Double bond	Reaction partner
Single bond	Reactant
Oxygen atom (hetero atom)	Product
Lone pair/electrons	Alkyl group
Carbon atom	Reaction type
	Aromatic structure
	Substituent (functional group)
	Geometry
	Conjugated system
	Number of bonds

Appendix #3: overview of the different resources and their level of granularity



Phenomenological

- Resonance structures are weighted differently
- The more resonance structures, the better
- What is more, reacts favourably
- Substituent influences reactivity

Structural

- Aromatic compounds are stable
- The higher substituted, the more stable
- The longer the molecule, the better electrons can be distributed
- Similarly connected molecules react similarly
- Steric hindrance makes attack more difficult
- sp^2-Hybridization enables resonance to occur
- Conjugated systems enable resonance to occur

Electronic

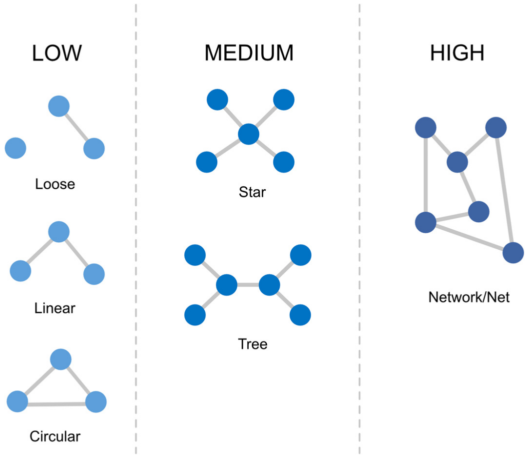
- Like charges repel
- Unlike charges attract
- Electron-donating property increases electron density
- Electron-withdrawing property decreases electron density
- M-effect outweighs I-effect
- Electron density distribution is good for stability
- Electron-rich centre attacks electron-deficient centre
- Charges are unfavourable
- Full octet is good
- Octet rule must not be violated
- The closer the charge, the higher the electronic property
- Electron-withdrawing property removes charges
- Product-like electron distribution is favourable
- +M-effect enables resonance
- Total charge results from the sum of single charges
- Charge distribution according to electronegativity is favoured

Energetic

- The more stable, the more reactive
- The less stable, the more reactive
- Stable is energetically favourable
- Energetically favoured reaction has a lower activation energy

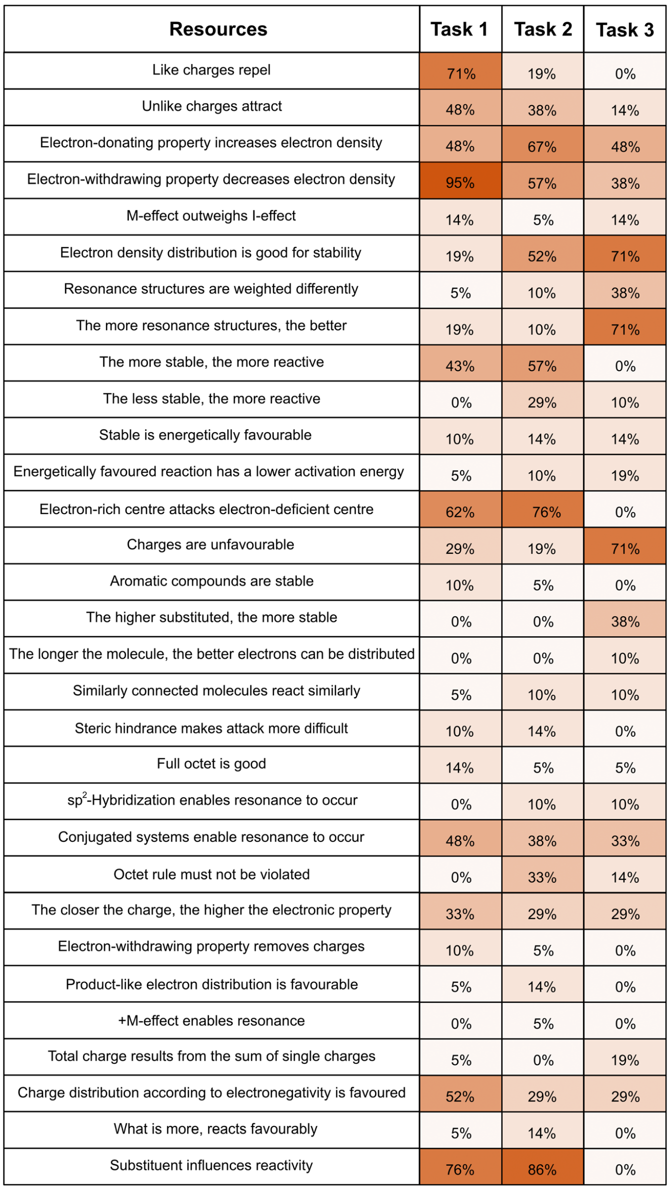
According to Deng and Flynn (2021), the phenomenological granularity level is describing chemical phenomena arising from molecules and atoms' interactions because of their properties. Thus, the ideas arise as a result of the granularity levels below. For example, by activating the resource *The more resonance structures, the better*, one states a common rule grounded in electronic and energetic considerations, *i.e.*, the consideration of electron density distribution and its linkage to energetics. The structural level describes resources that target structural features of molecules or atoms (*e.g.*, steric bulk, which refers to the composition of a molecule). The granularity level below, the electronic level, captures ideas referring to electronic features of molecules and atoms (*e.g.*, electron-donating effect, the description of electron density distribution, or the reference to charge interaction). Lastly, the energetic level captures ideas targeting thermodynamic and kinetic considerations, thus, referring to the energetics of a reaction (*e.g.*, the evaluation of varying stabilities in terms of the reaction pathway). In our data, some resources are a mixture of different granularity levels, which we classified in dependence of which level is in the foreground. For instance, the resource *Aromatic compounds are stable* targets both the structural and energetic levels. However, here, the structural consideration outweighs the energetic one because the conjugated ring system gives rise to higher stability.

Appendix #4: classification of students' resource graphs



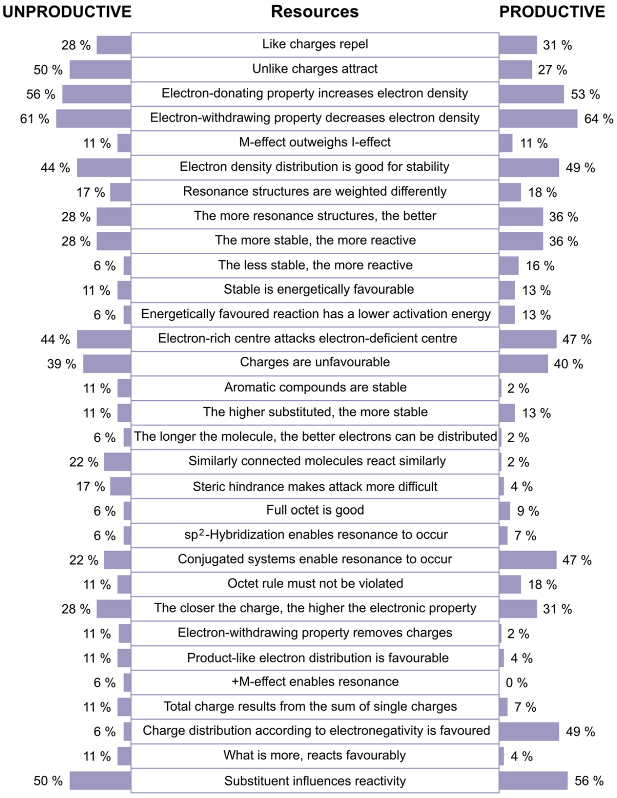
To classify students' resulting resource graphs, we adapted Yin *et al.*'s (2005) coding system for the structure complexity in concept maps. As such, students' resource graphs were classified as a whole, *i.e.*, in dependence of their overall structure with regard to (inter-)connectedness of the different activated resources.

Appendix #5: frequency of resource activation across the different contexts



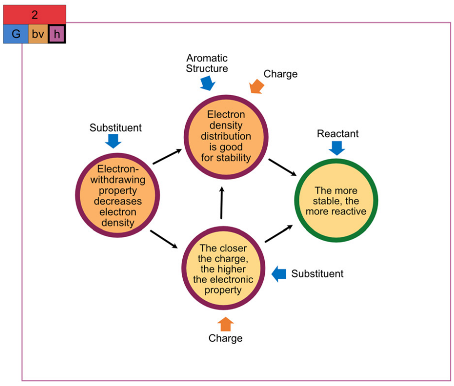
Resources	Task 1	Task 2	Task 3
Like charges repel	71%	19%	0%
Unlike charges attract	48%	38%	14%
Electron-donating property increases electron density	48%	67%	48%
Electron-withdrawing property decreases electron density	95%	57%	38%
M-effect outweighs I-effect	14%	5%	14%
Electron density distribution is good for stability	19%	52%	71%
Resonance structures are weighted differently	5%	10%	38%
The more resonance structures, the better	19%	10%	71%
The more stable, the more reactive	43%	57%	0%
The less stable, the more reactive	0%	29%	10%
Stable is energetically favourable	10%	14%	14%
Energetically favoured reaction has a lower activation energy	5%	10%	19%
Electron-rich centre attacks electron-deficient centre	62%	76%	0%
Charges are unfavourable	29%	19%	71%
Aromatic compounds are stable	10%	5%	0%
The higher substituted, the more stable	0%	0%	38%
The longer the molecule, the better electrons can be distributed	0%	0%	10%
Similarly connected molecules react similarly	5%	10%	10%
Steric hindrance makes attack more difficult	10%	14%	0%
Full octet is good	14%	5%	5%
sp^2-Hybridization enables resonance to occur	0%	10%	10%
Conjugated systems enable resonance to occur	48%	38%	33%
Octet rule must not be violated	0%	33%	14%
The closer the charge, the higher the electronic property	33%	29%	29%
Electron-withdrawing property removes charges	10%	5%	0%
Product-like electron distribution is favourable	5%	14%	0%
+M-effect enables resonance	0%	5%	0%
Total charge results from the sum of single charges	5%	0%	19%
Charge distribution according to electronegativity is favoured	52%	29%	29%
What is more, reacts favourably	5%	14%	0%
Substituent influences reactivity	76%	86%	0%

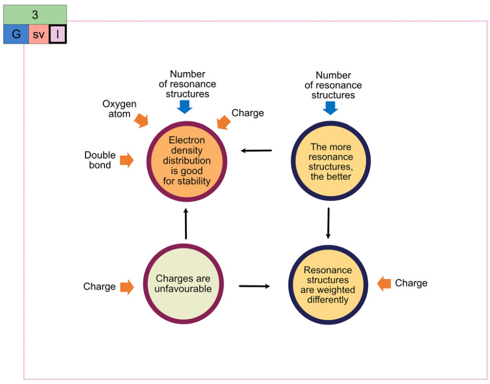
Appendix #6: relative frequency of resource activation in dependence of the productivity of the concept projection

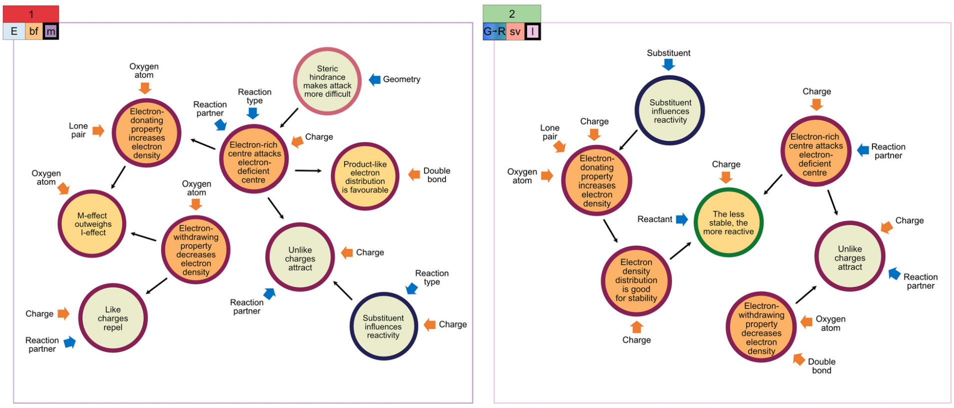


Appendix #7: exemplary students' resource graphs for different tasks

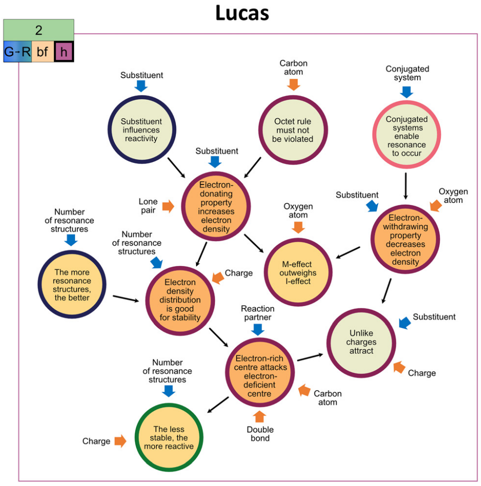
Benjamin



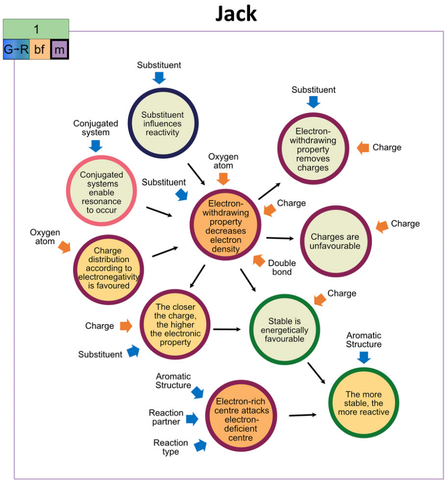




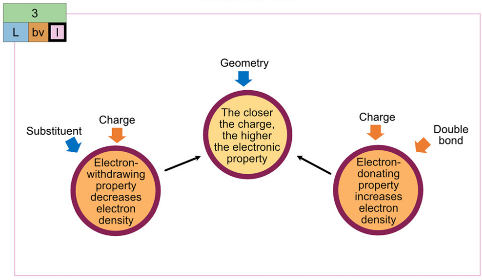
Claire



Lucas



Jack



Charlotte

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4. A Question of Pattern Recognition: Investigating the Impact of Structure Variation on Students’ Proficiency in Deciding about Resonance Stabilization

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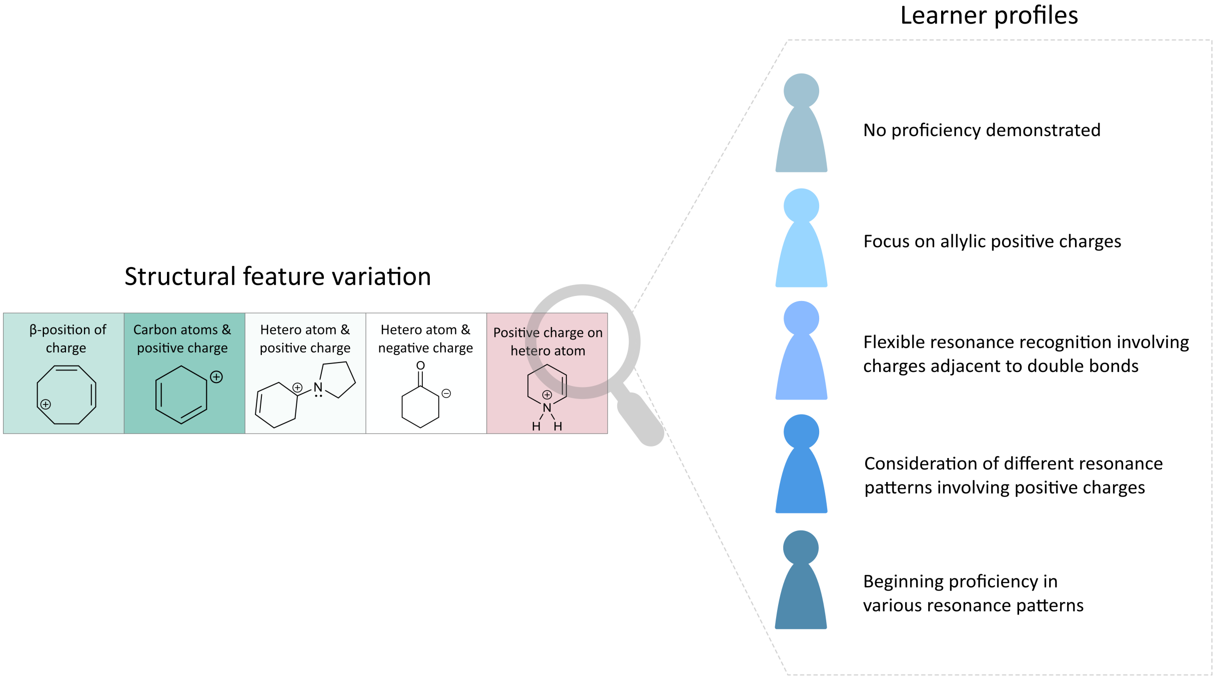

Braun, I., Lewis, S. E. & Graulich, N. (2025). A question of pattern recognition: investigating the impact of structure variation on students’ proficiency in deciding about resonance stabilization, *Chemistry Education Research and Practice*, *26*(1), 158-182. DOI: 10.1039/d4rp00155a

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A question of pattern recognition: investigating the impact of structure variation on students' proficiency in deciding about resonance stabilization

Irina Braun,[a] Scott E. Lewis[b] and Nicole Graulich*[a]

The ability to reason with representations is pivotal for successful learning in Organic Chemistry and is closely linked to representational competence. Given the visual nature of this discipline, this comprises competency in extracting and processing relevant visual information. With regard to the resonance concept, proficiency in identifying whether electron delocalization applies in a molecule is an essential prerequisite to using this concept in problem-solving. However, prior research shows that students struggle to recognize whether molecules profit from electron delocalization, and seldom use this concept in problem-solving. As it remains unclear how the variation of structural features affects students' consideration of resonance, this quantitative study seeks to identify characteristics regarding students' perception of electron delocalization. To this end, undergraduate students enrolled in an Organic Chemistry I course (N = 699) completed an online survey in which they had to decide on resonance stabilization for molecular structures with varying structural features. *K*-means cluster analysis was performed to explore patterns in students' proficiency in discerning resonance stabilization and how they relate to other performance variables (*e.g.*, time-on-task). The results suggest pattern recognition approaches with students' attention being guided by singular structural features or structures' visual similarity to familiar patterns (*i.e.*, allylic carbocations), with less attention to implicit features.

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Introduction

Much of the knowledge one acquires in Organic Chemistry relies on making sense of representations and visualizations. While one works through chapters in textbooks related to, for instance, specific reaction mechanisms or listens to instructors' explanations, the concepts and facts encountered are usually linked to specific representations, making imperceptible processes and abstract concepts accessible to the learner (Bodner and Domin, 2000; Justi and Gilbert, 2002; Gilbert, 2005). Representations are a crucial aspect of disciplinary discourse in chemistry (Hoffmann and Laszlo, 1991; Kozma *et al.*, 2000; Goodwin, 2008; Airey and Linder, 2009). They facilitate communication and serve as a sense-making tool in problem-solving. As such, various types of representations are used in Organic Chemistry to provide complementary information on chemical phenomena (Ainsworth, 2006; Rau *et al.*, 2015). The S_N2-reaction of 2-bromobutane with a hydroxide ion can serve as an example (Fig. 1). While the electron-pushing formalism in a mechanistic representation illustrates the processes and interactions between entities during the reaction, dash-wedge representations showcase the stereochemistry. In contrast, reaction coordinate diagrams reveal the energetic and kinetic aspects of this specific reaction type. Given that varying degrees of explicit and implicit information are encoded within representations, their processing may necessitate different cognitive operations and inferences (Cooper *et al.*, 2012a, 2012b; Talanquer, 2022). Learners must become adept in navigating through the varying complexity of representations (*e.g.*, a representation's granularity or iconicity) to successfully deal and reason with representations in Organic Chemistry (*e.g.*, choose suitable representations for problem-solving dependent on their affordances and limitations) (Kozma and Russell, 1997; Kozma and Russell, 2005; Talanquer, 2022). As part of that, learners must become proficient in decoding representations and linking relevant visual cues to chemical concepts (Rau, 2018; Talanquer, 2022). Resonance, for instance, is a concept that enables reasoning about electron density distribution in a molecule. As it is closely linked to the use of different representations, one must be able to decipher these representations, *e.g.*, connect the variation in colour

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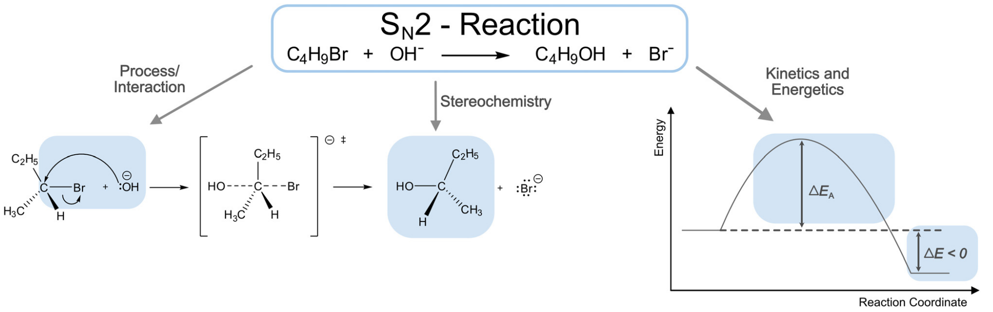


Fig. 1 Different representation types illustrate different aspects of a chemical phenomenon.

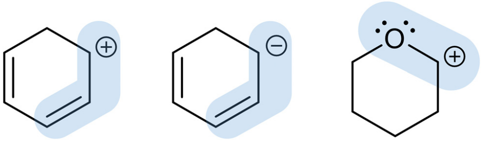


Fig. 2 Different structural features in a molecule enable resonance to occur.

in electrostatic potential maps to electron density distribution, or differentiate resonance hybrids from depictions of single resonance structures. When solving mechanistic problems in Organic Chemistry, learners usually encounter Lewis structures or skeletal formulas. To apply resonance, here, it is essential to be able to locate and recognize conjugated systems in structures in the form of different patterns (*e.g.*, allylic positive charges, lone pairs adjacent to positive charges), all indicating the possibility of electron delocalization (Klein, 2020) (Fig. 2).

Theoretical background

Sense-making skills and perceptual fluency as integral parts of representational competence

In general, successfully engaging with and using representations is governed by two broad, interrelated representational competencies: *sense-making skills* and *perceptual fluency* (Kellman and Massey, 2013; Rau, 2018). *Sense-making skills* refer to one's conceptual and procedural competencies in terms of a given representation. This involves, for instance, the knowledge and competency to connect or map visual features in representations to chemical principles and concepts, to make inferences based on representations, to explain the connections or differences between representations, and to choose particular representations for a specific purpose (Kozma and Russell, 2005; Rau, 2018; Talanquer, 2022). Thus, these skills pertain to one's knowledge of representations that can be explicitly verbally expressed (Rau, 2017).

Besides *sense-making skills*, fluency in decoding representations is also crucial for learning with representations. Hence, *perceptual fluency* builds another essential part of representational competence (Rau, 2018). It comprises the ability to effortlessly and quickly perceive and selectively attach meaning to relevant visual cues across varying representations as a result of experience-induced perceptual learning (Gibson, 2000; Kellman and Massey, 2013; Rau *et al.*, 2015). This competency refers to one's fluency in processing visual information in a specific type of representation (*e.g.*, recognizing patterns), one's use of representations to solve tasks (*e.g.*, distinguishing relevant from irrelevant visual features in a representation for further cognitive processing), and one's ability to automatically detect connections across different (types of) representations (*e.g.*, deciding at a glance whether two representations show the same or different entities) (Gibson, 2000; Kellman *et al.*, 2008; Airey and Linder, 2009; Koedinger *et al.*, 2012; Kellman and Massey, 2013; Rau, 2018). Unlike *sense-making skills*, which are acquired *via* explicit instruction such as (self-)explanations (Koedinger *et al.*, 2012; Rau, 2017), gaining fluency in perception undergoes a non-verbal, inductive process enhanced by extensive practice and exposure to representations in order to develop sensitivity to relevant perceptual features in a representation (Richman *et al.*, 1996; Koedinger *et al.*, 2012; Kellman and Massey, 2013). In fact, research across different disciplines has shown that the perception of representations distinguishes experts from novices. Experts are able to pick up relevant patterns in representations and abstract relationships which are invisible to novices (*e.g.*, Chi *et al.*, 1981; Richman *et al.*, 1996; Kellman and Garrigan, 2009; Gegenfurtner *et al.*, 2011; Kellman and Massey, 2013; Stieff *et al.*, 2020; Connor *et al.*, 2021). Being efficient in discerning patterns and extracting relevant information involves increased attentional filtering and automaticity in selecting meaningful features, which results in encoding visual information in the form of larger perceptual chunks, eventually decreasing cognitive load and freeing up cognitive capacity (Kellman and Garrigan, 2009; Rau *et al.*, 2015; Stieff *et al.*, 2020). This allows one to recognize familiar cases and categorize new instances with more ease, and to engage in higher-order conceptual reasoning such as solving more complex and creative problems or enabling more parallel processing (Richman *et al.*, 1996; Goldstone and Barsalou, 1998; Kellman *et al.*, 2008; Kellman and Garrigan, 2009; Kellman and Massey, 2013). *Perceptual fluency* is not limited to perceiving low-level sensory features in a representation (*e.g.*, discerning a certain functional group in a molecule), but also extends to detecting high-level, deeper structural *relations* within a given problem (*e.g.*, perceiving the possibility of reaction pathways given the arrangement of different entities in a system) (Kellman *et al.*, 2008; Kellman and Massey, 2013).

Developing proficiency in representational competence

Even though *sense-making skills* and *perceptual fluency* have built separate lines of research for years (Rau, 2017), perception and cognition are closely related (Goldstone and Barsalou, 1998; Wu *et al.*, 2001; Kellman *et al.*, 2010; Kellman and Massey, 2013). More specifically, with regard to representational competence in chemistry, the different skills discussed by Kozma and Russell (2005) involve both *sense-making skills* and *perceptual fluency*. For example, to translate representations (*e.g.*, draw different resonance structures), one must not only know the conventions for different representations but must also perceive specific, relevant cues and patterns in the starting representation (*e.g.*, identifying the conjugated system) to subsequently generate a corresponding representation. Consequently, besides conceptual knowledge about specific representations, fluency in extracting relevant information builds a crucial aspect underlying reasoning with representations (Kozma and Russell, 2005).

It becomes apparent that the interplay of *sense-making skills* and *perceptual fluency* characterizes proficiency in representational competence. It is not only crucial to have conceptual knowledge about a representation, but also necessary for this knowledge to be readily accessible in order to be flexibly applied across varying contexts. Given their mutually dependent character, it is not possible to characterize proficiency only in terms of *sense-making skills* or *perceptual fluency*. When reasoning with representations, it is important to be able to perceive relevant features in a representation in order to activate corresponding conceptual knowledge (DiSessa *et al.*, 2016); however, prior conceptual knowledge is required to attend to these features. Hence, they rather build integrated skills that develop on a continuum when learning chemistry and, furthermore, may be context-dependent. For instance, when learners have a sound conceptual understanding of a representation and have often encountered it in their courses, they can quickly make sense of the representation. In contrast, when learners have been introduced to a novel representation, they have not gained *perceptual fluency* yet; instead, their reasoning about this newly encountered representation rather relies on *sense-making*, requiring more time to come to a valid conclusion (*e.g.*, by explicitly thinking about the meaning of the representational features). Therefore, *perceptual fluency* (indicated by the time to answer tasks correctly) does not suffice to measure learners' developing representational proficiency, especially at the introductory level of Organic Chemistry, where novices are introduced to a number of new representation types (Anderson and Bodner, 2008). Instead, one can assume that the interplay of *sense-making skills* and *perceptual fluency* may increase one's performance (*i.e.*, learners' success in correctly answering tasks). Consequently, learners' performance scores across different tasks may reflect their developing proficiency in representational competence more adequately.

Developing proficiency in using different representations requires learners' repeated use and exposure to different types of representations when learning chemistry. However, traditional instruction often emphasizes learning facts and procedures, while the acquisition of *perceptual fluency* usually takes a minor, implicit role in teaching (Anderson and Bodner, 2008; Kellman *et al.*, 2008; Kellman and Garrigan, 2009). As a result, learners gain relevant knowledge about concepts or reactions but may not be able to successfully use and apply it (Wise *et al.*, 2000; Kellman *et al.*, 2010). Due to the tacit process of becoming perceptually fluent, beginners might face slow visual processing and cognitive overload when dealing with representations, eventually leading to superficial interpretations and a strong focus on salient, familiar features (Ealy and Hermanson, 2006; Anderson and Bodner, 2008; Hinze *et al.*, 2013). This may cause difficulties in extracting relevant information when interpreting representations.

Students' challenges in the extraction of resonance-related information

Throughout their Organic Chemistry courses, learners are introduced to a number of new representations. Despite unfamiliarity, they are expected to use these representations to learn about novel chemistry concepts (Rau, 2017). As a result, identifying relevant structural features and activating and integrating respective conceptual knowledge may be difficult for beginners in Organic Chemistry. This becomes even more challenging as representations might be used inconsistently and without explicit instructional training (Wise *et al.*, 2000; Graulich, 2015; Baldwin and Orgill, 2019; Patron *et al.*, 2021; Talanquer, 2022). Abundant literature in chemical education research reports that learners are often overwhelmed by this discipline's visual language and experience difficulties in extracting relevant information in representations, eventually hindering their problem-solving (*e.g.*, Keig and Rubba, 1993; Wu and Shah, 2004; Bhattacharyya and Bodner, 2005; Anderson and Bodner, 2008; Strickland *et al.*, 2010; Grove *et al.*, 2012; Anzovino and Bretz, 2016). This is problematic as the fluent extraction of relevant information builds the basis for reasoning with and learning of domain knowledge (DiSessa *et al.*, 2016). Concerning the resonance concept, in particular, proficiency in identifying whether electron delocalization occurs in a molecule builds an essential prerequisite to successfully apply this concept in problem-solving (*e.g.*, to draw reasonable resonance structures, to approximate the geometry of a molecule or to identify electrophilic or nucleophilic sites in a molecule to predict reaction pathways) (Carle and Flynn, 2020). However, several studies have shown that students face challenges while deciding if resonance applies, resulting in a scarce integration of this concept in their reasoning processes (Carle *et al.*, 2020;

Finkenstaedt-Quinn *et al.*, 2020; Petterson *et al.*, 2020; Braun *et al.*, 2022). In this regard, it has also been shown that students struggle to identify the correct place to start the electron movement, focus on unrelated structural features, or do not consider the octet rule or hybridization when generating resonance structures (Betancourt-Pérez *et al.*, 2010; Finkenstaedt-Quinn *et al.*, 2020; Petterson *et al.*, 2020; Braun *et al.*, 2022; Tetschner and Nedungadi, 2023). However, the structures' geometry, the saliency, and the explicitness of the given structural features (*i.e.*, lone pairs, hetero atoms) seem to influence whether learners can recognize and apply the resonance concept correctly, and how they distribute their visual attention to the structures (Carle *et al.*, 2020; Finkenstaedt-Quinn *et al.*, 2020; Braun *et al.*, 2022; Farheen *et al.*, 2024). Despite these exploratory results, it remains unknown how the variation of structural features affects students' consideration of resonance. While prior studies have identified general difficulties and pointed to potential influencing factors, the impact of varying structural features on students' ability to recognize and apply resonance has not been explored yet. Specifically, how differences in structural features make the recognition of resonance more difficult or what considerations guide students' resonance-related information extraction have not been systematically examined in previous studies. Such insights, however, are valuable in informing teaching practices and better supporting students in their learning process.

Research questions

Successfully learning Organic Chemistry necessitates a significant degree of proficiency in attending to and interpreting relevant features in representations, eventually affecting concept learning and use. Pertaining to this, learners' ability to perceive structural features indicating the possibility of electron delocalization builds the basis for successfully using resonance in problem-solving (Braun and Graulich, 2024). Even though literature provides insights into students' challenges in drawing and using resonance structures in problem-solving, it remains unclear how the variation of structural features impacts students' decision-making on resonance stabilization in molecules (*e.g.*, to which extent they pay attention to explicit and implicit structural properties when considering resonance), and how students' developing proficiency in resonance-related considerations is related to other performance metrics such as prior knowledge and time-on-task. To this end, the quantitative study presented herein is guided by the following research questions:

1. How do different combinations of structural features influence students' ability to discern resonance stabilization in molecules?
2. What trends regarding students' proficiency in making decisions on resonance stabilization in molecular structures emerge?
3. How do the emerging trends relate to other performance variables (*i.e.*, time-on-task, prior knowledge, cognitive load)?

Methods

Participants and research setting

The study was conducted at a large, research-intensive university in the southeastern region of the United States. The study population comprised first-semester Organic Chemistry students enrolled across five classes, taught by three different instructors using a common syllabus and textbook (Klein, 2020). Through lectures and discussion sections, the course covered fundamental concepts of structure, bonding, reactivity, and mechanisms of organic chemistry. All participants were informed about their rights and data handling beforehand. The students were recruited voluntarily *via* e-mail announcements and had a week to take the online survey (described below). As an incentive, the students received extra credit worth approximately 0.4% of their course grade upon survey completion, irrespective of consent to the study or the correctness of the provided answers to the tasks. Of 899 students enrolled in the Organic Chemistry I course, 699 students completed the survey giving informed consent for their data being anonymously analysed and published by the research team. As the survey was conducted near the end of the course, it followed the presentation of the resonance concept and the construction of resonance structures, which were covered within the first weeks of the course. Altogether, 1.5 lectures were delivered on the topic of resonance. The instruction followed the presentation of the concept in the textbook (Klein, 2020) and targeted different learning objectives. Students should be able to explain resonance stabilization and electron delocalization, use curved arrows to construct resonance structures, compare the significance of different resonance structures, construct resonance hybrids, and distinguish between delocalized and localized lone pairs in structures. Students were also expected to recognize the five resonance patterns described in the textbook (*e.g.*, lone pair adjacent to a carbocation) (Klein, 2020). Clicker questions during the lectures, virtual homework questions, and exam questions were used to assess whether students met the learning objectives. Furthermore, the Klein textbook offered students different scaffolded worked examples (*i.e.*, with an indication of step-by-step strategies) and practice problems for the various learning objectives (*e.g.*, how to draw significant resonance structures) (Klein, 2020).

Ethical considerations

Students were provided a written consent form detailing the data processing prior to study participation, and it was clarified to the students that they had the right to opt out from the survey at any time. No identifying information was collected that allowed participants to re-identify.

Research instrument and data collection

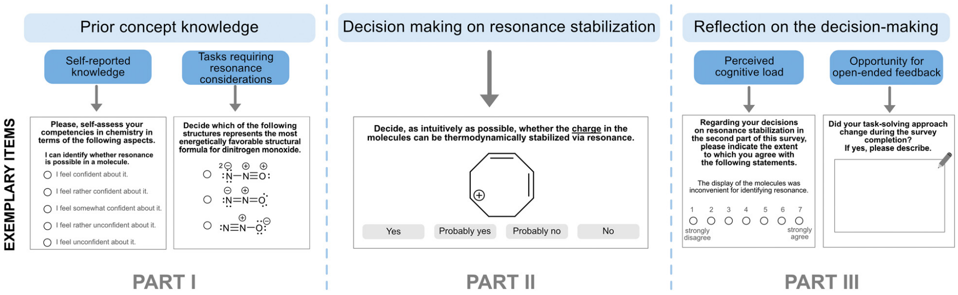
Data was collected *via* an online survey implemented in *Qualtrics*, which consisted of three parts (Fig. 3). The first part assessed students' conceptual prior knowledge of resonance. Based on the resonance-related learning outcomes described by Carle and Flynn (2020), students first self-assessed their confidence in dealing with different aspects around resonance (*e.g.*, "I can identify whether resonance is possible in a molecule", or "I can assess the thermodynamic stability of molecules based on their structural formulas") on a five-point Likert scale. Besides their self-reported knowledge, the students also solved different designed tasks to assess their understanding and use of resonance in concrete tasks (Fig. 3, part I). The tasks were informed by both Carle and Flynn's (2020) described learning outcomes on resonance, and conceptual difficulties regarding resonance reported in previous research studies (Taber, 2002; Kim *et al.*, 2019; Xue and Stains, 2020; Brandfonbrener *et al.*, 2021; Tetschner and Nedungadi, 2023; Braun and Graulich, 2024). For instance, students had to choose the energetically most favourable structural formula among different resonance structures of dinitrogen oxide, had to indicate the correct product of a reaction using the electron-pushing formalism (Flynn and Featherstone, 2017), or had to mark in a multiple-choice task all correct statements regarding resonance (*cf.* Appendix for the complete list of tasks). When designing the tasks, we avoided using structures similar to those in the subsequent survey part to avoid priming the students.

In the second part of the study (Fig. 3, part II), students were asked to decide whether a molecular structure profits from resonance stabilization. By deciding on resonance stabilization, students had to decide on the possibility of *reasonable* resonance structures. In some molecules, delocalization was theoretically possible but would result in energetically unfavourable resonance structures and would not contribute to charge stabilization. Applying resonance in these cases would not be reasonable. Following research on *perceptual fluency* (Kellman and Massey, 2013), the students were asked to decide whether resonance stabilization applies as intuitively as possible in order to avoid overthinking and consulting textbooks. To prevent fatigue effects, students were presented a subset of 37 molecules, one at a time, that were randomly selected from a database of 72 molecules. The first two molecules were identical for all students. When deciding on resonance stabilization, students could also express uncertainty by choosing among the answers *yes; probably yes; probably no*; or *no*. During this survey part, student log data was collected comprising their time spent on each item and the click count when answering the questions.

Finally, the third part of the survey (Fig. 3, part III) asked the participants to rate their perceived cognitive load on a seven-point Likert scale for different items regarding the second survey part. Specifically, the instrument developed by Klepsch *et al.* (2017) has been adapted to measure students' intrinsic, extraneous, and germane cognitive load. For instance, students had to decide to which extent they agreed that the display of the molecules was inconvenient for identifying resonance. In the end, the students were given open-ended questions to report on how their task-solving approach changed during the survey completion and to provide feedback. Due to the low response rate for the open-ended questions, they remain unconsidered in the following analysis. The students were asked to answer the entire survey without external help or any additional tools (*e.g.*, class material, textbooks). The median duration for completing the whole survey was 14 minutes and 29 seconds.

Item design

In the second part of the survey, the students had to decide whether electron delocalization (*i.e.*, resonance) contributes to charge stabilization for different molecular structures. Based on previous research on students' generation and understanding of structural representations, particularly involving resonance, the design of the molecular structures followed a systematic variation of different structural parameters, which could affect students' perception of resonance. This comprises the degree of explicitness of given information, the structures' complexity and geometry, and familiarity of structural features (Kraft *et al.*, 2010; DeFever *et al.*, 2015; Graulich and Bhattacharyya, 2017; Graulich *et al.*, 2019; Carle *et al.*, 2020; Finkenstaedt-Quinn *et al.*, 2020; Braun *et al.*, 2022; Talanquer, 2022). Specifically, in this study, the molecules differed in the indication of lone pairs of electrons, the explicit indication of bonds to hydrogen atoms, the distance of the charge to the conjugated system (*i.e.*, γ-, β-, or α-position), the type of charge (*i.e.*, positive or negative charge), the structure's carbon backbone (branched, linear, or cyclic structures), and the presence and familiarity of hetero atoms. For instance, 20 of the 72 items had a negative charge. Furthermore, some molecules required an explicit focus on additional aspects such as atoms' hybridization or violation of the octet rule in case of electron



Please, self-assess your competencies in chemistry in terms of the following aspects.

I can identify whether resonance is possible in a molecule.

○ I feel confident about it.
○ I feel rather confident about it.
○ I feel somewhat confident about it.
○ I feel rather unconfident about it.
○ I feel unconfident about it.

Decide which of the following structures represents the most energetically favorable structural formula for dinitrogen monoxide.

Decide, as intuitively as possible, whether the charge in the molecules can be thermodynamically stabilized via resonance.

Regarding your decisions on resonance stabilization in the second part of this survey, please indicate the extent to which you agree with the following statements.

The display of the molecules was inconvenient for identifying resonance.

Did your task-solving approach change during the survey completion? If yes, please describe.

Fig. 3 Survey design with exemplary items for every survey part.

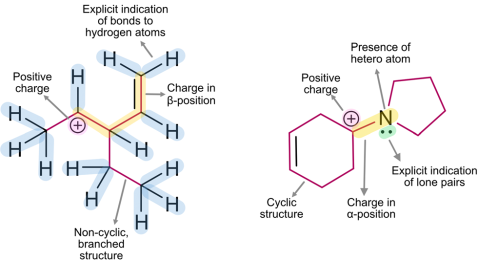


Fig. 4 Examples of structural variation for molecular structures.

delocalization. In general, all items had variations of the above-mentioned features, as indicated in the examples in Fig. 4.

Data analysis

Selection of considered structural features

To examine students' proficiency in dealing with different structural features when deciding on resonance stabilization, some decisions regarding the subsequent analysis (see section below) were made. Given that a molecule always fulfils multiple structural features (*cf.* Fig. 4), we simplified the data and reduced the number of initially encountered structural features to consider four structural characteristics that allowed the formation of distinct, non-overlapping combinations of structural features. While the integration of different structural parameters in the item design (see section *Item design*) permitted a variation of the molecular structures that might have affected students' overall decoding of the representations, previous research findings indicate that learners tend to focus on the most salient features in a representation when making decisions (Graulich *et al.*, 2019). Accordingly, we focused our analysis on rather salient, most meaningful structural characteristics that are directly related to electron delocalization, need to be considered, and, thus, might impact students' ability to discern resonance in a molecule: the distance of the charge to the conjugated system (*i.e.*, β- or α-position of the charge to the conjugated system, or the charge being on a hetero atom), the presence (or absence) of hetero atoms (*i.e.*, lack of hetero atoms indicated by the label "carbon atoms", or presence of hetero atoms, labelled as "hetero atom"), the type of charge (*i.e.*, positive or negative charge), and additional implicit aspects underlying the presence of conjugated systems and the plausibility of resulting resonance structures (*e.g.*, electronegativity, hybridization). Combining pairs of these abovementioned structural characteristics resulted in six categories that are exclusive in nature (*i.e.*, each item falls into one of these categories): 1. *β-position of charge* (20 items), 2. *carbon atoms & positive charge* (*i.e.*, allylic carbocations) (7 items), 3. *hetero atom & positive charge* (16 items), 4. *hetero atom & negative charge* (7 items), 5. *hetero atom & positive charge & implicit considerations* (7 items), and 6. *positive charge on hetero atom* (8 items) (*cf.* Fig. 5 for representative examples). Apart from the first and last category, the charge is adjacent to a hetero atom or double-bonded carbon atom for the remaining categories (α-position of the charge). As students were shown approximately 50% of all the items, some other possible combinations of structural features (*e.g.*, carbon atoms & negative charge, γ-position of the charge) were discarded from further analysis as less than five survey items would be assigned to these categories. Keeping these categories would mean that most students only saw between 1 and 2 items, which would distort obtained results in terms of students' performance on these variables. This would lead to extreme performance values (described in the section below). Consequently, of the initial 72 molecular structures, seven items were excluded from further analysis, overall resulting in 65 items included for cluster analysis (see section below).

Cluster analysis

Cluster analysis was performed to uncover patterns and describe characteristics of students' proficiency in recognizing resonance across different molecular structures. Cluster analysis is an exploratory statistical technique used to organize larger datasets by discovering meaningful groupings of objects (*i.e.*, clusters) based on their similarity in clustering variables (Everitt *et al.*, 2011). Irrespective of the specific clustering algorithm, the data is divided in a manner that objects similar in their characteristics are assigned to the same cluster. Objects within one cluster should, therefore, be as homogeneous as possible (*i.e.*, internal cohesion) but as distinct as possible from objects in other clusters (*i.e.*, external isolation) (Everitt *et al.*, 2011; Sarstedt and Mooi, 2014). Identifying a smaller number of groupings allows a concise description of patterns in the data, which can serve as a basis for further interpretation and prediction (Everitt *et al.*, 2011).

In the study presented herein, *K*-means clustering served as a clustering approach using Euclidean distance as a measure of distance. Unlike hierarchical clustering approaches, *K*-means clustering is robust to outliers and applies to larger sample sizes (above 500) (Sarstedt and Mooi, 2014). *K*-means is a non-hierarchical, partitioning cluster algorithm which iteratively relocates each object by minimizing their distance to cluster centroids (*i.e.*, grouping means). More specifically, the clustering process begins by dividing all objects simultaneously into a pre-specified number of clusters with a randomly selected initial cluster centre for each cluster. In the next steps, the cluster centroids are recalculated based on the objects forming the cluster, and the objects are successively reassigned to the closest cluster centroid. Objects can shift from one cluster to another during the clustering process to minimize the distance to the nearest cluster centroid. This process of cluster re-evaluation and optimization repeats until the cluster solution is stable, *i.e.*, the within-cluster variation is minimized, and the affiliation of objects to clusters does not change (Clatworthy *et al.*, 2005; Everitt *et al.*, 2011; Sarstedt and Mooi, 2014). Different steps were taken for the *K*-means clustering which are described in the following. All statistical analyses were conducted in SPSS version 29.0.

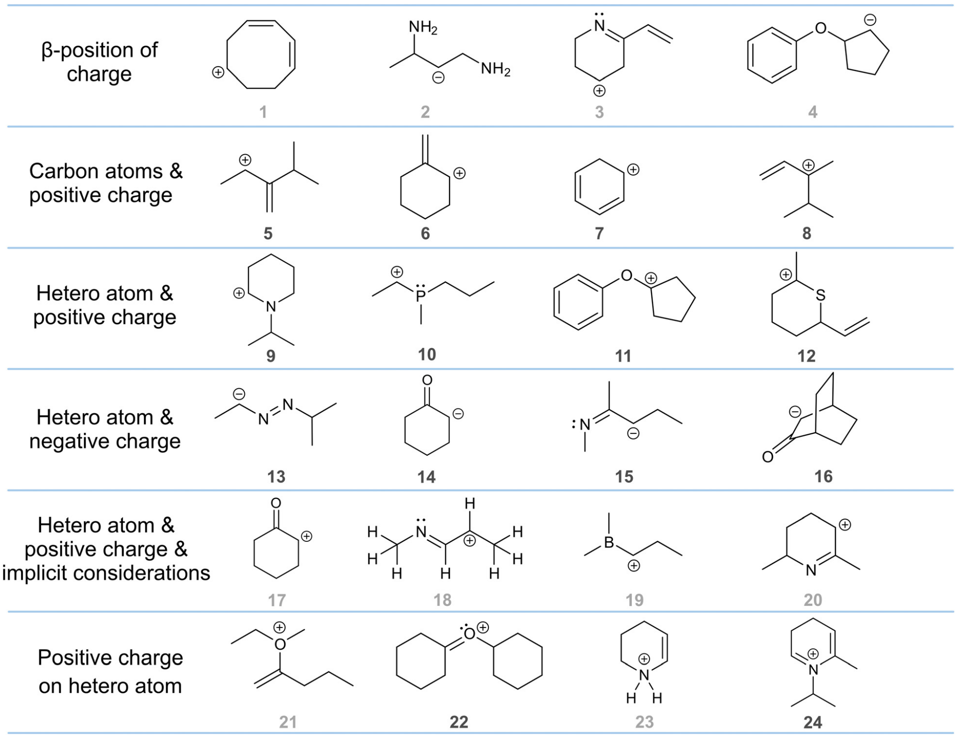


Fig. 5 Item examples for the different clustering variables. Dark numbers indicate the possibility of resonance stabilization, whereas molecular structures with light numbers do not profit from electron delocalization.

Scoring students' answers to the cluster variables. The inferred six categories of structural feature combinations (*cf.* section *Selection of considered structural features*) served as clustering variables (*i.e.*, characteristics to segment students into different clusters). The percentage of correct answers for each variable was calculated for each participant, based on students' individual number of answered items that belong to the set of each structural feature. For the analysis, we coded their answers as correct whenever their tendency toward resonance stabilization was correct (*e.g.*, *yes* or *probably yes* would be correct answers when resonance stabilization does apply for a molecule and *no* or *probably no* would be correct when resonance stabilization does not apply). Given the randomized item display, students were shown, on average, half of the items in each structural feature category (*e.g.*, 3–4 items for the category *hetero atom & negative charge* which encompasses 7 items altogether). Some students were not shown items of every clustering variable. Participants with missing data on any of the clustering variables were excluded from further analyses. The cluster analysis thus proceeded with a data set comprising N = 681 students (97% of consented students). Outliers were identified by looking for participants with more than two standard deviations from the sample mean on any cluster variable (see Table 1 in the *Results* section). The decision was made to retain the outliers in the analysis as they may provide meaningful information on students' difficulties and strengths regarding resonance recognition. After an initial cluster analysis, the decision was further made to remove items of the category *hetero atom & positive charge & implicit considerations* from the analysis. This variable had an overall low success rate for all students (35%) and was not differentiated by the clusters (*cf.* Table 8 in the Appendix for the initial cluster solution). The cluster analysis was redone with this variable removed, keeping 58 of the initial 72 survey items. The subsequent sections refer to the performed cluster analysis with the retained five variables (*i.e.*, 1. *β-position of charge*, 2. *carbon atoms & positive charge*, 3. *hetero atom & positive charge*, 4. *hetero atom & negative charge*, and 5. *positive charge on hetero atom*.)

Independence of clustering variables. Prior to clustering, the clustering variables were tested for independence. Although the categories were chosen to be distinct (*cf. Selection of considered structural features*), highly correlated variables (absolute correlations above 0.9) indicate insufficient uniqueness and lead to overrepresentation in the cluster solution

Table 1 Descriptive statistics for the different (combinations of) structural features

(Combination of) structural features	Mean (SD)[a]	Skewness[b]	Kurtosis[c]	Number of outliers[d]
β-Position of charge	65.34 *(25.61)*	−0.42	−0.69	22
Carbon atoms & positive charge	75.22 *(28.44)*	−1.03	0.35	35
Hetero atom & positive charge	55.46 *(27.28)*	−0.09	−0.82	26
Hetero atom & negative charge	54.37 *(32.23)*	−0.18	−0.99	0
Positive charge on hetero atom	43.55 *(28.82)*	0.20	−0.68	0

[a] $N = 681$. [b] Skewness standard error for this sample is 0.09. [c] Kurtosis standard error for this sample is 0.19. [d] More than two standard deviations from the mean.

(Sarstedt and Mooi, 2014). The correlation between all variables indicates a low level of collinearity among the variables (*cf.* Appendix, Table 9). Furthermore, the variance inflation factor (VIF) was calculated to inspect multicollinearity (*i.e.*, an indication of whether a variable has a strong linear relationship with the other variables), ascribing one variable as the dependent variable and regressing this variable to the other four variables. This was repeated for each variable. The VIF took values below 10 (maximum 1.09), indicating that multicollinearity does not pose problems for the cluster analysis (Field, 2013).

Decision on the number of clusters. As for the clustering procedure itself, the *K*-means clustering was started with eight clusters, which were successively reduced. The number of clusters was evaluated by inspecting each resulting cluster solution. The group means for each variable were compared to decide whether similar groups were merged in the process of decreasing the number of clusters. Finding similar clusters were merged led to an evaluation of the next cluster solution with one fewer cluster until distinct clusters were merged when the process stopped. This procedure led to a five-cluster solution for the given data, as a further combination of clusters resulted in the loss of important information. The final cluster solution was checked for reliability and validity and interpreted to infer meaningful group profiles.

Assessing the reliability and validity of the cluster solution. The reliability of the cluster solution was tested using a split-half approach (Clatworthy *et al.*, 2005; Sarstedt and Mooi, 2014). The dataset was randomly divided into two halves, and the *K*-means clustering was conducted independently for each half with $K = 5$ clusters. The qualitative comparison of the resulting cluster solutions (*cf.* Appendix, Table 10) yielded a similar cluster structure for each half of the dataset, thereby supporting the stability of the cluster solution. The validity of the cluster solution was assessed by comparing the cluster groups on different external variables that had not been included as variables during the clustering process. If significant differences for these variables exist among the clusters, the identified cluster solution is supported as providing meaningful information independent of the cluster solution (Clatworthy *et al.*, 2005; Sarstedt and Mooi, 2014). Students' prior concept-related knowledge, self-reported knowledge on resonance, average time spent on each item, and perceived cognitive load served as external variables. These comparisons are reported in more detail in the *Results* section. Students' answers for the tasks on their prior concept-related knowledge were scored so that the students could receive up to 15 points. Information regarding the task scoring can be found in the Appendix.

Results

Students' overall scores for the different structural feature categories

Descriptive statistics for the different categories were calculated and are displayed in Table 1 to describe students' overall scores in recognizing resonance stabilization in molecular structures for each structural feature. The relatively large standard deviations for all variables suggest a wide range of students' scores in answering the different items. Moreover, the variables exhibit a negative kurtosis, indicating a flatter data distribution than a normal distribution apart from the variable *carbon atoms & positive charge* (rather peaked distribution of the scores due to positive kurtosis). Regarding skewness, while the items belonging to the variable *positive charge on hetero atom* are positively skewed, *i.e.*, have a more pronounced distribution of the data toward the lower end of the possible value range, students' scores on the other variables show a negative skewness, thereby a higher rate of scores being clustered toward the higher end of the performance range with the tail pointing towards the lower end of the distribution range.

The mean values across the study population reveal that students scored highest for items belonging to the structural feature *carbon atoms & positive charge* (75%). Students also scored relatively high on items in *β-position of charge* (65%); therefore, they could relatively well decide on non-conjugated systems. Students' overall score on items involving hetero atoms was lower where students answered approximately half of the items correctly on average (55% for positive charge and 54% for negative charge). When additional implicit aspects (*i.e.*, hybridization, violation of the octet rule) had to be clearly considered for a correct decision on the stabilization of a positive charge (*i.e.*, *positive charge on hetero atom*), their score was relatively low at 44%. To test the statistical significance of these observed differences in students' success rates, a repeated-measures analysis of variance (ANOVA) was conducted to compare the overall mean scores of the clustering variables. As the Mauchly-test indicates a violation of the assumption of sphericity ($W = 0.89$, X^2 $(9) = 82.65$, $p < 0.001$), the Huynh–Feldt correction was applied. The repeated-measures ANOVA shows

Table 2 Paired-sample *t*-tests comparing students' success rate in the different cluster variables with indication of the effect size

Comparison	Mean difference	SE	*t*(680)	*p*[a]	*d*	Effect size[b]
Carbon atoms & positive charge – β-position of charge	9.88	1.34	7.39	< 0.001	0.28	Small
β-Position of charge – hetero atom & positive charge	9.88	1.52	6.52	< 0.001	0.25	Small
β-Position of charge – hetero atom & negative charge	10.97	1.50	7.29	< 0.001	0.28	Small
β-Position of charge – positive charge on hetero atom	21.79	1.54	14.18	< 0.001	0.54	Medium
Carbon atoms & positive charge – hetero atom & positive charge	19.76	1.35	14.67	< 0.001	0.56	Medium
Carbon atoms & positive charge – hetero atom & negative charge	20.86	1.62	12.91	< 0.001	0.50	Medium
Carbon atoms & positive charge – positive charge on hetero atom	31.67	1.60	19.76	< 0.001	0.76	Medium–large
Hetero atom & positive charge – hetero atom & negative charge	1.09	1.56	0.70	0.48	0.03	—
Hetero atom & positive charge – positive charge on hetero atom	11.91	1.52	7.86	< 0.001	0.30	Small
Hetero atom & negative charge – positive charge on hetero atom	10.82	1.70	6.35	< 0.001	0.24	Small

[a] Bonferroni-adjusted significance level at 0.005. [b] Effect size according to Cohen (1992).

that the overall scores for the different variables differ significantly with a large effect size [$F(3.82, 2599.75) = 123.37$, $p < 0.001$, $\eta^2 = 0.15$]. Follow-up paired-sample *t*-tests with a Bonferroni-adjusted α-level set at 0.005 as criterion for significance yielded significant differences ($p < 0.001$) between all categories except for the comparison of *hetero atom & positive charge* and *hetero atom & negative charge* (Table 2).

Cluster solution

K-means cluster analysis yielded a five-cluster solution reported in Table 3. It displays the means and standard deviations for each group's scores for each clustering variable and the distribution of students in each cluster. Finding the standard deviations within each cluster generally lower than the overall standard deviation supports the internal cohesion of the clusters.

Table 3 shows that each cluster can be characterized by the average scores on the different cluster variables. While cluster I shows rather moderate scores for all combinations of structural features not exceeding 52% on any variable, cluster II is characterized by relatively high scores for the variables *β-position of charge* (69%), *carbon atoms & positive charge* (80%), and *positive charge on hetero atom* (66%). In contrast, they score substantially lower on the remaining variables. Cluster III achieves even higher scores on the variables *β-position of charge* (80%) and *carbon atoms & positive charge* (81%), and also has a high average for the variable *hetero atom & negative charge* (79%). Cluster IV scores high on the variables *carbon atoms & positive charge* (89%) as well as *hetero atom & positive charge* (76%), but shows, compared to clusters II and III, a lower score for the variable *β-position of charge* (63%) and low scores for the remaining cluster variables (<31%). Finally, similar to cluster IV, cluster V shows a lower average for the variable *β-position of charge* (62%). While students in this cluster score well on the variables *carbon atoms & positive charge*, *hetero atom & positive charge*, and *hetero atom & negative charge* (>75%), average scores for *positive charge on hetero atom* were lower (62%). These cluster-specific score differences permit the inference of different profiles regarding students' proficiency in dealing with structural features. They are portrayed in detail in the *Discussion* section.

Relationship to other variables

Cluster assignments were related to other external variables as evidence of external validity; that is, the clusters represent meaningful groupings of students. The external variables investigated were the average time spent on the items, students' prior conceptual knowledge, students' confidence, and their perceived cognitive load when solving the tasks. The expectation is that higher performance on the resonance tasks will be associated with higher prior conceptual knowledge, higher

Table 3 Descriptive summary of the cluster solution with indication of average scores for all clustering variables and standard deviations

Cluster	*N* (%)	β-position of charge	Carbon atoms & positive charge	Hetero atom & positive charge	Hetero atom & negative charge	Positive charge on hetero atom
I	109 (16%)	49.42 *(21.92)*	27.94 *(21.91)*	48.23 *(21.28)*	51.21 *(26.35)*	50.72 *(23.38)*
II	128 (19%)	68.95 *(23.48)*	79.62 *(20.20)*	36.00 *(21.29)*	22.77 *(20.48)*	66.08 *(22.37)*
III	149 (22%)	79.72 *(18.65)*	80.72 *(20.50)*	37.49 *(21.56)*	78.89 *(19.20)*	19.26 *(18.10)*
IV	144 (21%)	62.77 *(24.43)*	88.83 *(16.29)*	75.54 *(19.30)*	30.55 *(20.95)*	24.08 *(19.46)*
V	151 (22%)	62.04 *(28.81)*	87.24 *(17.70)*	75.76 *(19.10)*	81.96 *(17.47)*	61.82 *(22.53)*
Overall	681	65.34 *(25.61)*	75.22 *(28.44)*	55.46 *(27.28)*	54.37 *(32.23)*	43.55 *(28.82)*

Table 4 Means (and standard deviations) for students' prior conceptual knowledge in dependence of their cluster affiliation

Cluster	I	II	III	IV	V	Overall
Prior knowledge score	7.51 *(2.23)*	8.09 *(2.04)*	8.05 *(2.04)*	8.53 *(2.03)*	8.50 *(2.13)*	8.17 *(2.12)*

confidence, and lower perceived cognitive load. Furthermore, informed by previous eye-tracking research contrasting decoding behaviours of experts and novices (*e.g.*, Gegenfurtner *et al.*, 2011; Lindner *et al.*, 2014), one can assume that clusters having more proficiency in discerning resonance stabilization will be associated with less time spent on the items. Inferential statistics were used to examine the extent of differences among the clusters on these external variables match these expected relationships.

Student prior knowledge. Table 4 shows the groupings' mean scores on the tasks assessing their resonance-related conceptual understanding (*cf.* Fig. 3, part I). Depending on students' affiliation to the five identified clusters, differences regarding their prior knowledge score arise with an overall increase from cluster I to cluster V. A one-way ANOVA with students' prior knowledge score as the dependent variable and cluster affiliations as the independent variable reveals significant differences among the cluster groupings with small effect sizes [$F(4, 676) = 4.87$, $p < 0.001$, $\eta^2 = 0.028$]. Follow-up pairwise comparisons using a Tukey test resulted in significant differences between clusters I and V ($p = 0.001$, $d = 0.45$), and I and IV ($p = 0.002$, $d = 0.48$) with small to medium effect sizes (Cohen, 1992). Students' knowledge of different competencies related to discerning resonance stabilization was self-reported (*cf.* Fig. 3, part I). Table 5 shows the competencies directly related to resonance-related decision-making for the tasks (see Appendix for complete list). The general trend shows clusters III to V having higher confidence ratings on each competency than clusters I and II. To test whether the differences are of statistical significance, Kruskal–Wallis tests were performed for each item. To control the Type I error resulting from multiple comparisons, a Bonferroni correction was applied, adjusting the α-value to 0.01 as criterion for significance. Despite the qualitative differences, the Kruskal–Wallis tests yielded no significant differences among the clusters. Among all items, *Identify whether resonance is possible in a molecule* ($H(4) = 12.70$, $p = 0.013$), the competency most directly applicable to the task clusters were based on, almost reached the threshold for significance.

Average time-on-task. On average, students' time spent on the items differs greatly. Table 6 shows the means and standard deviations for each cluster grouping. A one-way ANOVA exhibits statistically significant differences between the clusters with small effect sizes [$F(4, 676) = 6.50$, $p < 0.001$, $\eta^2 = 0.037$]. Tukey *post hoc* pairwise comparisons reveal significant differences between the clusters I and IV ($p < 0.001$, $d = 0.40$), I and V ($p = 0.004$, $d = 0.50$) and III and V ($p = 0.004$, $d = 0.43$) with small to medium effect sizes (Cohen, 1992). Similar to students' performance on prior knowledge, the average time on an item increases from the first (5.15 seconds) to the fifth cluster (8.24 seconds), except for cluster III (5.95 seconds).

Perceived cognitive load. At the end of the survey, students were asked to assess their perceived cognitive load regarding answering the items on resonance stabilization, and indicate their confidence in correctly answering them (*cf.* Fig. 3, part III). The clusters' mean values on the different variables can be found in Table 7. A Kruskal–Wallis test with a Bonferroni-adjusted α-value of 0.008 serving as significance criterion to control the Type I error yielded no significant differences between the clusters for any variable. However, the item *The problem-solving process was very complex* approached the

Table 5 Students' self-reported knowledge of competencies (1 = unconfident, 5 = confident) related to the decision on resonance stabilization in molecules in dependence of their cluster affiliation with indication of the standard deviation

Cluster	Identify resonance in molecules	Assess thermodynamic stability of molecules	Determine atoms' hybridization	Draw curved electron arrows	Define the resonance concept	Assess the influence of electron delocalization on molecule stability
I	3.78 *(0.99)*	3.42 *(1.11)*	3.86 *(1.07)*	4.01 *(0.94)*	3.76 *(1.02)*	3.55 *(1.11)*
II	3.91 *(1.02)*	3.41 *(1.08)*	3.98 *(1.07)*	4.20 *(0.97)*	3.95 *(1.05)*	3.68 *(1.06)*
III	4.15 *(0.86)*	3.56 *(1.00)*	4.03 *(1.06)*	4.29 *(0.83)*	4.02 *(0.93)*	3.80 *(1.03)*
IV	4.12 *(0.86)*	3.52 *(1.06)*	4.01 *(1.06)*	4.33 *(0.84)*	4.03 *(0.97)*	3.78 *(1.01)*
V	4.01 *(0.94)*	3.62 *(1.05)*	3.98 *(1.04)*	4.28 *(0.96)*	4.07 *(0.96)*	3.75 *(1.07)*
Overall	4.01 *(0.94)*	3.51 *(1.06)*	3.98 *(1.06)*	4.23 *(0.91)*	3.98 *(0.99)*	3.72 *(1.05)*

Table 6 Average time spent on each item (with standard deviations) for the different clusters. The time is measured in seconds

Cluster	I	II	III	IV	V	Overall
Time on item	5.15 *(5.46)*	6.64 *(5.07)*	5.95 *(3.55)*	7.67 *(6.83)*	8.24 *(6.59)*	6.82 *(5.74)*

Table 7 Students' reported perceived cognitive load and confidence regarding the completion of the second survey part (1 = strongly disagree, 7 = strongly agree) in dependence of their cluster affiliation with indication of the standard deviation

	Intrinsic cognitive load			Extraneous cognitive load		Germane cognitive load	
Cluster	Difficult to recognize resonance	Molecules were complex	Problem-solving process was complex	Inconvenient display of molecules	Exhausting to find important information	Effort in task solving	Confidence
I	4.46 *(1.46)*	4.29 *(1.54)*	4.23 *(1.45)*	3.58 *(1.73)*	3.88 *(1.59)*	4.86 *(1.67)*	3.22 *(1.64)*
II	4.42 *(1.51)*	4.48 *(1.63)*	4.29 *(1.53)*	3.48 *(1.86)*	3.90 *(1.72)*	4.72 *(1.45)*	2.90 *(1.41)*
III	4.44 *(1.30)*	4.30 *(1.37)*	3.99 *(1.44)*	3.12 *(1.68)*	3.49 *(1.62)*	4.55 *(1.35)*	3.12 *(1.26)*
IV	4.44 *(1.31)*	4.12 *(1.44)*	3.69 *(1.32)*	3.19 *(1.61)*	3.57 *(1.50)*	4.42 *(1.47)*	3.03 *(1.25)*
V	4.44 *(1.47)*	4.34 *(1.63)*	4.15 *(1.62)*	3.35 *(1.80)*	3.64 *(1.76)*	4.58 *(1.38)*	3.29 *(1.42)*
Overall	4.44 *(1.40)*	4.30 *(1.52)*	4.06 *(1.49)*	3.33 *(1.74)*	3.68 *(1.65)*	4.61 *(1.46)*	3.11 *(1.39)*

adjusted threshold for significance ($H(4) = 13.33$, $p = 0.010$). While the germane and intrinsic cognitive load (*i.e.*, the inherent difficulty and complexity of the items (Sweller *et al.*, 1998)) are comparable among the clusters, there is a slight tendency of decreasing extraneous cognitive load with clusters I and II exhibiting higher values than clusters III to V. The extraneous cognitive load explicitly targets the difficulty of processing information extraneous to the conceptual understanding of resonance, therefore addressing more specifically the design of the items (*i.e.*, the perception of the molecular structures in terms of structural features) (Sweller *et al.*, 1998). These qualitative differences may indicate that it becomes easier for students to perceive and process the given molecular features in certain clusters; however, no significant differences could be found. As such, it appears that overall, the perceived cognitive load was comparable across all clusters. Students' confidence for correctly deciding on resonance stabilization slightly varies among the clusters, even though they remain altogether relatively low (3.11/7).

Discussion

RQ 1: How do different combinations of structural features influence students' ability to discern resonance stabilization in molecules?

A closer inspection of the variables' mean values (*cf.* Table 1) indicates that different structural features make it significantly easier or more challenging for the students to correctly decide on resonance stabilization. While students across the entire study cohort achieved high scores for items belonging to the variable *carbon atoms & positive charge* (*i.e.*, allylic carbocations) (75%) and were also relatively proficient in deciding on no application of resonance stabilization in molecular structures bearing a charge in β-position to the conjugated system (65%), items involving hetero atoms related to lower scores (<56%). If, additionally, implicit aspects such as the violation of the octet rule had to be clearly considered to correctly decide on resonance stabilization, students' scores decreased even more (44%).

An analytic consideration of the molecular structures' characteristics and affordances could explain this varying performance. Given that items belonging to the category *β-position of charge* do not represent conjugated systems (*cf.* Fig. 5, items 1–4), resonance stabilization is not possible here. To answer these items correctly, one must have basic knowledge of conjugated systems, *i.e.*, that they represent arrays of aligning p-orbitals, resulting in π-bonding overlap along the whole system and enabling electron delocalization. Consequently, when the chain is interrupted (*i.e.*, positions of carbon atoms with sp^3-hybridization), no conjugated system is possible. With regard to the molecular structures and the processing of structural features, one must be proficient in estimating the distance of the charge, *i.e.*, knowing that the charge must be in direct adjacency to an electron-donating or -deficient source.

While one needs to be able to differentiate between a conjugated system and a non-conjugated system by analysing a broader part of the structure, items with the charge being in α-position need the learner to inspect the given structural features in more detail to decide on the possibility of resonance stabilization. In terms of the category *carbon atoms & positive charge*, items in this variable only involve allylic positive charges (*cf.* Fig. 5, items 5–8), which often serve as introductory examples for resonance (stabilization) (*e.g.*, in some textbooks such as in Ogilvie *et al.*, 2018; Klein, 2020). Allylic carbocations are also often encountered and discussed when addressing aromaticity (*e.g.*, electrophilic aromatic substitutions). As such, students' higher success in deciding on resonance stabilization for items belonging to the variable *carbon atoms & positive charge* could stem from their familiarity. By containing chains of a *single* type of atom (*i.e.*, carbon atoms), they require less information processing than those molecular structures comprising atoms other than carbon and hydrogen atoms. In these cases, the number of aspects to encounter exceeds the amount of information necessary to keep in mind when dealing with cations only involving carbon atom chains (*i.e.*, the same atom type). Logically, the more information must be processed, the more difficult the answering of items can become (Paas and van Merriënboer, 2020). Consequently, answering items that only involve carbon atoms (and hydrogen atoms) appears less demanding and easier to process.

Handling different atom types necessitates, for instance, the estimation of an atom's hybridization or the calculation of atoms' octets, thereby requiring a closer inspection and connection of different structural cues (*i.e.*, bonds, and lone pairs of electrons), which, possibly, need to be inferred first when not explicitly depicted (Cooper *et al.*, 2012a, 2012b; Graulich *et al.*, 2019). For instance, molecular structures belonging to the category *hetero atom & positive charge* necessitate more implicit structural considerations as all items in this variable depict single bonds adjacent to the charges (*cf.* Fig. 5, items 9–12). Unlike the previous category with the explicit indication of double bonds, here, learners have to reflect on the structures and possible π-bonding interactions (*e.g.*, by explicitly paying attention to electron pairs of the hetero atom as a source for electron delocalization). Consequently, to answer these items correctly, one must master a different pattern of molecular structure (Klein, 2020).

Items in the category *hetero atom & negative charge* involve the depiction of double bonds, similar to the allylic charges (*cf.* Fig. 5, items 13–16). However, here, a different approach is necessary. First, unlike items belonging to *carbon atoms & positive charge*, items in this category necessitate a broader consideration of the conjugated system due to the greater abundance of delocalized π-electrons. In contrast to allylic positive charges, these items require the electron delocalization in the reverse direction, thus not in the direction of the positive charge but starting from the negative charge towards the depicted double bonds. Second, as indicated by the two curved arrows in Fig. 6, one must mentally keep track of the electron delocalization, thereby, the hetero atoms must be taken closer into account (*e.g.*, fulfilment of the octet rule) (*cf.* Fig. 6). Hence, this pattern in electron delocalization is more complex than, for instance, allylic carbocations.

Items in the category *positive charge on hetero atom* require to include even more aspects when deciding on resonance stabilization. Here, one has to consider the feasibility of electron delocalization with regard to the hetero atom's properties. The protonated 1,2,3,4-tetrahydropyridine can serve as an example (Fig. 5, item 23). On a surface level, this structure resembles an allylic positive charge (*cf.* the variable *carbon atoms & positive charge*); nonetheless, electron delocalization is impossible because the nitrogen atom's octet would be exceeded. Unlike this example, the charged enamine compound (1,2,3,4-tetrahydro-6-methyl-1-(1-methylethyl)pyridine) (*cf.* Fig. 5, item 24) would profit from electron delocalization given the sp^2-hybridization of the nitrogen atom. Altogether, these analytic considerations illustrate that the items' inherent characteristics may account for students' varying ability in recognizing the possibility of resonance stabilization.

Despite these overall tendencies in students' performance on different structural features, the cluster analysis suggests that this trend does not necessarily apply to all students equally (*cf.* Table 3). Instead, differences in students' proficiency to deal with varying structural features prevail. These cluster-specific characteristics will be discussed next to identify underlying patterns within the wide range of student performance scores.

RQ 2 & 3: What trends regarding students' proficiency in making decisions on resonance stabilization in molecular structures emerge and how do they relate to other performance variables (*i.e.*, time-on-task, prior knowledge, cognitive load)?

A closer look into the groupings' average performance scores on the various clustering variables (*cf.* Table 3) allows a qualitative description of emerging characteristics and difficulties within the five clusters. While cluster I does not show pronounced proficiency in any structural feature, the other four clusters are reasonably proficient in discerning no possibility of resonance stabilization with the charge being in β-position and with recognizing resonance stabilization for allylic carbocations (*i.e.*, items belonging to the variable *carbon atoms & positive charge*). With regard to hetero atoms, cluster III is also proficient with the structural features *hetero atom & negative charge*, whereas cluster IV shows higher proficiency for *hetero atom & positive charge*. Cluster V is proficient in both *hetero atom & positive charge* and *hetero atom & negative charge*. This permits the inference of different profiles regarding students' guiding principles in deciding on resonance stabilization, and to

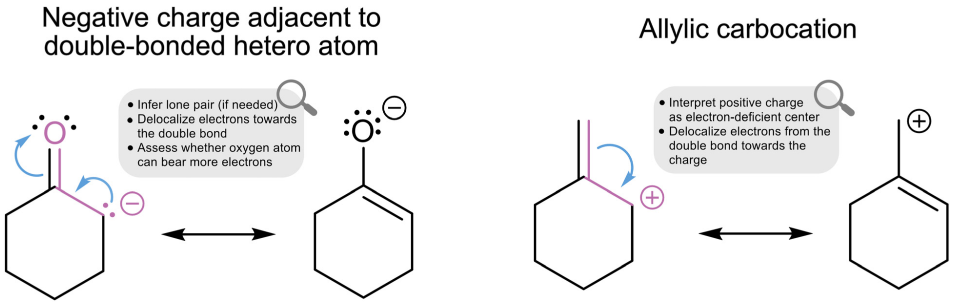


Fig. 6 Varying complexity and approaches when delocalizing a negative or positive charge adjacent to double bonds (*e.g.*, allylic carbocation or double-bonded hetero atom).

characterize students' proficiency in handling different structural features related to resonance.

Cluster I: no proficiency demonstrated

Cluster I, comprising 16% of the students (Table 3), is denoted by a score on most clustering variables that approach the chance guessing mark of 50%. The substantial deviation from chance guessing was with *carbon atoms & positive charge* (28%). This variable was scored the highest by the overall sample and markedly distinguished this cluster from the other clusters. It is possible that these students were enacting an alternative process for identifying resonance that led to predictions inconsistent with the canonical process or that these students were not engaging with the survey meaningfully. It is not possible to distinguish these explanations with the current data. Students in cluster I spent markedly less time on the task (5.15 seconds) compared to the other clusters, which could evidence either possibility. However, the consideration of the other external variables supports the assumption that students in cluster I might perceive difficulties in conceptualizing and, consequently, applying resonance, which might have induced a fast decision-making and chance-guessing approach. Students in cluster I show a substantially lower score on tasks targeting students' conceptual understanding of resonance (7.51) compared to the other clusters. Moreover, even though not differing significantly, they self-report the lowest resonance-related competencies for all items among the clusters (*cf.* Table 5). This emerging conceptual uncertainty reflects potential difficulties in their *sense-making skills* (*e.g.*, knowing how resonance can be encoded in structural features). Consequently, students might have found it harder to focus on the structural information necessary to make decisions on resonance stabilization, accounting for their lower performance in the various variables. Overall, these observed difficulties align with different studies showcasing that difficulties in understanding resonance hinder its successful application in problem-solving (*e.g.*, Petterson *et al.*, 2020; Brandfonbrener *et al.*, 2021; Braun *et al.*, 2022).

Cluster II: focus on allylic positive charges

Approximately 19% of the students belong to this cluster (Table 3). It is characterized by above average scores on the variables *β-position of charge* (69%), *carbon atoms & positive charge* (80%), and *positive charge on hetero atom* (66%), whereas showing low scores for the remaining two variables involving hetero atoms (*i.e.*, *hetero atom & positive charge* and *hetero atom & negative charge*) ($<37\%$). This indicates that students within this group are proficient in discerning conjugated systems and are more adept in dealing with molecules without hetero atoms. When comparing the different characteristics with regard to the molecular structures' features, it becomes evident that students in this cluster are guided by specific structural features when deciding on resonance stabilization. They approach the items in a visual way. More concretely, they seem to base their decision on the presence of allylic positive charges, therefore relying on one specific pattern of electron delocalization. As such, they achieve relatively high scores in identifying resonance stabilization for molecules of the variable *carbon atoms & positive charge*. The guiding principle of allylic positive charges might also explain students' scores on the other variables. Half of the items belonging to the variable *positive charge on hetero atom* involve double-bonded hetero atoms bearing a positive charge, whereas the remaining items in this variable resemble the allylic carbocation pattern except for the presence of a hetero atom (*cf.* Fig. 5, items 21–24). Given the students' relatively high proficiency with this variable, it may be that the pattern of allylic carbocation has cued students to correctly decide on resonance stabilization, either triggered by the explicit presence of a double bond next to a positive charge (*i.e.*, deciding in favour of resonance stabilization for items such as items 22 and 24 in Fig. 5), or being irritated by the presence of a charged hetero atom adjacent to a double bond. Consequently, even though items might resemble allylic carbocations (such as items 21 and 23 in Fig. 5), it is possible that students correctly decided against resonance stabilization being bothered by the presence of a hetero atom. This suggests that students might make a difference between molecular structures involving only a carbon backbone, and structures additionally comprising hetero atoms when deciding on resonance stabilization. Although students' strategies in handling items in this variable cannot be ultimately determined, and require further investigation, it is reasonable to assume that students base their decision-making regarding these items on structural features inherent to allylic carbocations. This assumption is further strengthened by the low scores on the other variables involving hetero atoms. While the items in the category *hetero atom & positive charge* comprise single bonded hetero atoms and require another pattern of electron delocalization, items belonging to *hetero atom & negative charge* necessitate the delocalization of electrons in the reverse direction (*cf.* Fig. 6), therefore making it impossible to apply the typically used resonance pattern in this cluster (*i.e.*, delocalizing a double bond toward a positive charge). Lastly, being cued by *adjacent* positive charges to double bonds, students might have found it easier to estimate the distance of the charge and, therefore, to recognize conjugated systems regarding the variable *β-position of charge*.

The emergent strategy in decision-making, focusing solely on allylic positive charges, might also stem from uncertainty. Though not differing significantly, students in this cluster indicated the lowest confidence for correctly solving the tasks (2.90/7) and rated the perceived complexity of the molecules and the problem-solving process (*i.e.*, intrinsic cognitive load) higher than the other clusters (*cf.* Table 7). This suggests that students might have found it more difficult to decide on resonance stabilization and, therefore, possibly recurred to a familiar pattern of electron delocalization. As students in cluster II might have searched for the presence of allylic carbocations, they limited their attention to structural features, thereby facilitating the decision on resonance stabilization due to processing less information (Paas and van Merriënboer, 2020).

Cluster III: flexible resonance recognition involving charges adjacent to double bonds

This cluster group (22% of students, Table 3) is characterized by an even more pronounced proficiency in handling the β-position of charges (*i.e.*, discerning conjugated systems) (80%) and dealing with allylic carbocations (*i.e.*, *carbon atoms & positive charge*) (81%) than cluster II. In contrast to the previously presented clusters, students within this group also perform better on items related to the variable *hetero atom & negative charge* (79%), whereas with a lower score on the variable *hetero atom & positive charge* (37%). Among all clusters, they score lowest on the variable *positive charge on hetero atom* (19%). With regard to the structural properties of the molecules, it becomes evident that the students in this cluster are also guided by the presence of double bonds when deciding on resonance but are able to operate with different charges more flexibly, indicating a higher proficiency over various structural features. More specifically, most items bearing a negative charge comprise double bonds, resembling the allylic carbocations pattern. However, unlike allylic carbocations, which permit a *source-to-sink* – approach by delocalizing electron density towards electron-deficient centres (*i.e.*, the positive charge) (Bhattacharyya, 2013), delocalizing a negative charge requires a different approach, with the negative charge being the starting point to delocalize electron density. As such, the delocalization of the π-electrons in the reverse direction necessitates more complex thinking (*i.e.*, interrelated consideration of structural features, *cf.* Fig. 6). This reflects an important learning outcome described by Carle and Flynn (2020), as students in this cluster seem to be able to track electron delocalization. This assumption matches students' relatively fast decision-making (5.95 seconds), suggesting that students in this cluster might show beginning fluency in dealing with molecules involving positive and negative charges adjacent to double bonds. In this regard, being able to keep track of the electrons in the molecular structure is an important learning objective. Betancourt-Pérez *et al.* (2010) have shown that students who master electron movement can better compare stabilities of different Lewis structures. This arising proficiency in dealing with different charges in this specific structural motive might also be leveraged by students' perceived competence in identifying resonance in molecules (4.15/5), with a score being the highest among all clusters.

Being guided by patterns involving double bonds might also explain students' varying scores in the other variables. While the presence of charges adjacent to double bonds might facilitate the decision on electron delocalization for molecular structures belonging to the variable *β-position of charge*, it might be conversely responsible for students' relatively low scores for items bearing a positive charge adjacent to a hetero atom. These molecular structures are displayed with single bonds and might cause confusion for not following the same pattern (Fig. 5, items 9–12). Interestingly, students show, among all clusters, the lowest performance in correctly answering items belonging to the variable *positive charge on hetero atom*, even though these items also comprise double bonds and charges. An explanation for this might be the more reflective consideration of potential electron delocalization. It might be that students have applied learnt patterns involving allylic charges without further reflecting on the actual *possibility* of electron delocalization. Therefore, they might not have thoroughly examined the nature of involved atoms in the conjugated systems. This reinforces previous studies related to the fragmented use of resonance when reasoning through different organic chemistry tasks (Brandfonbrener *et al.*, 2021; Braun and Graulich, 2024). Another explanation for students' challenges with the variables *hetero atom & positive charge* and *positive charge on hetero atom* might be the hetero atoms' hybridization. Unlike the other variables, displaying sp^2-hybridized hetero atoms, all items in *hetero atom & positive charge* and half the items of *positive charge on hetero atom* show sp^3-hybridized hetero atoms (*cf.* Fig. 5).

Cluster IV: consideration of different resonance patterns involving positive charges

About 21% of the students belong to cluster IV (Table 3). With regard to hetero atoms, unlike cluster III, cluster IV shows high proficiency in dealing with molecular structures involving positive charges adjacent to hetero atoms (*i.e.*, the variable *hetero atom & positive charge*). It appears that students in this cluster are able to deal more flexibly with positive charges when deciding on resonance. As such, unlike the previous clusters, they discern resonance in molecular structures displaying different patterns of electron delocalization in relation to positive charges, *i.e.*, also in molecules involving single-bonded hetero atoms in which the possibility of electron delocalization must be inferred (*e.g.*, in terms of delocalizable lone pairs of electrons, or the consideration of possible steric constraints regarding π-bonding interactions). While students in the third cluster also master different resonance patterns, overall, these patterns relate to double bonds (*i.e.*, double bonds adjacent to a positive or negative charge). In contrast to that, students' proficiency with different resonance patterns related to positive charges in cluster IV indicates that they seem to be considerate of different aspects and structural features and, therefore, might handle the structural features in a more interrelated, thorough manner (Betancourt-Pérez *et al.*, 2010). Being more proficient in considering different structural features could be associated with students' significantly higher score on tasks assessing their conceptual understanding (8.53) and their above-average self-reported competency in identifying resonance in molecules (4.12/5).

The more differentiated consideration of structural features might also account for their slightly lower mean score in discerning conjugated systems in contrast to the previous clusters (*i.e.*, *β-position of charge*). While other clusters could simply check by searching for certain features (*i.e.*, predominantly the presence of double bonds adjacent to charges), students in this group might experience more difficulties due to the higher degree of information to encounter and weigh (*e.g.*, estimate the distance and connection of charges to single-bonded hetero atoms), which may also be the reason for the higher amount of time spent on the items (7.67 seconds on average). Even though students seem to be more attentive to hetero atoms in terms of resonance, they seem to limit their consideration of resonance stabilization to the delocalization of positive charges. Given the low value for *hetero atom & negative charge* (31%), it seems that students in this group face difficulties in assessing the impact of resonance on the delocalization of negative charges. Thus, they might not associate resonance stabilization with the delocalization of negative charges, but instead with the compensation of electron deficiency with electron density. This is not surprising as delocalizing electrons from an electron-donating to a -deficient centre is a typical approach in (organic) chemistry, for instance, with regard to the electron-pushing formalism (Bhattacharyya, 2013; Flynn and Featherstone, 2017). Consequently, students' varying performance on items related to negative and positive charges indicates that students may mimic electron delocalization following a *sink-to-source* – approach but struggle to actually *interpret* the impact of electron delocalization (*i.e.*, the energetic meaning of delocalizing electron density and how negative charge distribution contributes to the molecule's stability). This assumption aligns with existing research emphasizing students' challenges in conceptual understanding of the resonance concept (*e.g.*, Kim *et al.*, 2019; Xue and Stains, 2020), their fragmented ideas about how resonance relates to stability and reactivity (Brandfonbrener *et al.*, 2021; Tetschner and Nedungadi, 2023), and might be related to an overall operational teaching of resonance in Organic Chemistry courses (Xue and Stains, 2020; Barakat and Orgill, 2024). Comparing the students' varying performance for the variables *hetero atom & positive charge* and *hetero atom & negative charge* and *positive charge on hetero atom* further indicates that students might perceive difficulties in dealing with sp^2-hybridized hetero atoms. More specifically, all items of the variable *hetero atom & negative charge* and half of the items in the variable *positive charge on hetero atom* show sp^2-hybridized hetero atoms.

Cluster V: beginning proficiency in various resonance patterns

This cluster, comprising 22% of the students, shows relatively high mean values for all variables (>61%) (Table 3). Consequently, students in this cluster combine the competencies regarding hetero atoms from clusters III and IV, with relatively high proficiency in dealing with both positive and negative charges adjacent to hetero atoms. As the items expose varying structural connectivity across the different variables, this showcases that students are more adept in handling different resonance patterns and dealing with different structural features in an interrelated manner (*e.g.*, inspecting hetero atoms in terms of de-localizable lone pairs to stabilize charges). This flexibility and beginning proficiency are supported by students' more advanced prior conceptual understanding (8.50), significantly outperforming other clusters. The students are also more confident in correctly answering the tasks on resonance stabilization (3.29/7), although this value does not differ markedly from the remaining clusters. Similar to cluster IV, being sensitive to different patterns and visual cues might also be the reason why students in this cluster perform slightly lower on items involving charges in β-position to the conjugated system (62%) and charged hetero atoms (62%). Processing and weighing more information in their interplay (instead of attending to mere structural features) might make the recognition of conjugated systems more difficult (Paas and van Merriënboer, 2020). This might account for students' spent time-on-task. Given that it took students in this cluster the longest to come to a decision (8.24 seconds), the amount of time spent might be interpreted as an indicator of the number of structural features considered and weighed during the problem-solving process. Consequently, even though students show proficiency for most variables with different structural features, they seem to still explicitly *make sense* of the molecular structures in terms of resonance stabilization.

General discussion

Different learning profiles can be inferred based on the clusters' varying proficiency with different structural features, which are summarized in Fig. 7. A more general comparison of the five clusters' characteristics and relationships with external variables permits the synthesis of different, broader inferences regarding students' development of proficiency in resonance-related structure decoding, how they deal with different structural features when deciding on resonance stabilization, and how underlying, guiding principles impact students' ability to discern resonance. These are described in the following.

Perceived cognitive load persists for all students. In general, the comparison of all clusters suggests no linear development in students' proficiency in recognizing resonance stabilization in molecular structures. Nevertheless, with increasing prior conceptual knowledge (as indicated by students' scores on tasks related to resonance-related learning outcomes), students' flexibility and proficiency to discern different possibilities of electron delocalization increases. They consider varying structural features in an interrelated way and recognize different resonance patterns, as opposed to focusing predominately on allylic charges. However, the consideration of students' perceived cognitive load revealed that more proficiency in discerning resonance stabilization does not relate to a decrease in neither intrinsic nor extraneous cognitive load, but remains similar for all clusters. It appears that students in this cohort keep finding it difficult to discern resonance, either due to general uncertainty in dealing with resonance (cluster I) or due to the emerging interconnectedness of different structural features (cluster V). The similar cognitive load for all students suggests that they are likely relying on *sense-making* processes when dealing with the various molecular structures, indicating that they have not gained *perceptual fluency* yet to focus their attention effortlessly on the most relevant structural features in the representations.

Fast decision-making relates to lower conceptual understanding. From the different cluster profiles, it becomes

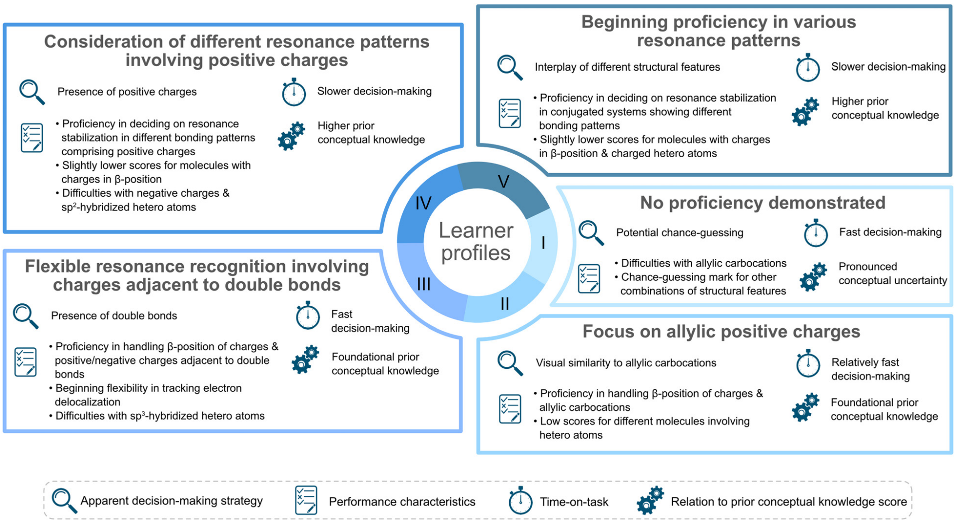


Fig. 7 Summary of the different learner profiles based on the cluster characteristics.

apparent that students' proficiency does not evolve linearly with prior knowledge and that students show different areas of emergent proficiency with regard to hetero atoms (*e.g.*, handling different charges, being able to recognize the possibility of electron delocalization when dealing with single-bonded hetero atoms). Students with significantly lower prior knowledge (cluster I) not only report higher uncertainty regarding competencies pertaining to resonance-related learning outcomes, but spent, on average, the least amount of time on the tasks, overall resulting in moderate scores across all variables. Therefore, students might have adopted a superficial guessing approach, perhaps due to uncertainty about which combinations of structural features allow electron delocalization to occur or how to proceed in solving the tasks (*e.g.*, in locating conjugated systems). In contrast, it could be shown that more proficiency in discerning resonance stabilization corresponds to more time to come to a decision, suggesting a more thorough inspection of the molecular structures. This indicates that students' proficiency in discerning resonance might depend on their conceptual understanding (including *sense-making skills*), but does not necessarily correlate with faster decision-making. Consequently, the initial assumption of higher proficiency relating to less time for decision-making has not been met.

Allylic carbocations serve as a blueprint for resonance considerations. Besides focusing on the presence of hetero atoms, more than 40% of the students (cluster II and III) seem to base their consideration of resonance on double bonds, visually resembling allylic carbocations which are often the first to encounter when introducing resonance stabilization. Due to this visual similarity, this approach may lead to a first reliance on double bonds as a guiding principle. This is leveraged by high scores on items in the variable *carbon atoms & positive charge*, being the only variable in which students overall show high proficiency (75%). This suggests that students in this cohort find it easier to solve resonance tasks involving allylic carbocations, possibly due to its familiarity and reduced amount of information to process. This combination of structural features might serve as a structural blueprint to decide on resonance stabilization in other molecular structures. This finding suggests that students first pay attention to simpler patterns, before gaining more proficiency in identifying different patterns of resonance and more thoroughly including hetero atoms in their consideration of resonance. Similarly, dealing with negative charge in terms of resonance stabilization does not seem as straightforward as with positive charge for at least 40% of the students (clusters II and IV), suggesting that students might be primed by associating resonance stabilization with the compensation of positive charges.

Inaccessibility of molecular structures requiring implicit considerations. The cluster analysis further revealed that all students, irrespective of cluster affiliation, had difficulties in correctly deciding on resonance stabilization for items necessitating a more profound analysis of the structures. This is not only reflected by their overall low success rate on items belonging to the initially considered, but later excluded variable *hetero atom & positive charge & implicit considerations* (35%), but also extends to students' overall lower score for the variable *positive charge on hetero atom* (44%). The low scores suggest that the operationalization of resonance (*i.e.*, mechanical application of resonance when visually suitable structural features are adjacent to a charge) seems easier to activate for the students than a more nuanced consideration of implicit aspects that are not immediately apparent. This reinforces students' operational approach to the resonance concept previously reported in several studies (*e.g.*, Xue and Stains, 2020; Brandfonbrener *et al.*, 2021). As such, students in this cohort have yet to demonstrate flexibility in identifying resonance patterns and to apply different learning outcomes for resonance (Carle and Flynn, 2020). For instance, from a qualitative perspective, students across all clusters self-assess their competency relatively high for assessing the hybridization of atoms (3.98/5). However, the scores on the variable *positive charge on hetero atom* remain quite low across all clusters. This indicates that they do not always consider hybridization when deciding on resonance – a crucial aspect that instructors of organic chemistry expect students to do when reasoning about resonance (Barakat and Orgill, 2024). Staying on the level of surface pattern recognition is, not surprisingly, cognitively less demanding than reflecting on the plausibility or possibility of resonance structures. This aligns with a large body of research in Organic Chemistry education (*e.g.*, Domin *et al.*, 2008; Graulich and Bhattacharyya, 2017; Graulich *et al.*, 2019; Demirdöğen *et al.*, 2023) and suggests that students do not necessarily link structural to electronic and energetic accounts, when it is not reinforced and assessed in teaching. This observation contributes to previous studies related to learners' limited competency in linking structure to energetics when dealing with chemical reactions (Caspari *et al.*, 2018; Pölloth *et al.*, 2023).

Students' limited consideration of further, implicit features could also be related to the presentation of resonance in the textbook used in the course. Compared to other common Organic Chemistry textbooks, on average, the Klein textbook addresses more representational competencies (*e.g.*, the interpretation, translation, generation, and limitations of representations) and offers a higher degree of highly scaffolded worked examples and practice problems to build these skills (Gurung *et al.*, 2022). However, a closer look into the corresponding practice problems for the course's resonance-related learning objectives reveals that the exercises are limited to the identification and use of resonance patterns, in which resonance does apply. At least in the textbook chapter introducing and explicitly practising resonance, no exercises use examples in which resonance is *not* possible (Klein, 2020). Therefore, when answering these exercises, students were not required to question the feasibility of resonance structures when locating resonance patterns (*e.g.*, deciding on the violation of the octet rule) apart from few exercises focusing on valid curved arrows (Klein, 2020). This may account for students' lower success rate for items requiring such considerations.

Higher prior knowledge may cause uncertainty. Clusters associated with significantly higher conceptual understanding (clusters IV and V) showcase more pronounced structural flexibility in recognizing resonance stabilization across different molecular structures by paying attention to various structural features. By performing better on variables comprising different types of atom connectivity and bonding, these students seem to think about different interrelated structural features to a greater extent and more thoroughly, as also indicated by more time spent on the tasks. However, as more information needs to be considered, multiple structural information may also result in overthinking, confusion, and uncertainty (Linn, 2005). This manifests in a relatively weaker performance on items in the variable *β-position of charge* (clusters IV and V), thereby possibly confusing students in locating conjugated systems – a critical step in solving more complex problems in organic chemistry. Following that, even students with a higher degree of prior knowledge in this cohort seem not fully proficient in discerning resonance in all cases yet, even though they showed proficiency across various variables.

Conclusion

The quantitative study presented herein aimed at exploring how the variation of structural features affects students' consideration of electron delocalization and which (combinations of) structural features render students' recognition of resonance stabilization difficult. Using *K*-means clustering, different profiles and characteristics regarding students' proficiency and strategies in discerning resonance could be determined. Altogether, the data suggests no clear linear progression in terms of proficiency in recognizing resonance in molecular structures but rather indicates different paths in terms of emerging proficiency. While it became evident that dealing with allylic carbocations is much easier for the majority of students than with hetero atoms, a closer analysis of the different cluster affiliations revealed different individual challenges with regard to discerning resonance stabilization, which affect the time spent on items, and which relate to students' conceptual understanding of resonance. Some students seem to base their decision on the possibility of electron delocalization on the presence of singular features (*i.e.*, allylic systems), either due to low conceptual understanding and uncertainty or because of the visual resemblance of the structures to allylic carbocations. Moreover, across all clusters, it became apparent that students had difficulties in correctly answering items requiring further implicit considerations. However, students' perceived cognitive load remained similar across all clusters. Based on these findings, different implications for teaching and future research can be inferred.

Implications for practice

To successfully recognize and apply resonance across different types of molecular structures, one must be proficient in dealing with various structural features. While this study revealed that most students correctly decide on resonance stabilization for allylic carbocations, most students faced challenges in correctly deciding for molecules comprising other (combinations of) structural features (*e.g.*, hetero atoms), even with increased prior knowledge. This is problematic as chemical problem-solving requires students to deal with more complex structures and flexibly use (implicit) structural information to consider the possibility of electron delocalization on their own (*e.g.*, without explicitly indicating features such as lone pairs of electrons). In this regard, it is questionable whether students truly gain competence in discerning resonance by focusing on learning simple patterns of electron delocalization. Even though the students in this study learned about different critical aspects underlying resonance considerations in their Organic Chemistry I course (*e.g.*, evaluate the significance of resonance contributors), the findings of the cluster analysis indicate that students had not fully applied their acquired knowledge to decide on resonance stabilization, both with regard to the recognition of resonance patterns and the plausibility of resulting resonance structures. At a broader level, the results implicate that it is crucial to reinforce and practice resonance considerations on a regular basis in order to promote learners' connection and activation of concept-related resources, thus making them more available when confronted with molecular structures (DiSessa *et al.*, 2016). However, at a more local level, students' affiliation to the different clusters reveals different stages of proficiency in discerning resonance stabilization, requiring different approaches to enhance their *sense-making skills* and *perceptual fluency*. Based on that, specific implications can be derived for each cluster to develop their resonance-related proficiency.

Since cluster I exposed conceptual difficulties, resulting in a low performance across all cluster variables, students in this cluster would benefit from *sense-making activities* (Rau *et al.*, 2017). In this regard, Rau and colleagues (2017) and Rau (2018) have shown that *sense-making activities* should precede *fluency-building activities* when learners do not have sufficient prior knowledge. Consequently, these students could be supported with exercises explicitly making sense of electron delocalization and actively seeking explanations for resonance (Rau *et al.*, 2017). Instead of a mere superficial recognition of resonance patterns, at this early stage of developing proficiency, emphasis should be placed on a thorough reflection on how different visual cues in the molecular structures relate to resonance (*e.g.*, whether they build a conjugated system), and *why* the different structural feature combinations actually permit electron delocalization (Seufert, 2003; Xue and Stains, 2020). The concurrent consideration of aspects such as atoms' electronegativity, hybridization, or the energetic impact of electron delocalization on hetero atoms could be discussed to a greater extent to connect existent different conceptual knowledge pieces (Betancourt-Pérez *et al.*, 2010; DiSessa *et al.*, 2016). In other words, instead of simply learning and applying different patterns, which may result in an overreliance on singular features resembling specific patterns, one could, at the beginning, inspect the molecular structures in more detail to raise students' awareness of why electron delocalization is possible and energetically favourable; laying the ground for a more reflective approach to subsequent pattern recognition. One could also integrate different, complementary representations to illustrate the impact of electron delocalization and, therefore, support students' understanding of electron density *distribution* (*e.g.*, use of electrostatic potential maps) (Ainsworth, 2006; Rau, 2017). In this regard, it could be also addressed that electron delocalization does not necessarily equalize the compensation of positive charge but may also encompass the delocalization of negative charge (*i.e.*, as shown by the reverse direction of curved electron arrows).

Students in clusters II to IV are more proficient in deciding on resonance stabilization, but they did not demonstrate proficiency with different structural feature combinations involving hetero atoms. To support these students, scaffolding (Kranz *et al.*, 2023) or stepped-supporting tools (Hermanns and Schmidt, 2018) addressing these difficulties could be offered. For instance, when deciding on resonance stabilization for various molecular structures, students could be provided with different impulse questions and solution strategies (*e.g.*, to consider the hybridization of (hetero) atoms, to determine the presence of conjugated systems, to check whether the octet rule is violated, or to expand the molecular structures to make atoms' features more explicit). Accordingly, students can determine on their own whether they need help, ultimately allowing them to foster their *sense-making* of specific bonding patterns of resonance they still struggle with. Furthermore, different contrasting examples of (im-)plausible resonance structures with similar structure motives could be weighed and discussed in the classroom (*cf.* Fig. 6 for examples) (Graulich and Schween, 2018). For instance, eliciting comparisons of a positively and negatively charged molecular structure in terms of resonance stabilization could help students understand that in both cases, electron delocalization contributes to its stability (*cf.* cluster IV) but that negatively charged compounds require a different approach. Moreover, to enhance these students' *perceptual fluency*, thus, being able to quickly focus on relevant structural cues, highlighting what to focus on (*i.e.*, conjugated systems) could be a helpful guidance and prevent students from merely looking for singular structural features when deciding on resonance (*cf.* clusters II and III).

Finally, students in cluster V showed the most pronounced proficiency regarding resonance stabilization across varying combinations of structural features. However, in this cluster, it took the students the longest to come to a decision. This suggests that students' proficiency is based on *sense-making skills*, thereby showing the need to engage students at this proficiency stage more in *fluency-building activities* (Rau, 2018) to become more fluent in their decision-making. This could be accomplished with short classification exercises following the principles of perceptual learning (Kellman and Massey, 2013), *e.g.*, prompting students to decide on resonance for a sequence of molecules and providing immediate feedback. Here, existing practice exercises in Klein (2020) could be expanded by also exposing students to molecular structures where resonance is *not* applicable (*e.g.*, due to the β-position of the charge, or the violation of the octet rule). Categorizing a variety of molecular structures in terms of resonance stabilization, not only by discriminating the different bonding patterns of resonance but also by considering their applicability, could help students become sensitive to a more reflective use of resonance patterns regarding molecules exposing similar structural feature motives.

Lastly, common teaching approaches to introduce and use resonance should be revisited. Students' overall proficiency with allylic carbocations could stem from their familiarity with instructional contexts (*e.g.*, the introduction of electron delocalization and discussion of aromaticity). While easier examples are certainly necessary at the beginning to help understanding, using more diverse examples and exercises could support students to become more adept in deciding on resonance for various molecular structures.

Implications for research

While this study yields first insights into how different structural features impact students' consideration of resonance stabilization in a molecule, the analysis focused on a limited number of structural features in smaller, relatively simple molecular structures. Future work could delve deeper into more complex structures to further shed light on other (less salient) features, such as the impact of the familiarity of hetero atoms or the role of lone pairs on students' application of resonance. It would also be interesting to investigate students' strategies to perceive conjugated systems in more detail (*e.g.*, through eye-tracking) or to look deeper into students' certainty when answering different resonance tasks. Given that students in this study were explicitly prompted to consider and decide on resonance stabilization in provided structures, more research is needed investigating students' proficiency in resonance recognition within reaction contexts.

Not included in the analysis were changes in students' perceptions and strategies as a result of being presented with a sequence of molecular structures. In this regard, it could also be worthwhile to look in more detail into how students' proficiency develops across a semester or across different courses, *e.g.*, model a learning progression or uncover the differences between novice learners and advanced learners in terms of resonance-related decoding of molecular structures. While this study indicates that the clusters differ in conceptual understanding, future studies could more systematically investigate how prior conceptual knowledge affects students' proficiency in discerning resonance in molecular structures. Lastly, the effectivity of different teaching approaches needs to be investigated in more detail (*e.g.*, does instruction focusing on a stronger connection of different concepts, such as hybridization, energy, and resonance, result in more reflective pattern recognition? Does perceptual learning with feedback settings help students to become proficient in discerning resonance?). This also comprises a more thorough examination of how instructors' teaching practices impact learners' proficiency in discerning resonance stabilization in molecules, *e.g.*, whether they promote certain learning profiles.

Limitations

This quantitative study is explorative in nature; therefore, the results must be interpreted in light of several limitations. First, as the data were collected at one institution following a traditional curriculum, it remains unclear whether the findings can be generalized, given different teaching approaches at other universities. Second, the cluster analysis focused on a limited number of combinations of salient structural features, whereas each molecular structure also includes multiple less salient structural features (*e.g.*, the complexity of the structure's carbon backbone of the structures, the explicit indication of bonds to hydrogen atoms). As such, their overall interplay might have influenced students' decision-making on resonance as well. Given the reduction of structural features considered in the cluster analysis, students' proficiency in resonance considerations for structures involving negative charges could not be resolved entirely. For instance, it remains unclear whether students are proficient with negative charges when the

Table 8 Descriptive summary of the initial cluster solution comprising the variable *hetero atom & positive charge & implicit considerations* with indication of average scores for all clustering variables and standard deviations

Cluster	***N* (%)**	**β-position of charge**	**Carbon atoms & positive charge**	**Hetero atom & positive charge**	**Hetero atom & negative charge**	**Hetero atom & positive charge & implicit considerations**	**Positive charge on hetero atom**
I	130 (19%)	52.51 *(22.56)*	34.71 *(25.27)*	48.79 *(22.57)*	58.97 *(25.92)*	60.82 *(27.35)*	51.07 *(24.80)*
II	96 (14%)	74.72 *(21.16)*	78.52 *(21.55)*	32.95 *(22.23)*	21.61 *(20.30)*	48.35 *(29.74)*	68.36 *(23.69)*
III	142 (21%)	81.42 *(16.74)*	83.42 *(19.37)*	35.78 *(19.90)*	76.18 *(19.63)*	32.14 *(25.38)*	20.33 *(19.23)*
IV	158 (23%)	58.11 *(25.02)*	85.89 *(18.83)*	69.47 *(20.34)*	25.39 *(20.01)*	19.12 *(20.11)*	28.77 *(22.65)*
V	155 (23%)	62.94 *(28.41)*	88.78 *(16.98)*	78.76 *(17.63)*	80.35 *(18.52)*	24.37 *(25.38)*	58.23 *(23.99)*
Overall	681	65.34 *(25.61)*	75.22 *(28.44)*	55.46 *(27.28)*	54.37 *(32.23)*	35.11 *(29.61)*	43.55 *(28.82)*

molecules do not involve hetero atoms. Given the randomized display of about 50% of the items for each student, students solved different items that could have influenced the findings in light of the interplay of different structural features. Due to the study's quantitative character, students' proficiency with different structural features was inferred from patterns in the cluster solution and could not be complemented with qualitative data. The interpretations drawn would benefit from further student validation (*e.g.*, member checking) to verify the correctness of conclusions made regarding students' proficiency and difficulties. At the time of data collection, no concept inventory to assess students' prior resonance-related knowledge existed. Consequently, the assessment of students' conceptual understanding could not be based on established instruments. Lastly, the remote completion of the survey bears different limitations that might have affected the inferred findings. On the one hand, students' actual effort in solving the tasks remains unclear and could not be validated. For instance, although students were explicitly prompted to decide on the impact of electron delocalization on the molecule's stability, it remains unclear whether students interpreted the prompt as intended (*e.g.*, whether they tried to look for resonance stabilization or the mere possibility of delocalizing electrons). The hypothetical interpretation of the prompt as deciding on the formal possibility of electron delocalization would not affect the inferences made based on the clustering variables. The decisions on stability contribution align with the possibility of electron delocalization for the variables included in the cluster analysis (*cf.* Fig. 5). However, conclusions drawn on implicit considerations based on the variable *hetero atom & positive charge & implicit considerations* (excluded from the cluster analysis due to low performance scores across all clusters, *cf.* Table 8 and section *Cluster analysis*) should be viewed with caution. On the other hand, even though students were explicitly asked to take the survey without external helping tools, it is uncertain whether students answered the items intuitively or whether they used supporting tools (*e.g.*, lecture notes and textbooks). Eventually, the use of external tools might have affected students' cluster affiliation (*e.g.*, by more often correctly identifying resonance across the different cluster variables) and their cluster characteristics (*e.g.*, time spent on the tasks). Finally, the conclusions regarding students' proficiency in discerning resonance stabilization are constrained by being based on simple molecular structure items; therefore, it remains unknown whether they also apply to students' proficiency in identifying the possibility of electron delocalization in reaction contexts.

Author contributions

Irina Braun: conceptualization, investigation, methodology, formal analysis, writing – original draft, visualization. Scott E. Lewis: resources, methodology, writing – review and editing. Nicole Graulich: conceptualization, methodology, supervision, writing – review and editing.

Data availability

The data are not publicly available as participants of this study did not consent for their data to be shared publicly.

Conflicts of interest

Researcher SEL receives funding from the Royal Society of Chemistry (RSC). The RSC played no role in the data collection, analysis or presentation of the research.

Appendices

Tasks assessing students' prior resonance-related knowledge

Based on the learning outcomes defined by Carle and Flynn (2020) and reported alternative conceptions on resonance (*e.g.*, Brandfonbrener *et al.* (2021), Xue and Stains (2020)), nine tasks have been designed to assess students' conceptual understanding of resonance (Fig. 8). For each correct answer, students received 1 point (altogether 15 points). Solutions are indicated in blue.

Initial cluster solution

The cluster analysis was initially performed with six clustering variables (Table 8). However, the variable *hetero atom & positive charge & implicit considerations* did not differentiate the clusters with overall low scores for all clusters. Consequently, the cluster analysis was redone, omitting this variable (*cf.* Table 3).

Correlation matrix

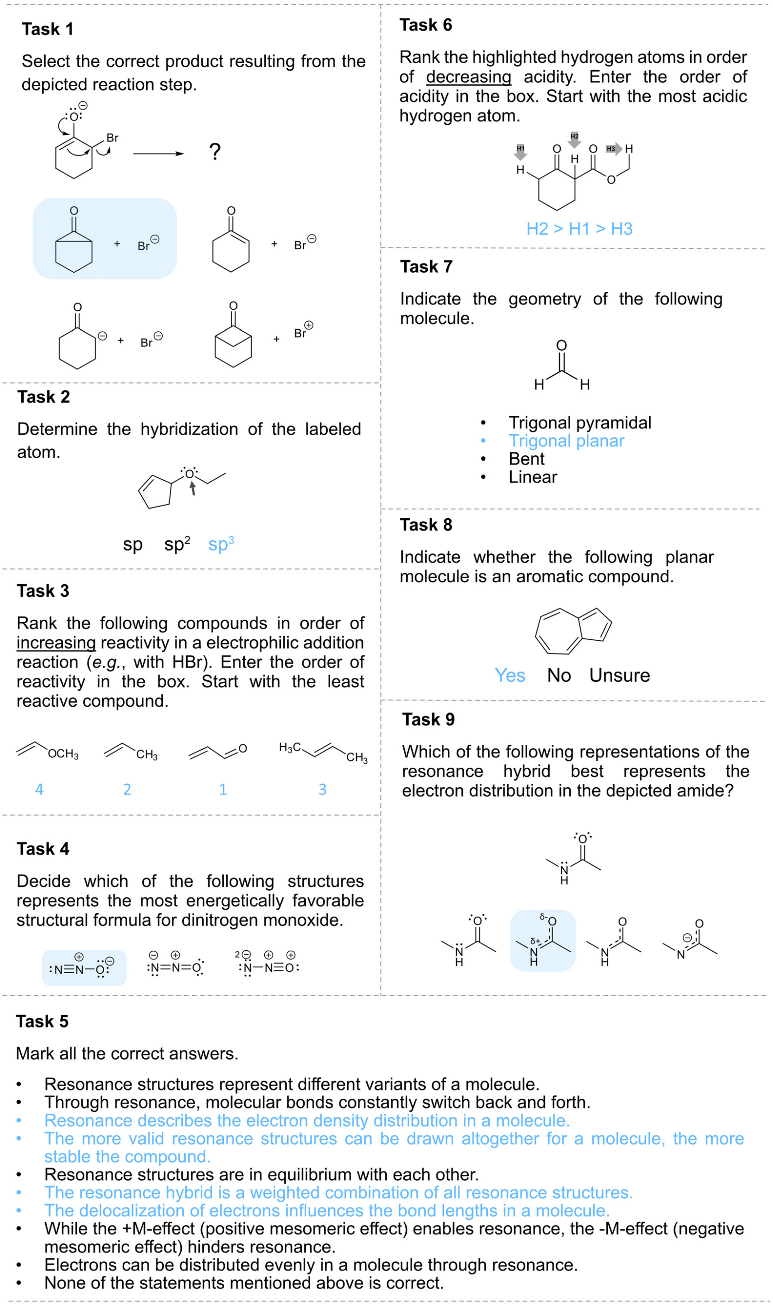
The clustering variables exhibited low correlations (<0.9). They are summarized in Table 9.

Split-half reliability of the cluster solution

To test for reliability of the cluster analysis, the data was randomly divided in half. On each half, a K-means cluster analysis with $K = 5$ clusters was performed independently. The results of each cluster analysis are summarized in Table 10. Inspecting and comparing the two cluster solutions (Clatworthy *et al.*, 2005), it was found that they agree qualitatively and correspond to the characteristics of the cluster solution reported in Table 3, thereby supporting the stability of the cluster analysis.

Self-reported knowledge

Students self-reported on different competencies related to resonance-specific learning outcomes in the first survey part (Fig. 3). While Table 5 reports on learning outcomes directly related to the decision-making in the second survey part (Fig. 3), Table 11 gives an overview of the clusters' self-assessment on the remaining items with indication of the means and standard deviations.



Task 1

Select the correct product resulting from the depicted reaction step.

Task 2

Determine the hybridization of the labeled atom.

sp sp^2 sp^3

Task 3

Rank the following compounds in order of increasing reactivity in a electrophilic addition reaction (*e.g.*, with HBr). Enter the order of reactivity in the box. Start with the least reactive compound.

Task 4

Decide which of the following structures represents the most energetically favorable structural formula for dinitrogen monoxide.

Task 5

Mark all the correct answers.

- Resonance structures represent different variants of a molecule.
- Through resonance, molecular bonds constantly switch back and forth.
- Resonance describes the electron density distribution in a molecule.
- The more valid resonance structures can be drawn altogether for a molecule, the more stable the compound.
- Resonance structures are in equilibrium with each other.
- The resonance hybrid is a weighted combination of all resonance structures.
- The delocalization of electrons influences the bond lengths in a molecule.
- While the +M-effect (positive mesomeric effect) enables resonance, the -M-effect (negative mesomeric effect) hinders resonance.
- Electrons can be distributed evenly in a molecule through resonance.
- None of the statements mentioned above is correct.

Task 6

Rank the highlighted hydrogen atoms in order of decreasing acidity. Enter the order of acidity in the box. Start with the most acidic hydrogen atom.

H2 > H1 > H3

Task 7

Indicate the geometry of the following molecule.

- Trigonal pyramidal
- Trigonal planar
- Bent
- Linear

Task 8

Indicate whether the following planar molecule is an aromatic compound.

Yes No Unsure

Task 9

Which of the following representations of the resonance hybrid best represents the electron distribution in the depicted amide?

Fig. 8 Overview of the designed tasks to assess students' resonance-related prior knowledge.

Table 9 Pearson correlation matrix for the six clustering variables

(Combinations of) structural features	β-Position of charge	Carbon atoms & positive charge	Hetero atom & positive charge	Hetero atom & negative charge
Carbon atoms & positive charge	0.17**			
Hetero atom & positive charge	−0.12**	0.21**		
Hetero atom & negative charge	0.09*	0.04	0.07	
Hetero atom & positive charge & implicit considerations	−0.03	−0.29**	−0.20**	0.01
Positive charge on hetero atom	−0.08*	−0.07	0.01	−0.06

**Significance level p = 0.01. *Significance level p = 0.05.

Table 10 Split-half reliability of the cluster solution

Cluster	% of *N*	β-Position of charge	Carbon atoms & positive charge	Hetero atom & positive charge	Hetero atom & negative charge	Positive charge on hetero atom
I	16.3	52.04	23.15	47.67	41.93	47.65
II	14.3	74.19	84.46	46.56	25.78	73.59
III	22.7	80.90	76.44	29.66	77.02	22.66
IV	23.0	61.49	89.13	74.53	25.33	22.64
V	23.6	56.81	82.00	77.88	80.86	55.10
Overall	*343*	*65.09*	*71.04*	*55.26*	*50.18*	*44.33*
I	16.0	43.67	35.62	49.69	56.94	52.79
II	20.1	66.07	75.64	29.15	26.76	67.45
III	24.0	76.11	86.23	46.10	80.66	20.09
IV	18.0	67.41	88.03	67.20	25.59	24.02
V	21.9	68.24	90.90	78.52	79.28	65.38
Overall	*338*	*64.3*	*75.28*	*54.13*	*53.85*	*45.95*

Table 11 Students' self-reported knowledge of competencies (1 = unconfident, 5 = confident) on different resonance learning outcomes in dependence of their cluster affiliation with indication of standard deviations

Cluster	Estimate molecules' geometry	Determine aromaticity in a molecule	Estimate acid and base strength of molecules	Assess the influence of electron delocalization on molecule's reactivity
I	3.83 (1.05)	3.97 (1.11)	3.60 (1.05)	3.50 (1.07)
II	3.89 (1.09)	4.08 (1.21)	3.58 (1.10)	3.63 (1.16)
III	3.90 (1.03)	4.25 (1.02)	3.56 (1.07)	3.85 (1.04)
IV	4.01 (0.99)	4.26 (1.10)	3.62 (1.02)	3.74 (0.90)
V	3.95 (1.02)	4.07 (1.11)	3.49 (1.06)	3.75 (1.03)
Overall	3.92 (1.03)	4.14 (1.11)	3.57 (1.06)	3.71 (1.04)

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5. The More Explicit, the Better? How the Indication of Electron Lone Pairs Affects Students' Consideration of Resonance in Organic Chemistry

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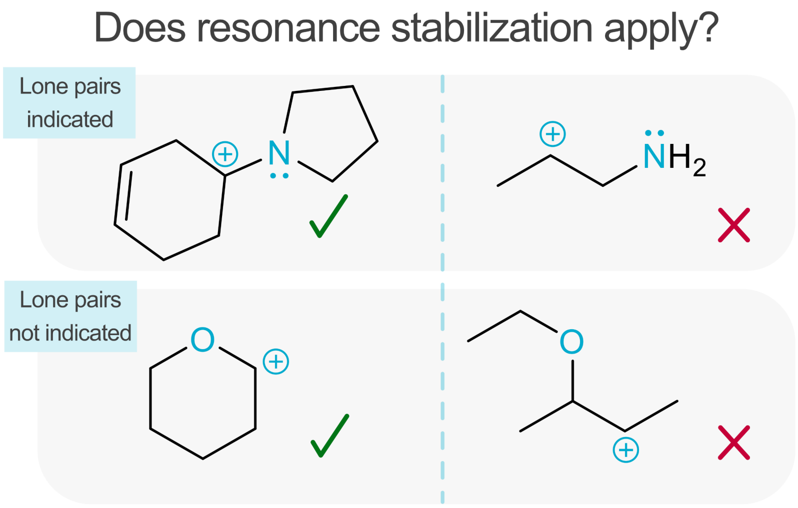

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The More Explicit, the Better? How the Indication of Electron Lone Pairs Affects Students' Consideration of Resonance in Organic Chemistry

Irina Braun and Nicole Graulich*

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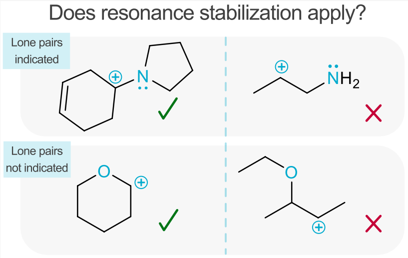

ABSTRACT: Proficiency in decoding and interpreting representations plays a critical role in learning in Organic Chemistry. However, abundant research within and beyond chemistry education suggests that learners tend to focus their attention on surface features and struggle to discern and use relevant features in solving tasks. With regard to the resonance concept, it has been shown that learners have difficulties in identifying the possibility of electron delocalization in molecular structures, eventually resulting in a limited integration of this concept in problem-solving. While the explicit display of lone pairs has been recommended and is typically used in teaching to indicate the source of electron-pushing arrows, explorative results across different studies yield ambiguous findings about its helpfulness for learners in successfully discerning the possibility of electron delocalization. To substantiate these findings, a quantitative study was conducted with undergraduate students ($N = 699$) enrolled in an Organic Chemistry I course. Students solved an online survey in which they had to decide on the possibility of resonance stabilization for different molecular structures varying in their structural features. Using paired-sample *t*-tests, differences in students' performance on their resonance-related decision-making for items (not) exhibiting electron lone pairs were examined. Results suggest that students' perception of resonance stabilization significantly depends on the display of lone pairs, highlighting the necessity of teaching resonance-related pattern recognition in a more reflective way.

KEYWORDS: *Second-Year Undergraduate, Organic Chemistry, Problem Solving/Decision Making, Molecular Properties/Structure, Resonance Theory*

INTRODUCTION

The proficient use of representations builds a crucial component of mastery in Organic Chemistry.[1,2] Successful problem-solving in this discipline is closely tied to the inspection and interpretation of various representations. For instance, to make claims about reaction pathways, one must decode mechanistic representations in terms of explicit features (e.g., presence of hetero atoms), and based on that, make inferences about implicitly encoded properties (e.g., electronegativity).[3] Even though explicit features can be directly perceived in a representation, the consideration of both explicit and implicit information is a critical prerequisite for successful reasoning in Organic Chemistry.[4−7] Consequently, students must be able to see beyond a representation.[5] However, abundant research in chemistry education[8−11] and other disciplines[12−15] has demonstrated that learners strongly rely on explicit features rather than implicit, underlying features when solving tasks. To illustrate, students focused on surface features when judging the similarity in reactivity of different organic compounds,[5] or associated nucleophiles with the presence of charges and lone pairs.[16] Learners' tendency to attend to explicit features is not surprising as they are easier to process due to their saliency.[17] Nevertheless, research has also shown that the allocation of attention to salient features may be problematic, as they can be irrelevant in a certain task context and, therefore, may interfere with one's problem-solving, eventually encouraging incorrect answers.[18] Consequently, competence in dealing with representations entails "relational conceptual understanding" (Graulich et al. 2019, p. 926),[5] thus being able to distinguish between more and less relevant representational features in certain contexts. Even though explicit features can be misleading, they may also be

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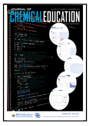

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helpful in guiding learners' reasoning and support the processing of information. For instance, DeCocq and Bhattacharyya[19] showed that the indication of explicit information (i.e., providing the products of a reaction) helped students to activate relevant knowledge when reasoning about reactions. Representations that contain more explicit features (e.g., expanded bond-line structures) may decrease intrinsic cognitive load (i.e., the inherent complexity of a task).[20] For example, it might be easier to decide on a hetero atoms' octet when the electron pairs are indicated, as all necessary information is already explicitly depicted and can be readily connected and used in a problem context. In contrast, leaving out the electron pairs requires learners not only to more carefully consider the atom type and the bonds in a molecule but also to infer the implicit nonbonding electrons.

■ ELECTRON LONE PAIRS AS EXPLICIT FEATURES IN RESONANCE CONTEXTS

A concept that is closely related to the use of representations is the resonance concept. It is used to describe the delocalization of π-electrons in molecules that cannot be adequately represented by a single Lewis structure. As such, resonance structures display different bonding descriptions based on the distribution of π-electrons among overlapping p-orbitals on adjacent atoms in a conjugated system. Their construction can help in inferring the molecule's structure and properties.[21] From former studies, it is known that this concept imposes a high cognitive load on learners[22−26] and that learners seldom consider this concept when solving problems.[27−29] As a potential source, it has been demonstrated that learners are not always able to identify the possibility of electron delocalization in a molecule.[27−30] This is problematic, as more advanced applications of this concept (e.g., determine electrophilic sites in a molecule) build upon this competency.[31] Specifically, students seem to search for specific explicit cues (e.g., hetero atoms, lone pairs, double bonds) when deciding on the application of resonance.[28−30,32] For instance, both in the context of acid−base and addition reactions, Shultz and colleagues[28,29] showed that students more often succeeded in applying resonance in tasks when electron pairs were explicitly depicted in molecular structures. Therefore, the authors advocate for displaying electron lone pairs as explicit cues to support students in considering resonance in a molecule.[29] Other authors also conclude that students at the introductory Organic Chemistry level may benefit from the explicit indication of electrons to help the decoding of molecular structures.[10,33−35] Indeed, in introductory chemistry, the use of Lewis dot structures, explicitly displaying atoms' electrons, is an effective instructional tool to explain, for instance, chemical bonding or Lewis acids and bases.[36,37] In accordance with that, to facilitate learning, different textbooks in Organic Chemistry explicitly display lone pairs when introducing resonance and showing examples of resonance structures, and advise learners to pay attention to these structural features.[38,39] Ultimately, this results in different structural patterns (e.g., allylic lone pairs, lone pair adjacent to positive charge),[38] which should support students in narrowing their attention to relevant explicit features when deciding on resonance. Such patterns are also often emphasized by Organic Chemistry instructors when introducing and teaching this concept.[23,40] However, with regard to the successful use of resonance in solving Organic Chemistry tasks (e.g., predicting mechanistic pathways), relying on explicit features is not enough. It is crucial that learners are able to flexibly and fluently discern the possibility of electron delocalization in a molecule, irrespective of the explicit display of electron pairs, as not every representation that they may encounter depicts electron lone pairs. In fact, the indication of electron lone pairs may substantially guide students' decisions about resonance and, therefore, may be misleading in terms of their helpfulness in structure decoding. In this regard, a recent study by Farheen et al.[35] showed in the context of locating electrophilic and nucleophilic regions that some students falsely invoked resonance for ethyl amine being cued by indicated lone pairs. In this example, lone pairs were distracting for students when they inferred structural properties.

■ THE ROLE OF REPRESENTATIONAL COHERENCE FORMATION FOR CONCEPT CONSIDERATIONS

The ability to decode representations and use structural features across different representations is essential for reasoning in Organic Chemistry, as chemical information is intricately linked to the surface features of representations.[5] As such, it is essential for learners to learn how representations are connected to chemical concepts and how those can be mapped onto features of (various) representations.[41] Within these cognitive mapping processes (i.e., sense-making activities),[41] coherence formation comes into play.[42,43] When being exposed to a specific representation during knowledge acquisition processes, learners extract relevant, inherent elements in a representation and establish relations between those elements to learn how they can be connected to a concept (local coherence formation).[42] With regard to resonance, that would mean that learners realize that conjugated systems are a prerequisite for electron delocalization to occur (e.g., represented in the form of allylic carbocations as the combination of a positive charge adjacent to double-bonded carbon atoms). However, learning Organic Chemistry encompasses dealing with different representations, such as in its simplest form, various molecular structures and mechanistic representations.[44] Consequently, during learning processes, learners also begin to interconnect different representations by creating referential connections between corresponding elements of different representations (global coherence formation).[42] With regard to resonance, by dealing with different molecular structures enabling electron delocalization, learners encounter different combinations of structural features (e.g., allylic carbocations, hetero atoms with lone pairs adjacent to a positive charge), which correspond to one another in the sense of representing different forms of conjugated systems. Identifying relations within and across different representations allows learners to form coherent knowledge structures and build an integrated mental representation of a concept.[42] Learning how a concept can be encoded across varying representations may facilitate the recognition of underlying perceptual patterns across representations.[41,42] Eventually, these built knowledge structures may substantially govern learners' visual attention to structural features when considering concepts during problem-solving. Besides bottom-up approaches (i.e., characterized by stimuli's saliency) and top-down approaches (i.e., explicit application of knowledge, influenced by one's mental representation of a concept), Theeuwes[45] highlights that previous experiences build an essential factor driving visual attention due to their priming function. As such, one's repeated exposure to certain features leads to an efficient selection in subsequent contexts as

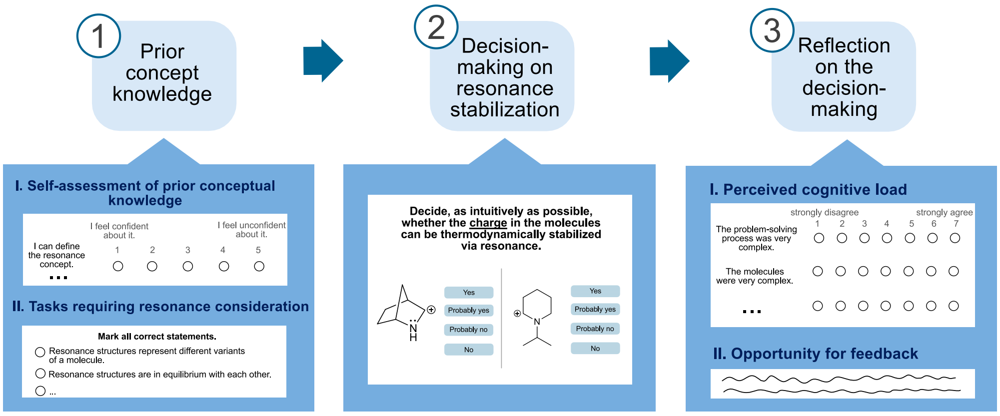

Figure 1. Overview of the study design.

these features gain saliency.[45] With regard to resonance, being often exposed to examples of molecular structures displaying lone pairs might not only narrow learners' mental representation of resonance (i.e., what they associate with this concept), but also influence how they visually attend to representations when deciding on resonance. In contrast, exposure to molecular structures varying in their structural features in a teaching context could result in more flexible use and recognition of resonance.

■ RESEARCH QUESTION

Given the varying explorative results on students' consideration of resonance when dealing with molecular structures bearing electron lone pairs, the study presented herein aims to explore in more depth how Organic Chemistry students at an introductory level deal with lone pairs when discerning resonance in molecules by examining whether the indication of lone pairs affects students' decision differently. More specifically, we aim to address the following research question:

How does the indication of electron lone pairs impact students' decision-making on resonance stabilization?

Due to students' overall reliance on surface features in (Organic) Chemistry, as demonstrated in previous chemistry education research, we hypothesize that students' decision-making on resonance stabilization is substantially led by the indication of explicit features (e.g., discern resonance when lone pairs are indicated, whereas not recognizing resonance when lone pairs are lacking) (H1).

■ METHODS

Context and Participants

The study took place at a southeastern public university in the United States. Undergraduate students enrolled across five different introductory Organic Chemistry I classes, taught by different instructors but using a common syllabus and textbook,[38] participated in this study. No IRB approval was required for data collection, from either the German university at which the study was affiliated or the American university where the data collection took place. However, the study followed ethical guidelines. All participants, being voluntarily recruited via e-mail announcements, were informed about their rights and data handling beforehand and it was clarified to the students that they had the opportunity to withdraw from the study at any time. No identifying information was collected that would allow a reidentification of the participants. The students were asked to complete an online survey (see section below) within a week. Upon survey completion, irrespective of consent to the study or the correctness of the given answers, all students received a small amount of extra credit worth approximately 0.4% of their course grade as an incentive. Of 899 students enrolled in Organic Chemistry I, 699 students completed the survey, giving informed consent for their data being anonymously analyzed and published by the research team. The survey was administered near the end of the semester. As resonance and the construction of resonance structures were covered within the first weeks of the course, the students were already introduced to this concept.

Survey Design and Data Collection

As research instrument, an online survey[46] consisting of three parts was implemented in *Qualtrics* and is displayed with example items in Figure 1. The first survey part (Figure 1) served to examine students' prior resonance-related knowledge via tasks based on resonance-specific learning outcomes[31] and previous research on concept-related alternative conceptions.[23,26,47−49] Furthermore, students were asked to self-assess their prior knowledge on defined learning outcomes for resonance[31] on a five-point Likert scale. In the second, main part of the survey, students had to decide for 72 molecular structures, each item being shown one at a time, whether resonance applies to stabilize the indicated charge (see Figure 1, part 2 for examples). As such, students had to decide on reasonable (i.e., possible and energetically favorable) resonance structures. To avoid fatigue effects, each student was shown a randomized subset of 37 molecules with the first two items being identical for all students. When designing the survey, we were also interested in capturing students' uncertainty in dealing with different molecular structures. As such, students could express uncertainty by choosing among the answers *yes*; *probably yes*; *probably no*; or *no* when completing this survey part, thereby still expressing a tendency. However, in the scope of this work, students' uncertainty was not taken into account during the subsequent data analysis to enhance the accessibility

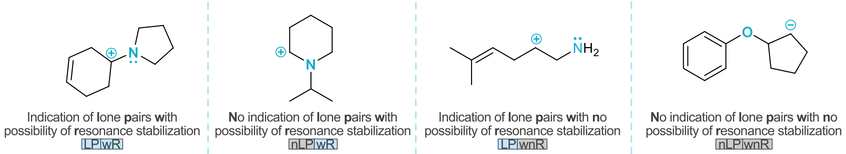

Figure 2. Exemplary survey items that vary in the indication of lone pairs and the possibility of electron delocalization.

Table 1. Descriptive Statistics for Each Structural Feature Category (N = 691)

Category	LPwR	nLPwR	LPwnR	nLPwnR
Mean (SD)	65.73 (27.44)	50.99 (24.21)	60.65 (32.55)	68.38 (29.26)
Skewness[a]	−0.51	0.02	−0.32	−0.60
Kurtosis[b]	−0.47	−0.63	−0.99	−0.64

[a] SE of 0.09. [b] SE of 0.19.

of the results. Consequently, the answer options *yes* and *probably yes* as well as *no* and *probably no* were merged when analyzing the data. Answers to the different items were considered correct when students' tendency in decision-making was correct. In general, the molecular structures were systematically varied in their degree of explicitness of given information, their complexity and the familiarity of structural features.[5,6,9,29,30,50,51] In the third survey part, students answered different items[52] on a 7-point Likert scale to gain insight into their perceived cognitive load during the second survey part (Figure 1, part 3). Furthermore, they had the opportunity to provide open feedback. The students were asked to complete the survey without the use of additional tools (e.g., textbooks and lecture notes). Overall, the median for the survey completion was 14 min and 29 s.

Data Analysis

For the scope of this article, we focus our analysis on the second survey part and concentrate on the variation of one structural feature: the indication of electron lone pairs. The impact of other (combinations of) structural features on students' competency in discerning resonance stabilization is reported elsewhere.[46] In the first step of the analysis, the 72 items were reviewed. Items in which the indication of lone pairs is not possible (e.g., allylic carbocations) were excluded. Second, the items were classified into four categories: 1. *indication of lone pairs with possibility of resonance stabilization* (LPwR) (10 items); 2. *no indication of lone pairs with possibility of resonance stabilization* (nLPwR) (17 items); 3. *indication of lone pairs with no possibility of resonance stabilization* (LPwnR) (8 items); and 4. *no indication of lone pairs with no possibility of resonance stabilization* (nLPwnR) (9 items). Overall, 44 items were included in the analysis. Items requiring further implicit considerations (i.e., exceeding octet) or with charges being in the γ-position to the conjugated system were not included in the analysis. Thus, items in which resonance stabilization does not apply display charges in the β-position to the conjugated system. Figure 2 provides item examples for each category.

In the third step, the percentage of correct answers for each student and each category was calculated. For instance, students' answers for molecules not enabling resonance stabilization were correct when they selected as answers *no* or *probably no*. As the items were presented in a randomized order, not all students saw the same number of items for each category. Eight students were excluded from the analysis, not being shown any items on one of the four categories. As such, the number of participants included in the analysis was reduced to 691. Finally, we compared students' competency in discerning resonance stabilization for the four structural feature categories using paired-sample t-tests. All statistical analyses were conducted in SPSS, version 29.0.

■ RESULTS

Students' average scores for each structural feature category were calculated and are indicated in Table 1. Furthermore, Figure 3 visually depicts students' performances across the different categories.

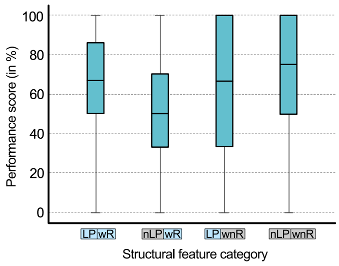

Figure 3. Boxplots for students' performance on the different structural feature categories (LPwR = indication of lone pairs with possibility of resonance stabilization; nLPwR= no indication of lone pairs with possibility of resonance stabilization; LPwnR = indication of lone pairs with no possibility of resonance stabilization; nLPwnR = no indication of lone pairs with no possibility of resonance stabilization).

The descriptive statistics suggest that the indication of lone pairs seems to affect students' competency in discerning resonance stabilization in molecular structures, with the highest performance scores for items enabling resonance stabilization and exhibiting lone pairs (LPwR, 66%) and items not enabling resonance and lacking explicit lone pairs (nLPwnR, 68%) (Table 1). To investigate whether these emergent trends in students' performance are statistically significant, paired-sample t-tests were performed between the four categories. The assumption of normal sampling distribution for the differences between the scores of the four categories was confirmed visually using QQ-plots, as the Shapiro−Wilk test tends to yield significant results even for small departures from normality in larger sample sizes.[53] To control the familywise error rate (Type I error) as a result of multiple comparisons, a Bonferroni correction of the α-value was made. As such, the criterion for significance was set to $p_{\text{crit}} = 0.05/6 = 0.0083$ for each t-test.

The results of the paired-sample t-tests, which are summarized in Table 2, yield significant differences in students' performance for almost all category comparisons. More specifically, students' scores on items profiting from resonance stabilization were much higher when lone pairs were indicated (LPwR, 66%), and significantly lower when they remained implicit (nLPwR, 51%). This difference, being of medium effect size (Table 2), indicates that students are more successful in deciding in favor of resonance when lone pairs are explicitly provided. A similar inference can be made with regard to the comparison of nLPwR and nLPwnR (Table 2), highlighting that students found it easier to decide against resonance stabilization when lone pairs were lacking in the molecular display. From students' scores, it also became apparent that the indication of lone pairs more often misguided students to decide on resonance stabilization when its application is not possible in a molecule (LPwnR, 61%), compared to their scores on items in which electron pairs were not displayed (nLPwnR, 68%) (cf. Table 2, significant differences with small effect size). Students' tendency to rely on lone pairs when considering resonance is also reflected in the varying scores for the categories LPwR and LPwnR. This comparison shows that even if the lone pairs were in the β-position to the charge (LPwnR), and did not belong to a conjugated system, students were more often biased to falsely invoke resonance stabilization. However, this difference is rather small and has a small effect size. Students' relatively higher performance scores for the categories LPwR and nLPwnR (≥65%) (cf. Table 1) finally show that students' decision on resonance stabilization is facilitated when the display or lack of explicit structural features is congruent to the possibility of electron delocalization. Overall, these findings underline that the students in this cohort were significantly influenced by the indication of lone pairs when deciding on resonance stabilization. That supports the confirmation of hypothesis H1.

Table 2. Results of the Paired-Sample t-Tests between the Different Structural Feature Categories with Indication of the Effect Sizes[a]

Comparison	Mean difference	SE	$t(690)$	p[b]	d	Effect size[c]
LPwR − nLPwR	14.74	1.14	12.91	**<0.001**	0.49	medium
LPwR − LPwnR	5.08	1.65	3.09	**0.002**	0.12	small
nLPwnR − LPwR	2.65	1.51	1.75	0.08	0.07	–
LPwnR − nLPwR	9.66	1.59	6.07	**<0.001**	0.23	small
nLPwnR − nLPwR	17.39	1.58	11.00	**<0.001**	0.42	small−medium
nLPwnR − LPwnR	7.73	1.21	6.39	**<0.001**	0.24	small

[a] Significant differences are highlighted in bold. [b] Bonferroni-adjusted significance level of 0.0083. [c] Effect sizes according to Cohen.[54]

■ DISCUSSION AND CONCLUSION

The quantitative study presented herein aimed to examine how the indication of lone pairs impacts students' consideration of resonance stabilization. The results suggest that students were affected by the indication of lone pairs, namely, that they were more proficient in correctly deciding on the possibility of resonance stabilization when lone pairs were indicated (LPwR) than when not indicated (nLPwR). When resonance stabilization was not possible in a molecule, students more often made a correct decision when the lone pairs were lacking (nLPwnR), whereas the indication of lone pairs tended to be more distracting in these cases (LPwnR). These findings suggest that a continuous indication of lone pairs may not support students in considering resonance in problem-solving, as previously advised in different studies.[10,29,34] Relying on the presence of lone pairs may cause challenges or misguided decisions in problem-solving when lone pairs are not indicated in tasks. Indeed, students were more successful when the indication of lone pairs favored the decision on resonance, but whenever the indication was incongruent with the required decision, students were significantly less successful. As such, the findings add to the abundant literature on students' reliance on surface features when solving problems in Organic Chemistry[5,16,55] and further suggest, with regard to the resonance concept, that students seem to approach resonance tasks based on surface pattern recognition, with less attention to structural details[22] and to connecting different pieces of structural information to the underlying concept of resonance. Stated differently, students seem to rely more on the available structural cues when deciding on resonance stabilization[5] than on inferring implicit properties (e.g., considering the possibility of not displayed lone pairs) or assessing the actual existence of a conjugated system. This observation might be related to the focus on teaching approaches that emphasize the recognition of resonance patterns over conceptual understanding (e.g., understanding of a conjugated system).[23,40] The findings might also be tied back to the common representation of molecular structures in textbooks frequently displaying lone pairs when introducing and practicing resonance structures. As students may typically encounter resonance with the explicit exposure of lone pairs, they might create referential connections between these explicit features and resonance, which may impact their mental representation of this concept,[43] and thus may guide their recognition of resonance in problem-solving tasks. Commonly found resonance patterns in textbooks[38] that explicitly emphasize the presence of lone pairs may further reinforce this established association.

Ultimately, these results show that we as instructors must be aware of the effects that indicating explicit features on molecular structures can have, as students tend to rely on these features when solving resonance tasks. Eventually, this might hinder students in identifying the possibility of electron delocalization and hence restrict the application of this concept in more complex structures and in more advanced tasks (e.g., solving mechanisms).[31] Given Organic Chemistry instructors' expectations of students becoming proficient in resonance pattern recognition and competent in further distinguishing between delocalized and localized electron pairs,[40] these results call attention to shifting the teaching of pattern recognition from a mere operational to a more nuanced approach (e.g., more explicitly discuss the presence and inference of implicit electron pairs,[35] more often vary the display of molecular structures when practicing and dealing with resonance [for instance, by implementing a variety of different structures in digital educational games[56]], and explicitly focus on molecular structures with lone pairs where resonance is not present) to help learners become more flexible pattern recognizers and gain more practice with varying representations of resonance structures.

LIMITATIONS

Some limitations should be considered with regard to the reported findings. First, note that the survey was administered at only one institution so that the generalization of these findings to other cohorts is limited. Second, with regard to the remote survey administration, it remains unclear if students put effort into solving the tasks and whether they solved the tasks without external tools. Lastly, students' identified patterns in resonance recognition might be affected by subsequently answering 37 items (i.e., testing effect).

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Notes

The authors declare no competing financial interest.

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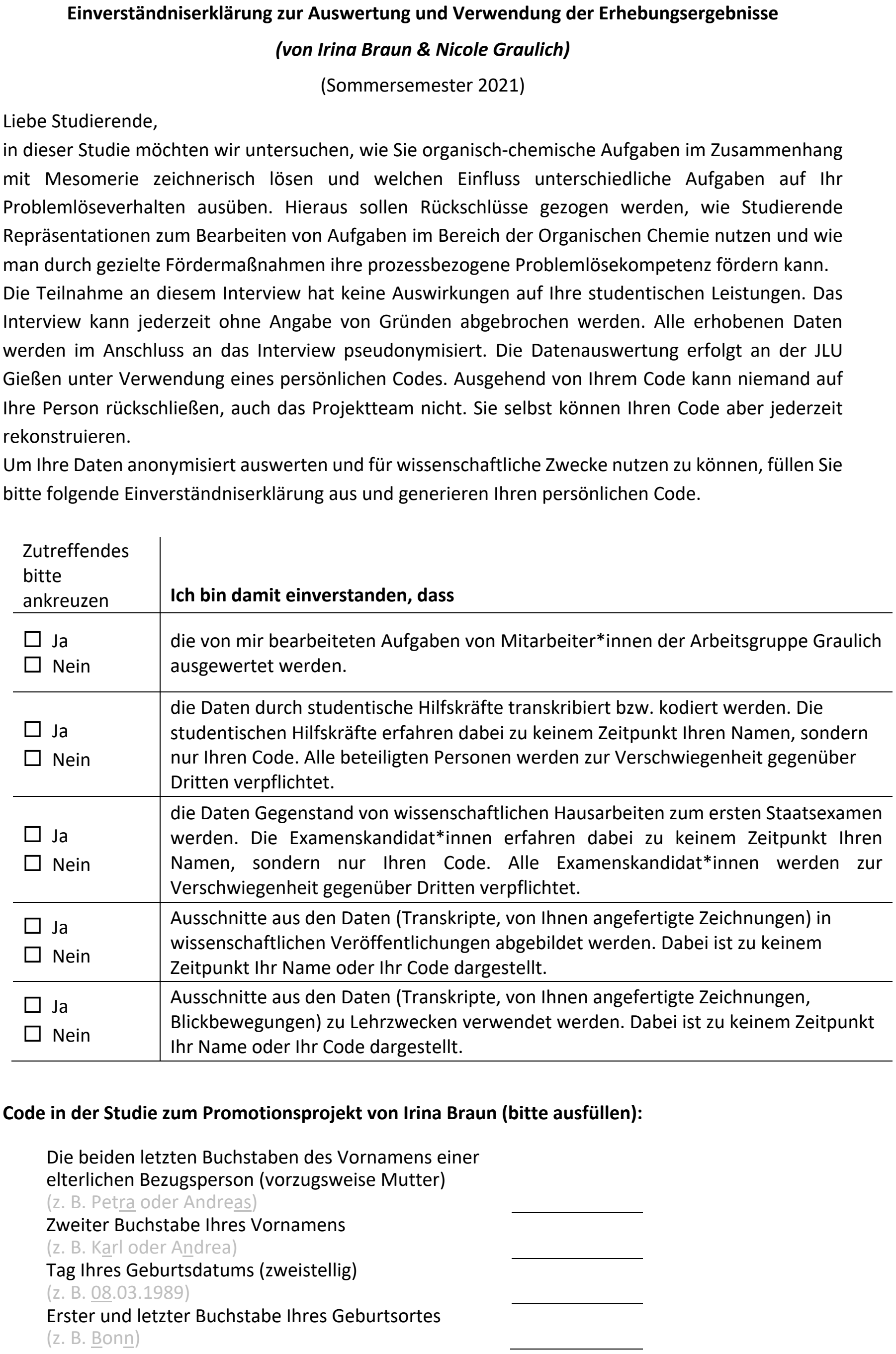
6. Appendices

6.1 Supporting Information Study 1

6.1.1 Consent Forms Used at the Justus-Liebig-University Giessen



Einverständniserklärung zur Auswertung und Verwendung der Erhebungsergebnisse

(von Irina Braun & Nicole Graulich)

(Sommersemester 2021)

Liebe Studierende,
in dieser Studie möchten wir untersuchen, wie Sie organisch-chemische Aufgaben im Zusammenhang mit Mesomerie zeichnerisch lösen und welchen Einfluss unterschiedliche Aufgaben auf Ihr Problemlöseverhalten ausüben. Hieraus sollen Rückschlüsse gezogen werden, wie Studierende Repräsentationen zum Bearbeiten von Aufgaben im Bereich der Organischen Chemie nutzen und wie man durch gezielte Fördermaßnahmen ihre prozessbezogene Problemlösekompetenz fördern kann.
Die Teilnahme an diesem Interview hat keine Auswirkungen auf Ihre studentischen Leistungen. Das Interview kann jederzeit ohne Angabe von Gründen abgebrochen werden. Alle erhobenen Daten werden im Anschluss an das Interview pseudonymisiert. Die Datenauswertung erfolgt an der JLU Gießen unter Verwendung eines persönlichen Codes. Ausgehend von Ihrem Code kann niemand auf Ihre Person rückschließen, auch das Projektteam nicht. Sie selbst können Ihren Code aber jederzeit rekonstruieren.
Um Ihre Daten anonymisiert auswerten und für wissenschaftliche Zwecke nutzen zu können, füllen Sie bitte folgende Einverständniserklärung aus und generieren Ihren persönlichen Code.

Zutreffendes bitte ankreuzen	**Ich bin damit einverstanden, dass**
☐ Ja ☐ Nein	die von mir bearbeiteten Aufgaben von Mitarbeiter*innen der Arbeitsgruppe Graulich ausgewertet werden.
☐ Ja ☐ Nein	die Daten durch studentische Hilfskräfte transkribiert bzw. kodiert werden. Die studentischen Hilfskräfte erfahren dabei zu keinem Zeitpunkt Ihren Namen, sondern nur Ihren Code. Alle beteiligten Personen werden zur Verschwiegenheit gegenüber Dritten verpflichtet.
☐ Ja ☐ Nein	die Daten Gegenstand von wissenschaftlichen Hausarbeiten zum ersten Staatsexamen werden. Die Examenskandidat*innen erfahren dabei zu keinem Zeitpunkt Ihren Namen, sondern nur Ihren Code. Alle Examenskandidat*innen werden zur Verschwiegenheit gegenüber Dritten verpflichtet.
☐ Ja ☐ Nein	Ausschnitte aus den Daten (Transkripte, von Ihnen angefertigte Zeichnungen) in wissenschaftlichen Veröffentlichungen abgebildet werden. Dabei ist zu keinem Zeitpunkt Ihr Name oder Ihr Code dargestellt.
☐ Ja ☐ Nein	Ausschnitte aus den Daten (Transkripte, von Ihnen angefertigte Zeichnungen, Blickbewegungen) zu Lehrzwecken verwendet werden. Dabei ist zu keinem Zeitpunkt Ihr Name oder Ihr Code dargestellt.

Code in der Studie zum Promotionsprojekt von Irina Braun (bitte ausfüllen):

Die beiden letzten Buchstaben des Vornamens einer elterlichen Bezugsperson (vorzugsweise Mutter)
(z. B. Petra oder Andreas) ______________
Zweiter Buchstabe Ihres Vornamens
(z. B. Karl oder Andrea) ______________
Tag Ihres Geburtsdatums (zweistellig)
(z. B. 08.03.1989) ______________
Erster und letzter Buchstabe Ihres Geburtsortes
(z. B. Bonn) ______________

Einwilligungserklärung zur Erhebung und Verarbeitung personenbezogener Daten für Forschungszwecke

1 Gegenstand des Forschungsprojektes

1.	Forschungsprojekt	Untersuchung des prozessorientierten Problemlösens in der Organischen Chemie am Kontext der Mesomerie
2.	Forschungszweck	Evaluation und Förderung der prozessbezogenen Problemlösekompetenz hinsichtlich der Nutzung organisch-chemischer Repräsentationen
3.	Durchführende Institutionen	Justus-Liebig-Universität Gießen, Institut für Didaktik der Chemie, Heinrich-Buff Ring 17, 35392 Gießen
4.	Projektleitung	Prof. Dr. Nicole Graulich (JLU Gießen, Tel.: 0641-9934600, E-Mail: Nicole.Graulich@didaktik.chemie.uni-giessen.de) Irina Braun (JLU Gießen, Tel.: 0641-9934631, E-Mail: Irina.Braun@didaktik.chemie.uni-giessen.de)
5.	Erhebungszeitraum	Sommersemester 2021
6.	Interviewerin	Irina Braun

2 Einwilligungserklärung

Hiermit willige ich ein, dass im Rahmen des unter (1) beschriebenen Forschungsprojekts Daten meiner Person erhoben und ausgewertet werden. Die Erhebung erfolgt zum einen durch **Eye Tracking-/Videoaufnahmen sowie Audioaufnahmen**, die in der Folge transkribiert werden. Zum anderen werden **schriftliche Aufzeichnungen** erhoben. Daten aus allen Erhebungsformaten werden unter Verwendung eines Codeworts vollständig pseudonymisiert und für wissenschaftliche Analysen und in der Folge für wissenschaftliche Veröffentlichungen verwendet und mindestens 10 Jahre lang gespeichert werden.

Über Art und Umfang von Erhebung und Auswertung wurde ich mündlich und in der schriftlichen Anlage zu dieser Erklärung umfassend informiert. Sofern ich Fragen zu dieser vorgesehenen Studie hatte, wurden sie mir vollständig und zu meiner Zufriedenheit beantwortet.

Die Mitglieder der beteiligten Arbeitsgruppen sind zur Verschwiegenheit gegenüber Dritten verpflichtet. Gleichermaßen erkläre ich Verschwiegenheit bezüglich der Aufgabeninhalte gegenüber Dritten.

Die Angaben in der Einverständniserklärung entsprechen meinem freien Willen.

Ihre Einwilligung ist freiwillig. Sie können die Einwilligung ablehnen, ohne dass Ihnen dadurch irgendwelche Nachteile entstehen. Ihre Einwilligung können Sie jederzeit gegenüber der durchführenden Institution widerrufen. Die weitere Verarbeitung Ihrer personenbezogenen Daten wird ab diesem Widerruf unzulässig. Dies berührt jedoch nicht die Rechtmäßigkeit der aufgrund der Einwilligung bis zum Widerruf erfolgten Verarbeitung. Relevante Definitionen der verwendeten datenschutzrechtlichen Begriffe sind in der Anlage Begriffsbestimmungen enthalten.

______________________________	______________	______________________
Vorname und Nachname in Druckschrift	Datum	Unterschrift

6.1.2 Demographic Questionnaire

Code: __ __ __ __ __ __ __

Demographischer Fragebogen

(von Irina Braun & Nicole Graulich)

(Sommersemester 2021)

Füllen Sie bei den Punkten 1-6 die für Sie zutreffenden Angaben aus.

1) Geschlecht ☐ weiblich ☐ männlich ☐ divers

2) Fachsemester ☐ 2 ☐ 4 ☐ 6 ☐ 8 ☐ 10 ☐ anderes: ______

3) Geburtsjahr ____________

4) Studiengang
   - ☐ Chemie (BSc.)
   - ☐ Lebensmittelchemie (Bsc.)
   - ☐ Materialwissenschaft
   - ☐ L3 Chemie
   - ☐ BBB Chemie
   - ☐ ____________________________

5) Ich belege das Modul „Chemie-BK23 Organische Stoffchemie (OC1)“ zum ersten Mal.

☐ ja ☐ nein

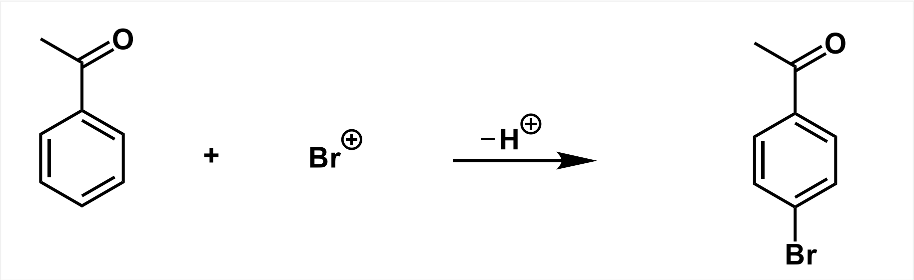
6) Ich habe das Modul „Chemie-BK23 Organische Stoffchemie (OC1)“ bereits bestanden.

☐ ja, Jahr: _______ ☐ nein

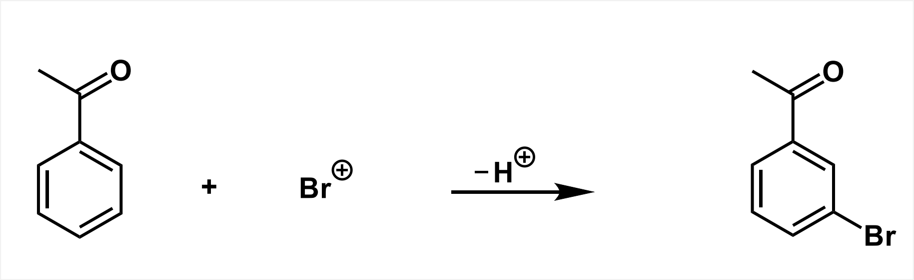
6.1.3 Original Tasks from the Qualitative Interview Study

1) **Begründen Sie zeichnerisch, welches Produkt bei der folgenden elektrophilen Substitution am Aromaten bevorzugt gebildet wird.**

A

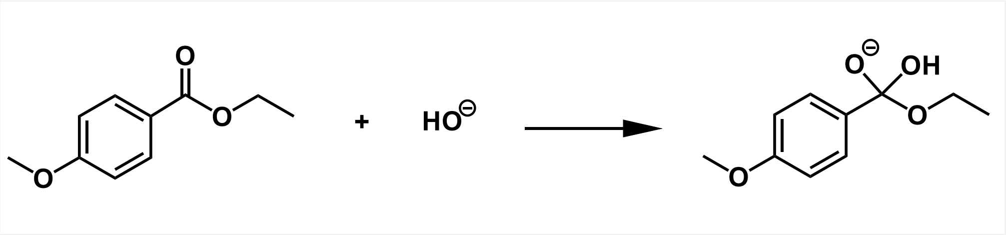


B

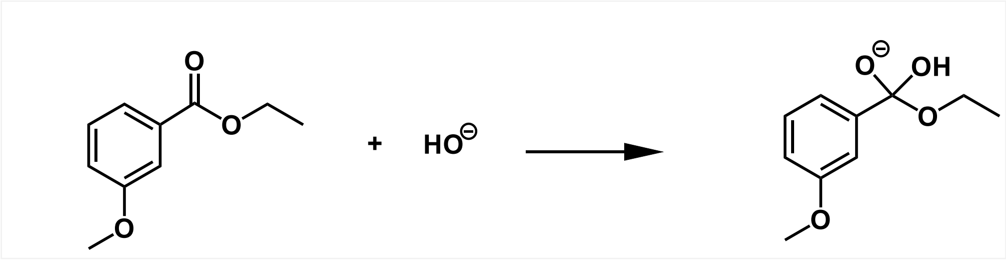


2) **Folgend ist der erste Schritt einer Reaktion dargestellt, in welcher ein Hydroxid-Ion nucleophil an einem Carbonylkohlenstoffatom angreift. Begründen Sie zeichnerisch, in welcher Verbindung der Angriff bevorzugt erfolgt.**

A

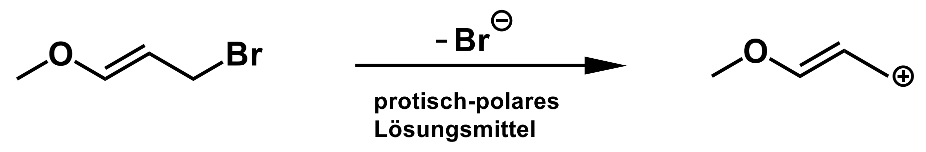


B

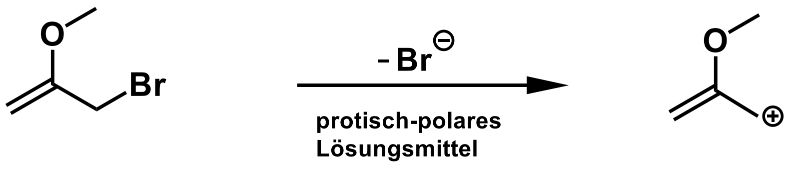


3) Begründen Sie zeichnerisch, welche Verbindung das stabilere Carbenium-Ion bildet.

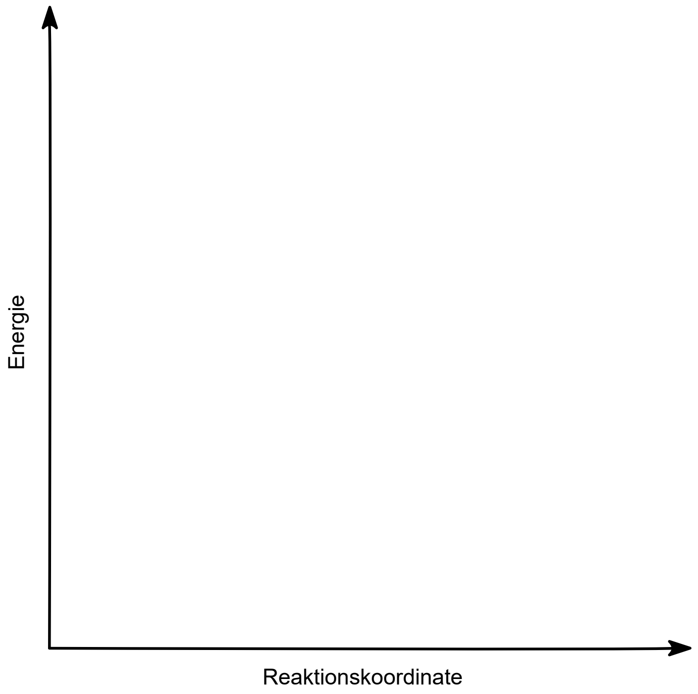
A



B



Code: __ __ __ __ __ __ __



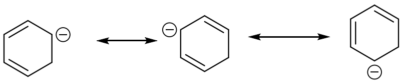
6.1.4 Interview Protocol

Allgemeines

- Datenschutzerklärung, Einverständniserklärung, demographischer Fragebogen
- **Kontext**: Problemlösen in der OC im Bereich der Mesomerie, zeichnerisches Erschließen
- Ablauf erläutern und Einweisung geben:
  - o Einige Vorwissensfragen zu diesem Thema
  - o Aufgabenbearbeitung mit Eye-Tracker (wird aufbehalten, Hartplastik, Eye-Tracking Setup)
    - ▪ Aufgaben so gut es geht lösen; es geht <u>nicht</u> um Wissensabfrage (keine Bewertungssituation)
    - ▪ Keine Unterbrechung, bis Aufgabe fertig bearbeitet (→ Bescheid geben)
      - ➔ Einige Fragen zu der Aufgabenbearbeitung
      - ➔ Antworten so ausführlich wie möglich, Denkschritte begründen, um die Gedankengänge zu erfassen
  - o evtl. werden Notizen gemacht
  - o Insgesamte Dauer: 90 Min.

Vorwissen

1. Was bedeutet Mesomerie/was fällt dir dazu ein? (→ anhand eines Beispiels erklären)
2. Kannst du mesomere Grenzformeln aufzeichnen?
   a. eigenes Beispiel, sonst:



   b. Falls Aromat: Tritt Mesomerie nur im Zusammenhang mit Aromatizität auf?
   c. Was „verschiebt“ sich? Wodurch unterscheiden sie sich? (elektronische Ebene)
   d. Wie gehst du beim Zeichnen von mesomeren Grenzstrukturen vor? (Bezug auf Beispiel) / Wie kommst du von einer zur anderen Strukturformel?
      i. Nach welchen Regeln gehst du vor/welche kennst du?
      ii. Bedeutung der Pfeile?
   e. An welchen strukturellen Merkmalen erkennst du, dass Mesomerie auftritt?
   f. Wie sieht das Molekül tatsächlich aus? (Zusammenhang zwischen mesomeren Grenzformeln)
3. Wozu zeichnet man mesomere Grenzformeln? Welche Informationen kann man aus diesen ableiten? (anhand Beispiel) (→ Reaktivität/Stabilität)
   a. Sind alle gleich stabil? Warum (nicht)? (Quantität vs. Qualität)

    b. Wo könnte es mit einem Nukleophil/Elektrophil reagieren? Woran machst du das fest? (Eigenschaften ablesen)
4. Welche elektronischen Effekte gibt es noch, die eine Reaktion beeinflussen, wo liegen die Unterschiede zu Mesomerie?

Retrospektive

1. Kannst du deine **einzelnen Denkschritte beschreiben und begründen**?
    a. Woher wusstest du, was zu tun war? (→ Anhaltspunkte/Suche nach welchen Unterschieden?)
    b. Wie bist du zu deiner Lösung gekommen?
    c. Kannst du deine angefertigten Zeichnungen chronologisch beschreiben (d.h., wie sind sie zeitlich entstanden)?
    d. Sofern neu angefangen: warum?
    e. Sofern Probleme aufgetreten: Was waren die Schwierigkeiten?
    f. Sofern ungenau: was heißt *ungünstig/besser/…* etc. in diesem Kontext?
2. **Warum hast du die Zeichnungen angefertigt**, d.h. wie haben sie dir geholfen, das Problem zu lösen/wie hast du mit ihnen gearbeitet?
    a. Was (und wie) hast du aus den einzelnen Zeichnungen abgeleitet?
    b. Was bedeuten die einzelnen Zeichenbestandteile für das Problem (z. B. Ladungen)?
    c. Warum hast du bestimmte Zeichnungen übersprungen/ignoriert im weiteren Verlauf?
    d. Wenn keine Zeichnungen angefertigt: Warum im Kopf gelöst?
3. **Wie sind einzelne Zeichnungen/mesomere Grenzformeln entstanden**?
    a. Aufgrund welcher Kriterien bist du von der vorherigen zur nächsten Grenzformel gekommen? Welche Überlegungen liegen ihnen zugrunde (Begründung)? Wie bist du zu deinen Zeichnungen gekommen?
    b. Woran machst du fest, dass die einzelnen mesomeren Grenzformeln valide sind?
4. **Skala von 1-5 (1 = leicht, 5 = schwierig)**, wie schwer ist dir die Bearbeitung der Aufgabe gefallen?
    a. Warum? Was fiel dir schwer?
    b. Warum war sie leichter/schwieriger als die anderen Aufgaben?

Energieprofil (Aufgabe 3)

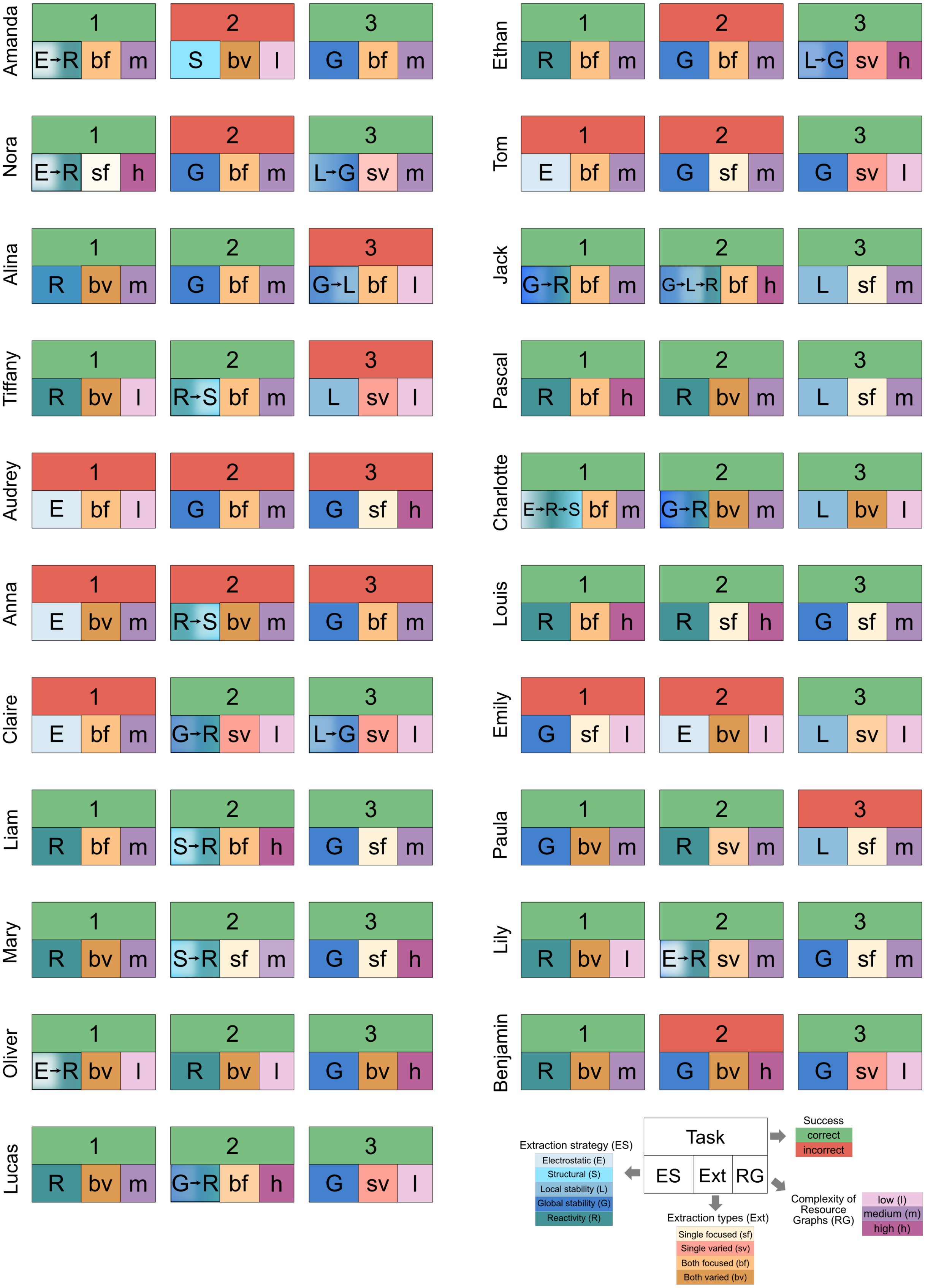
1. Kannst du für diese beiden Reaktionen ein Energieprofil zeichnen und beschriften?
    a. Was bedeuten die einzelnen Bestandteile im Energiediagramm? (Edukte/Produkte/E_A/ÜZ/Breite E_A/Höhe E_A)

2. Wie bist du zu den Energieprofilen gekommen? (→ Struktur-Zusammenhang / Vergleich)
    a. Woran machst du die Anordnung fest/Wie bist du auf die Zuordnung gekommen?
        i. Energetisch höher/tiefer? Endergonisch/exergonisch?
        ii. Unterschiede zwischen beiden Reaktionen im Energieprofil?
        iii. Wie sieht der ÜZ in der jeweiligen Reaktion aus?
3. Welche Reaktion verläuft schneller? Warum?
    a. Kann man überhaupt die Geschwindigkeit einer Reaktion am Energiediagramm ablesen/ableiten? Woran machst du das fest?

Allgemeine Reflexion

1. Ähnliche Aufgabenstruktur (Fallvergleiche): Was war deine Strategie bei diesen Aufgaben? Hast du eine allgemeine Lösungsstrategie für diese Aufgaben?
2. Wie oft zeichnest du persönlich im Rahmen der OC1-Veranstaltung?
    a. z. B. chemische Inhalte nochmal zur Übung und Vertiefung visualisieren, Inhalte aus dem Lehrbuch abschreiben, bei Übungen nochmal den Lösungsweg explizit angeben, oder nur das zeichnen, was unbedingt notwendig ist?
    b. Persönliche Vorlieben zum Medium zum Zeichnen (auf Papier/digital)?
    c. Holst du dir manchmal Feedback zu den Zeichnungen ein bzw. bekommst du welches (Kommiliton*innen, Dozierende)?
3. Was hat dir bei den Aufgaben allgemein Schwierigkeiten/Probleme bereitet?
4. Wobei hättest du dir grundsätzlich mehr Unterstützung gewünscht?
5. Weitere Kritik/Anmerkungen?

6.1.5 Students' Concept Projections for the Different Tasks



	1	2	3
Amanda	🟩 E→R bf m	🟥 S bv l	🟩 G bf m
Nora	🟩 E→R sf h	🟥 G bf m	🟩 L→G sv m
Alina	🟩 R bv m	🟩 G bf m	🟥 G→L bf l
Tiffany	🟩 R bv l	🟩 R→S bf m	🟥 L sv l
Audrey	🟥 E bf l	🟥 G bf m	🟥 G sf h
Anna	🟥 E bv m	🟥 R→S bv m	🟥 G bf m
Claire	🟥 E bf m	🟩 G→R sv l	🟩 L→G sv l
Liam	🟩 R bf m	🟩 S→R bf h	🟩 G sf m
Mary	🟩 R bv m	🟩 S→R sf m	🟩 G sf h
Oliver	🟩 E→R bv l	🟩 R bv l	🟩 G bv h
Lucas	🟩 R bv m	🟩 G→R bf h	🟩 G sv l
Ethan	🟩 R bf m	🟥 G bf m	🟩 L→G sv h
Tom	🟥 E bf m	🟥 G sf m	🟩 G sv l
Jack	🟩 G→R bf m	🟩 G→L→R bf h	🟩 L sf m
Pascal	🟩 R bf h	🟩 R bv m	🟩 L sf m
Charlotte	🟩 E→R→S bf m	🟩 G→R bv m	🟩 L bv l
Louis	🟩 R bf h	🟩 R sf h	🟩 G sf m
Emily	🟥 G sf l	🟥 E bv l	🟩 L sv l
Paula	🟩 G bv m	🟩 R sv m	🟥 L sf m
Lily	🟩 R bv l	🟩 E→R sv m	🟩 G sf m
Benjamin	🟩 R bv m	🟥 G bv h	🟩 G sv l

Figure 21. Overview of students' concept projections across the different task contexts (see Chapter 3 for tasks).

6.1.6 Students' Resource Graphs for the Different Tasks

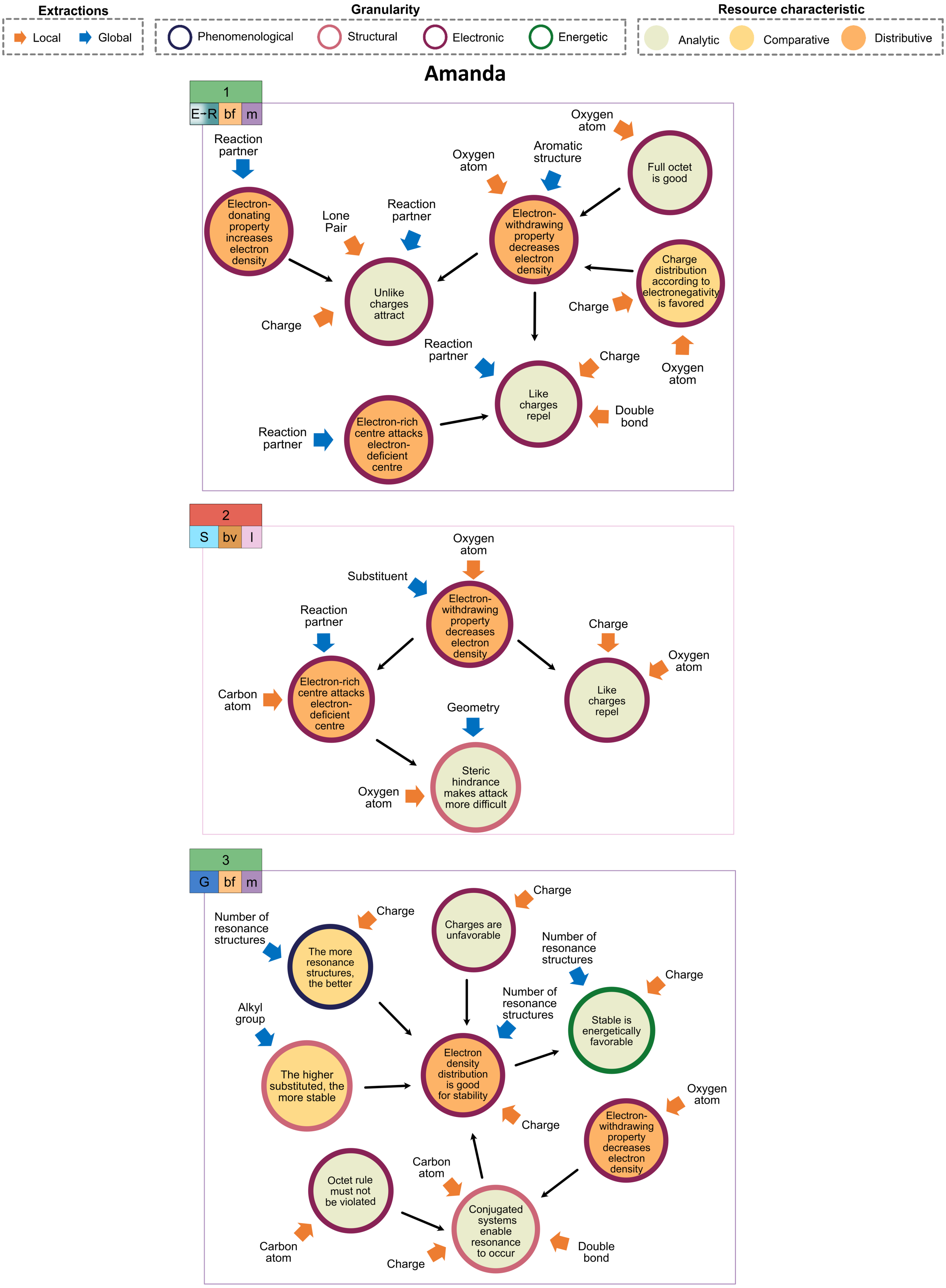


Figure 22. Amanda's resource graphs for the different tasks with explanation of the resource granularity (outer circles), resource characteristics (inner circles), and extraction (arrows).

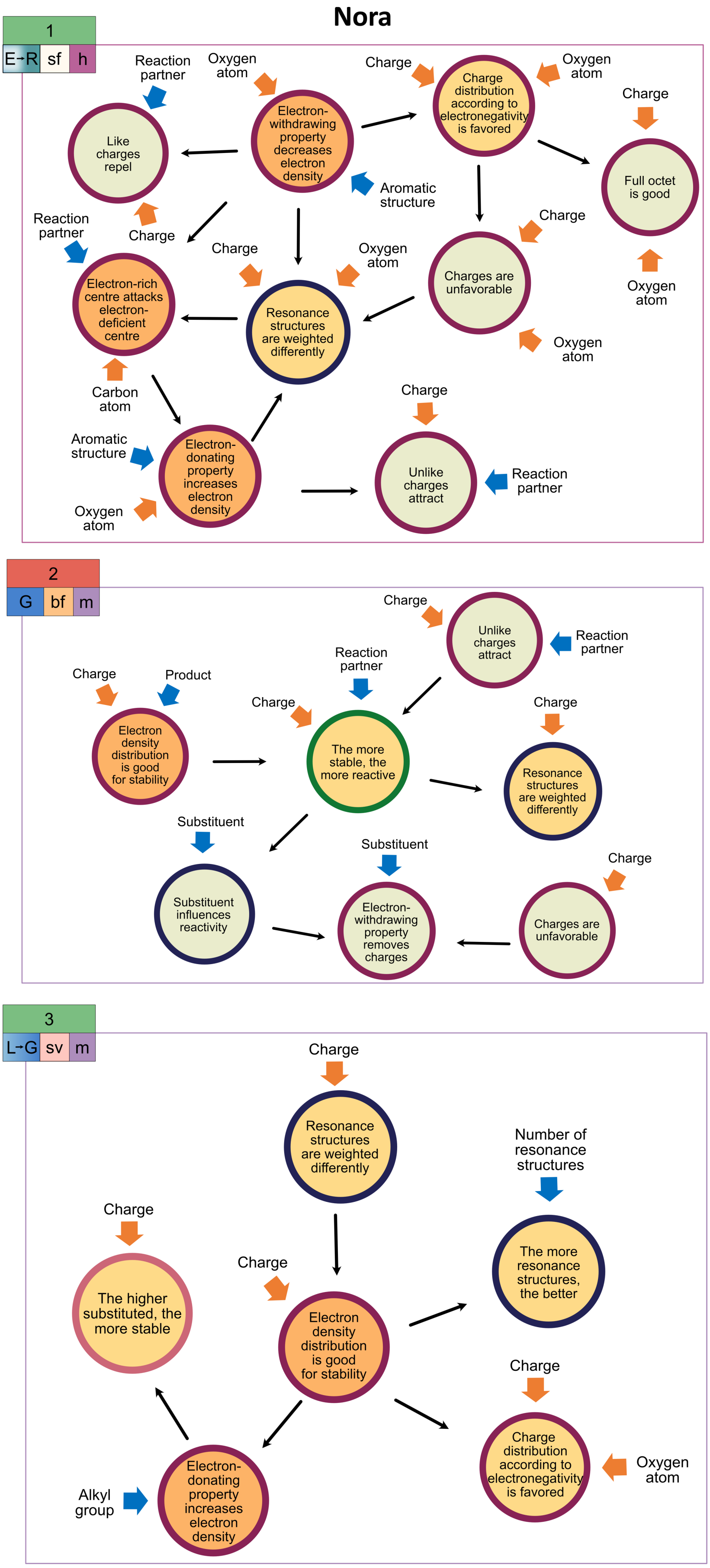


Figure 23. Nora’s resource graphs for the different tasks.

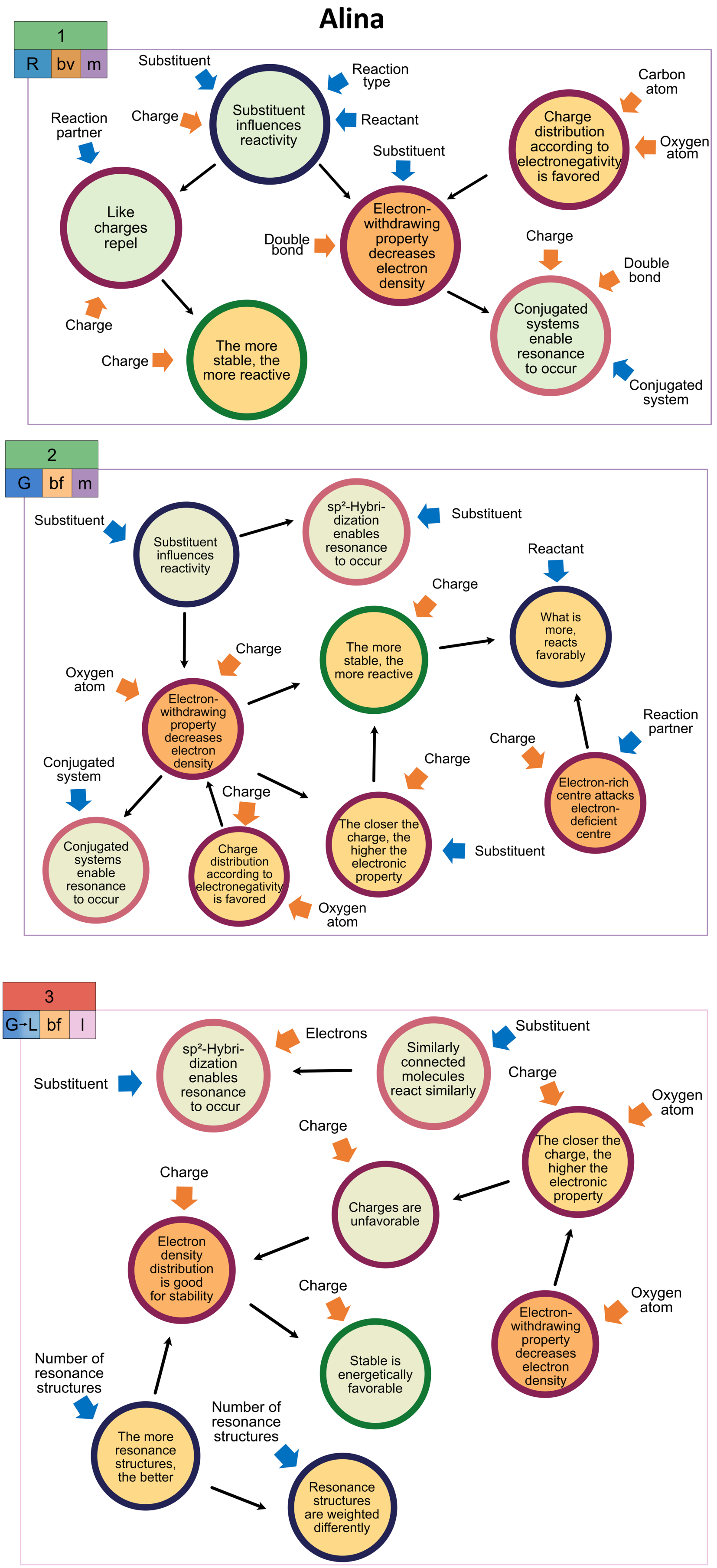


Figure 24. Alina’s resource graphs for the different tasks.

Tiffany

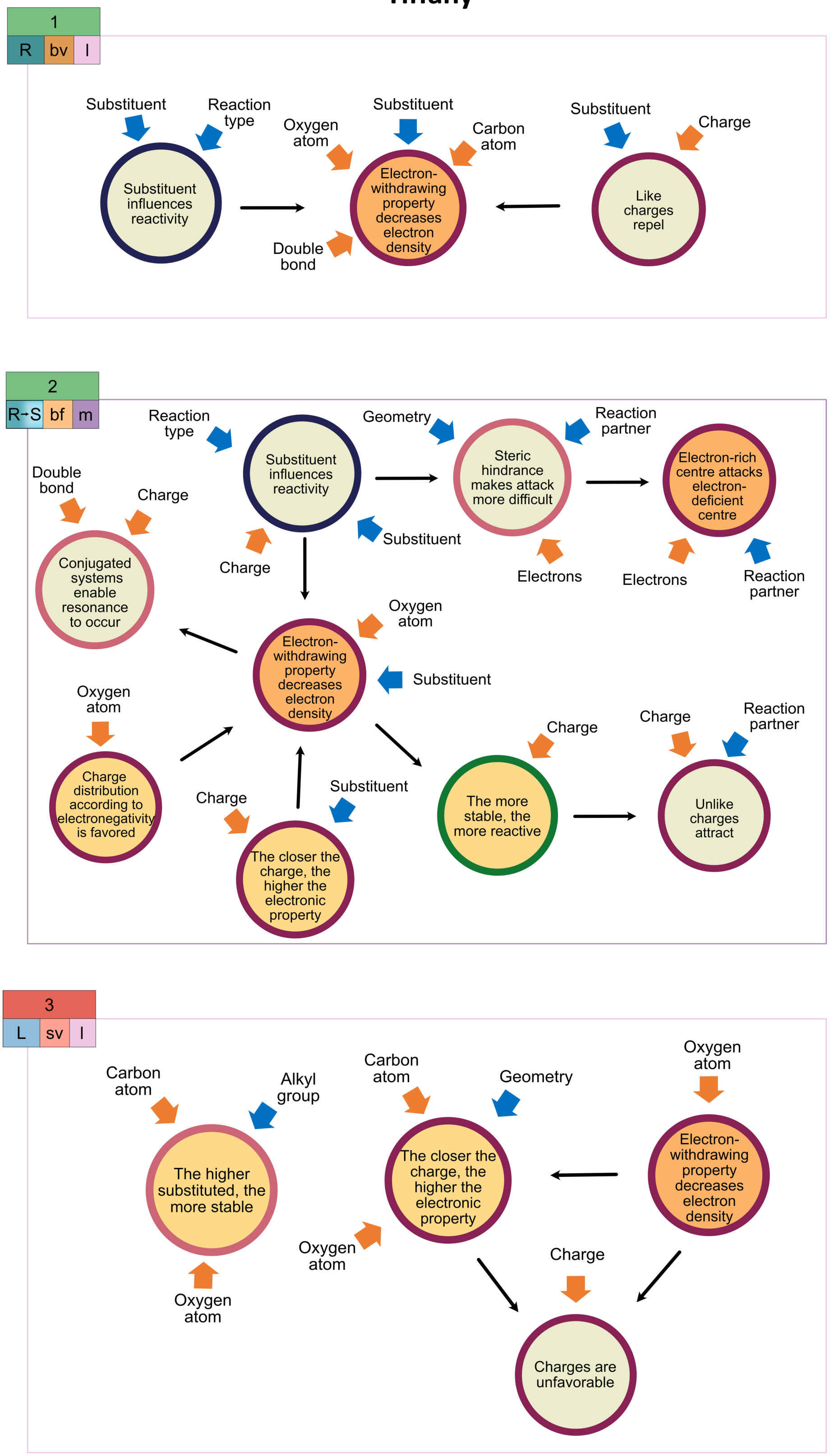


Figure 25. Tiffany's resource graphs for the different tasks.

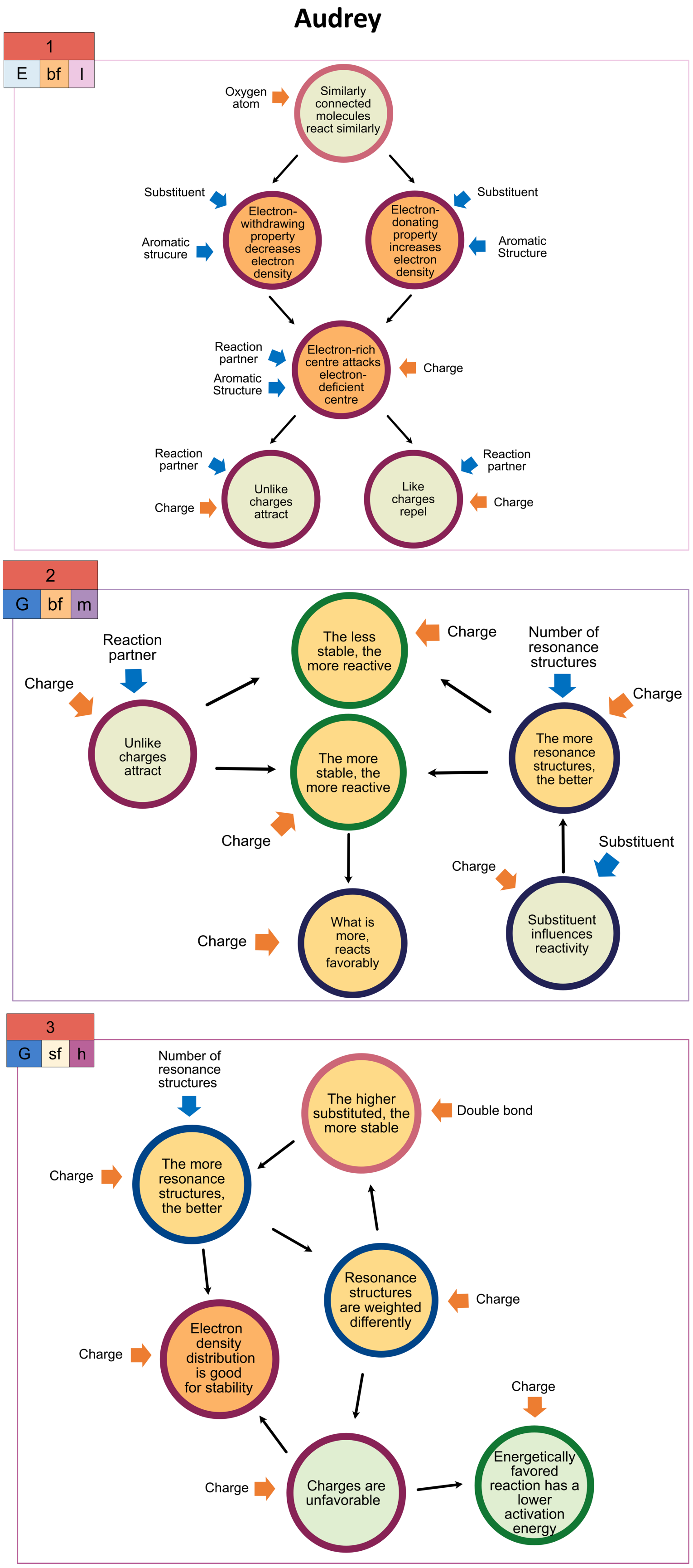


Figure 26. Audrey’s resource graphs for the different tasks.

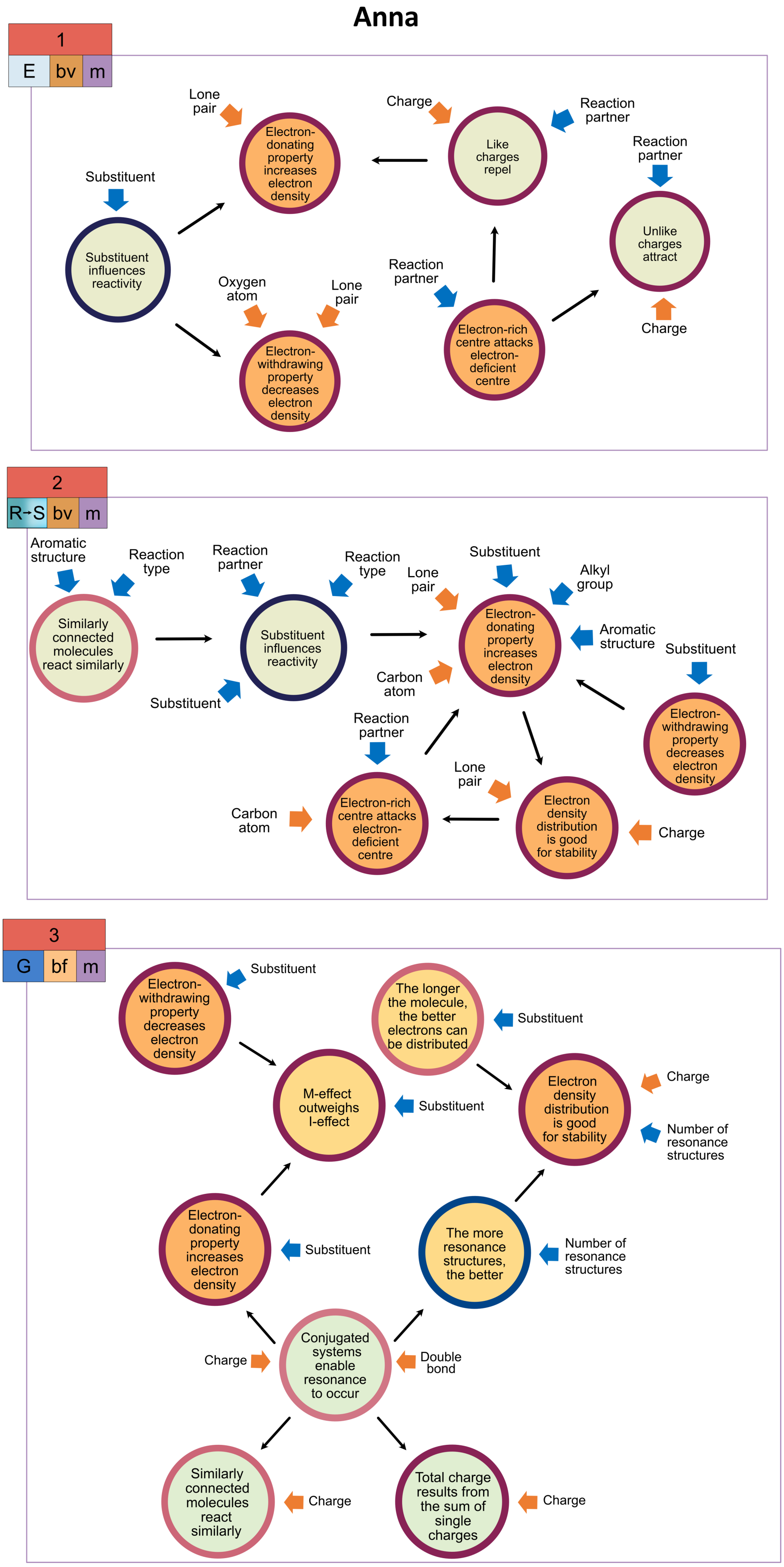


Figure 27. Anna’s resource graphs for the different tasks.

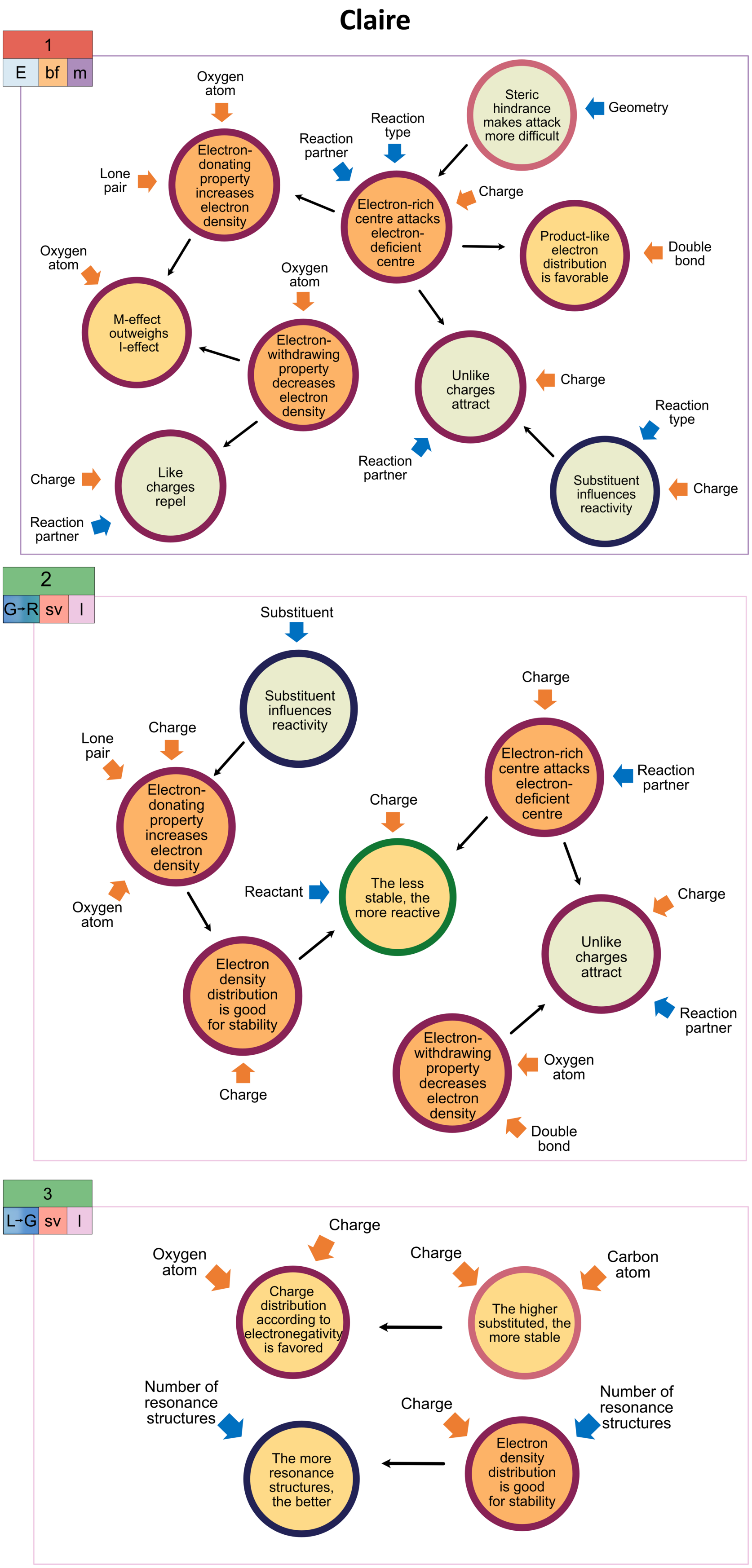


Figure 28. Claire's resource graphs for the different tasks.

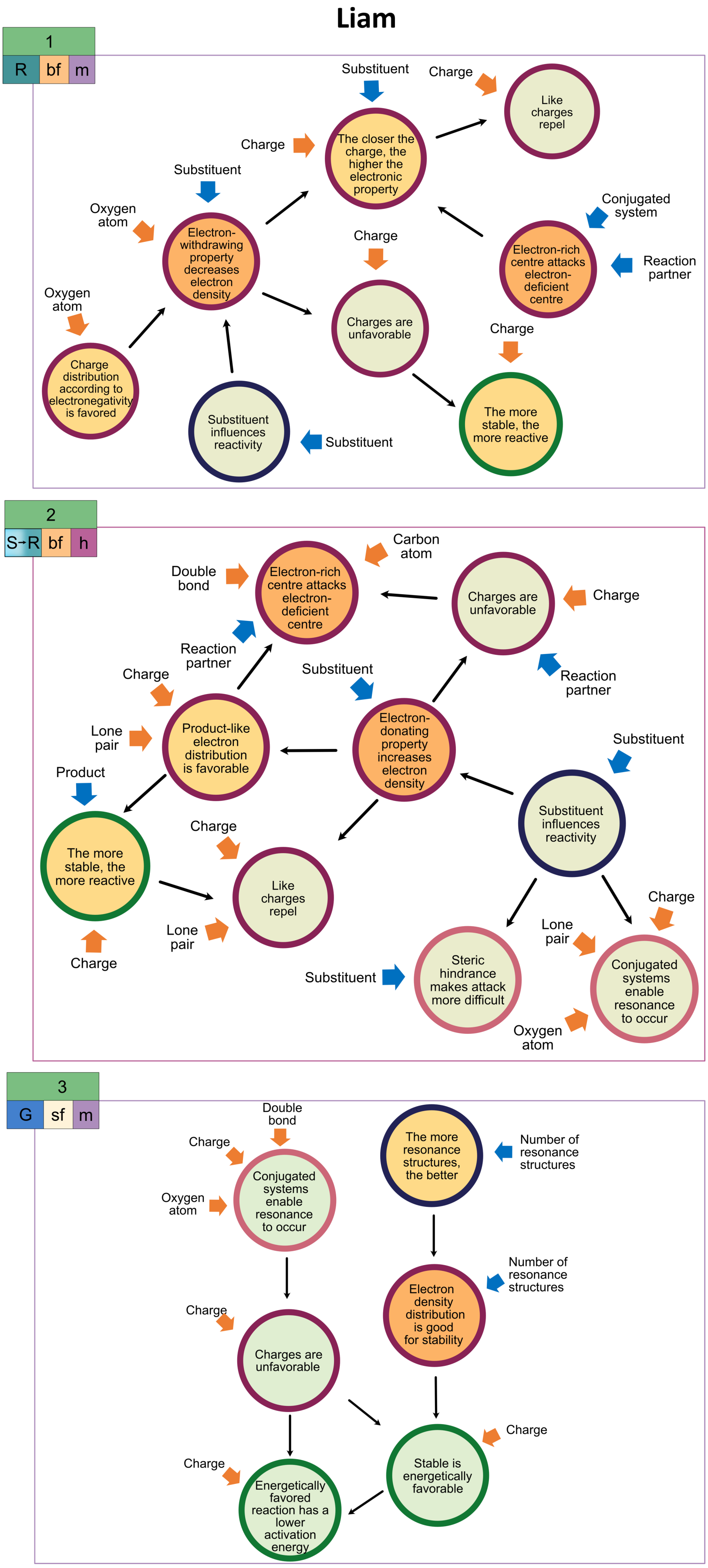


Figure 29. Liam's resource graphs for the different tasks.

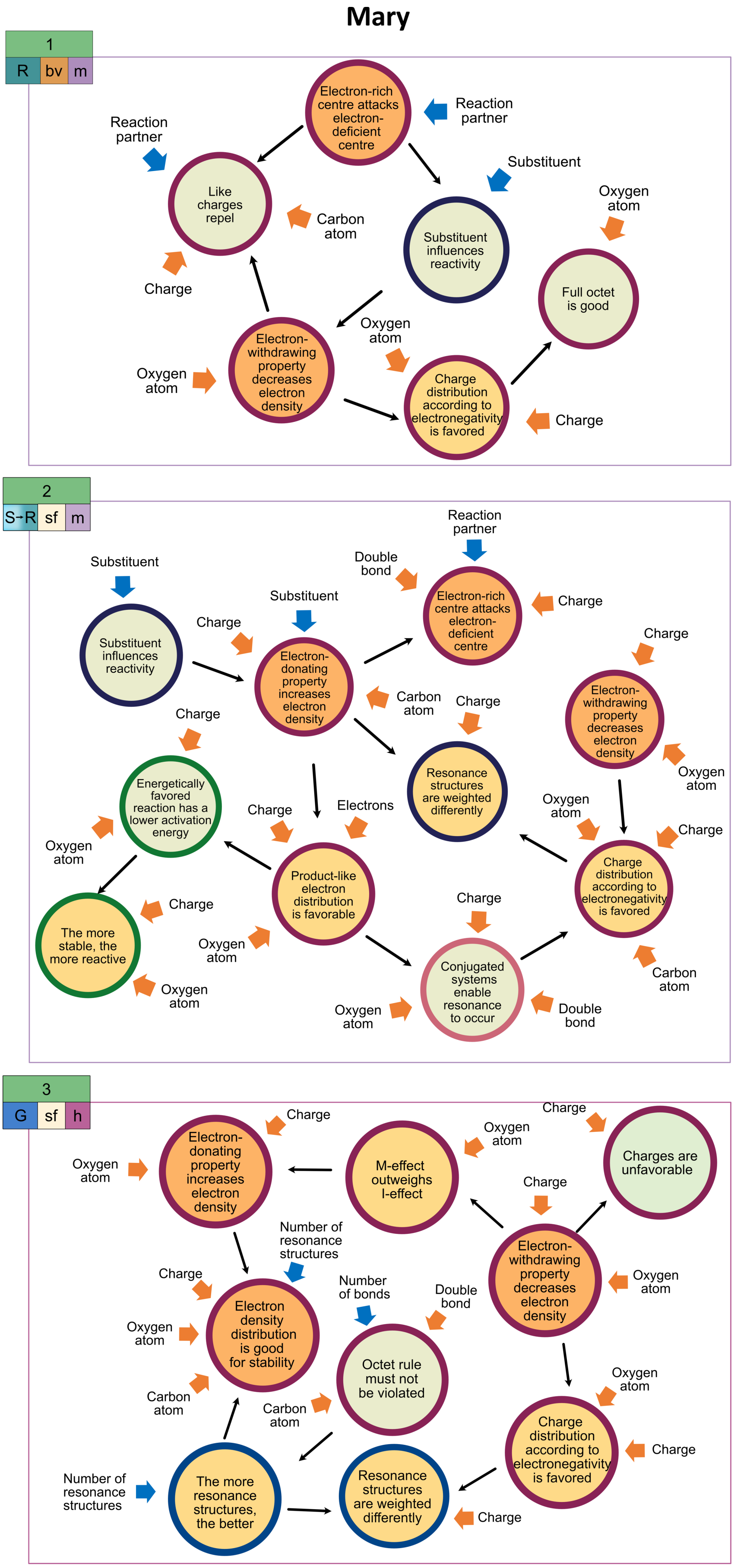


Figure 30. Mary's resource graphs for the different tasks.

Oliver

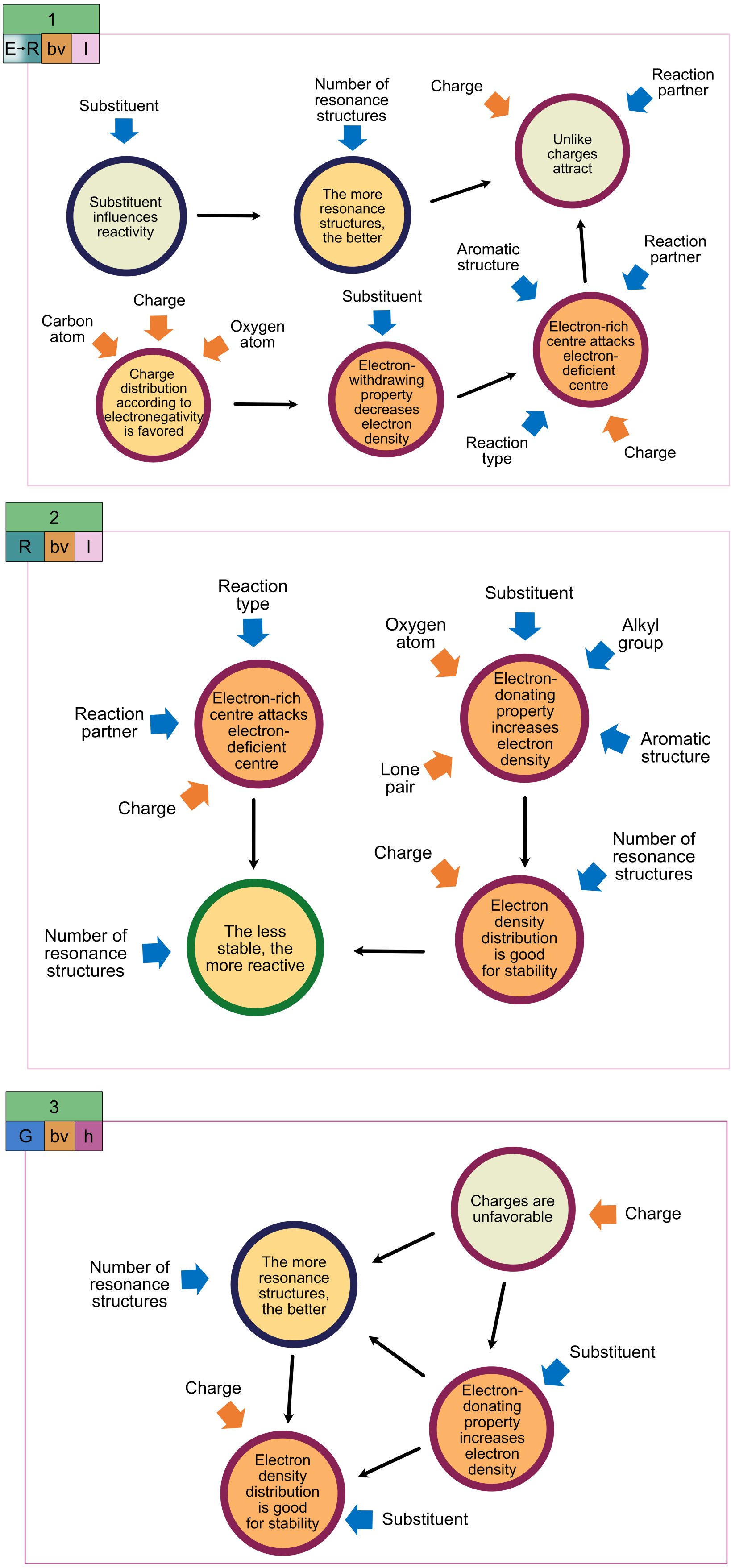


Figure 31. Oliver's resource graphs for the different tasks.

Lucas

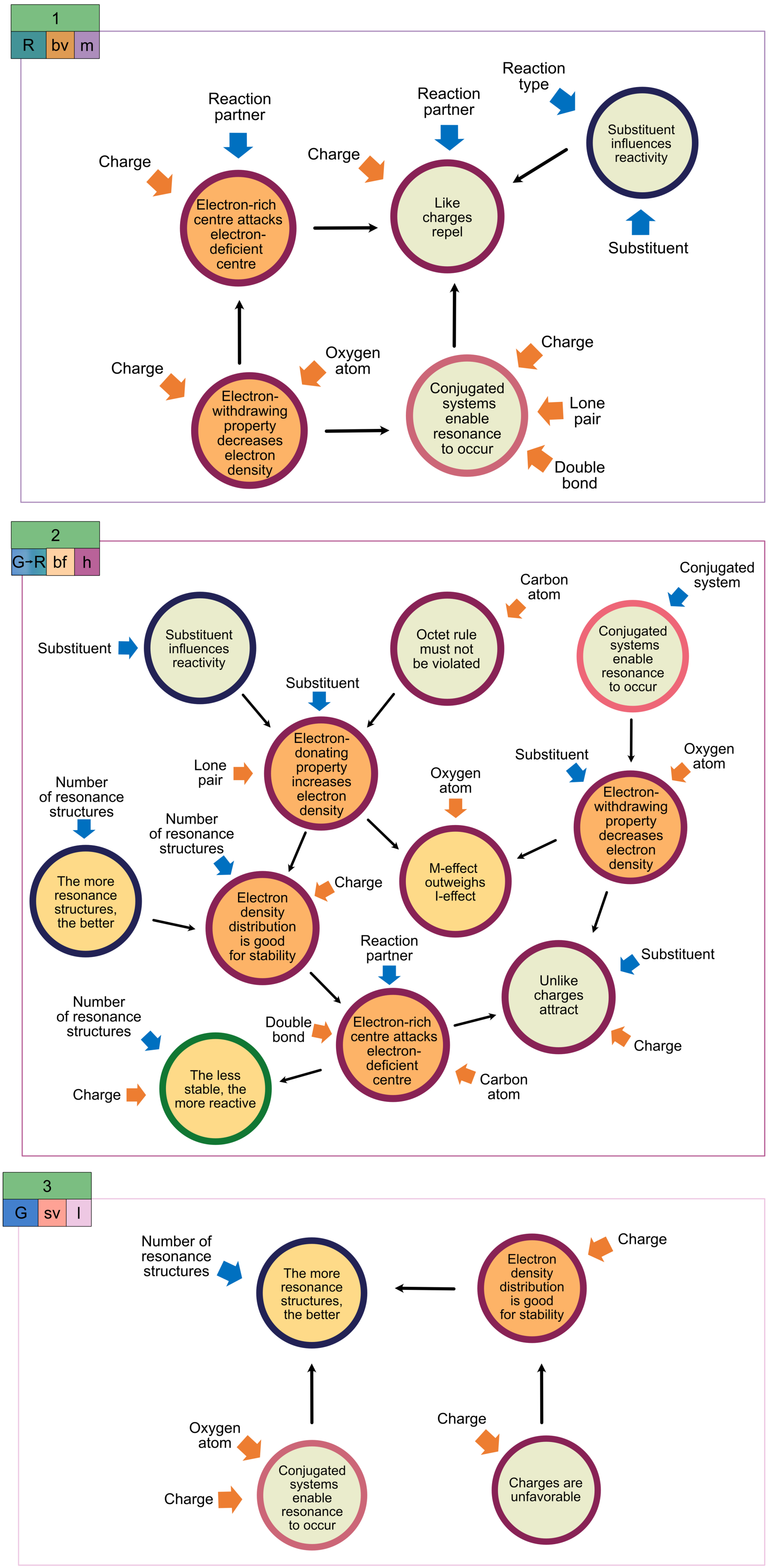


Figure 32. Lucas' resource graphs for the different tasks.

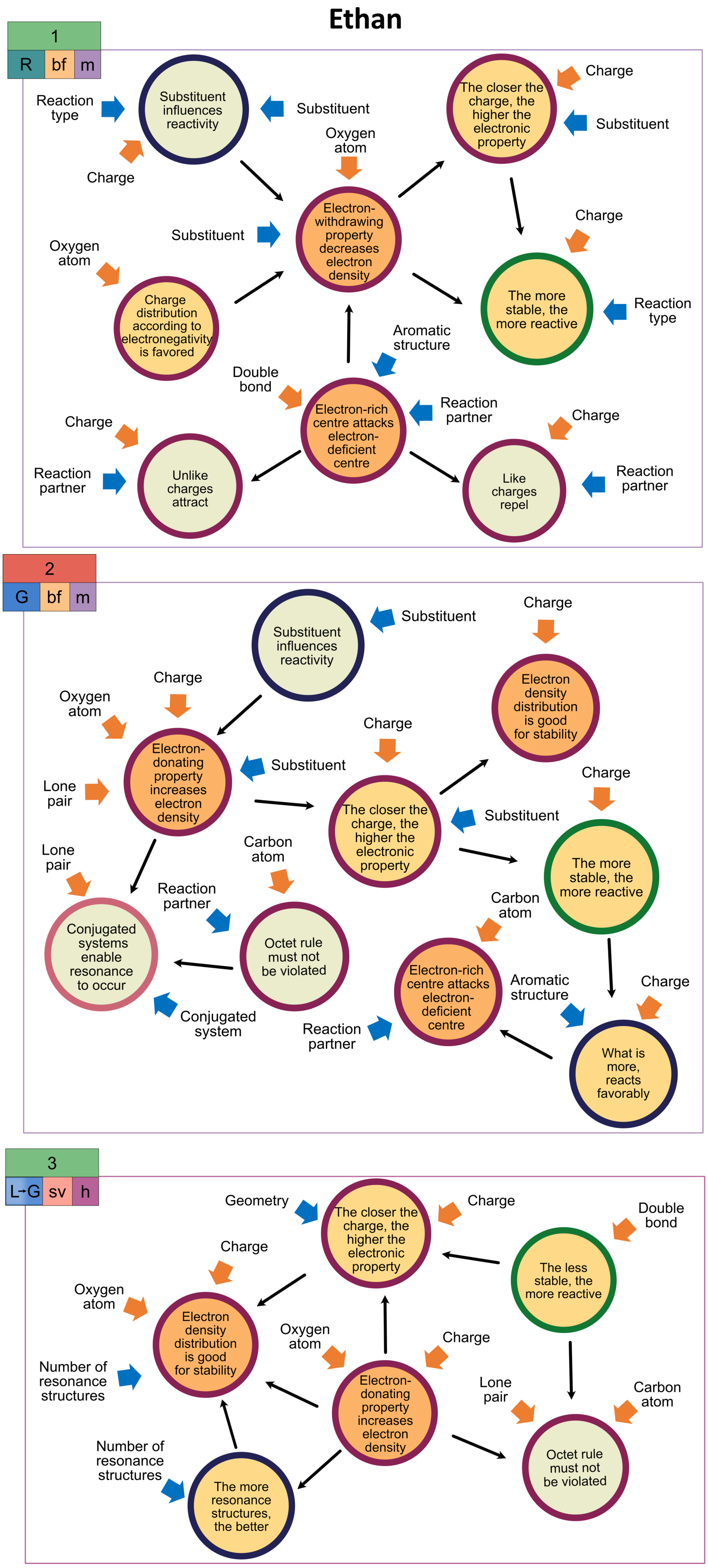


Figure 33. Ethan’s resource graphs for the different tasks.

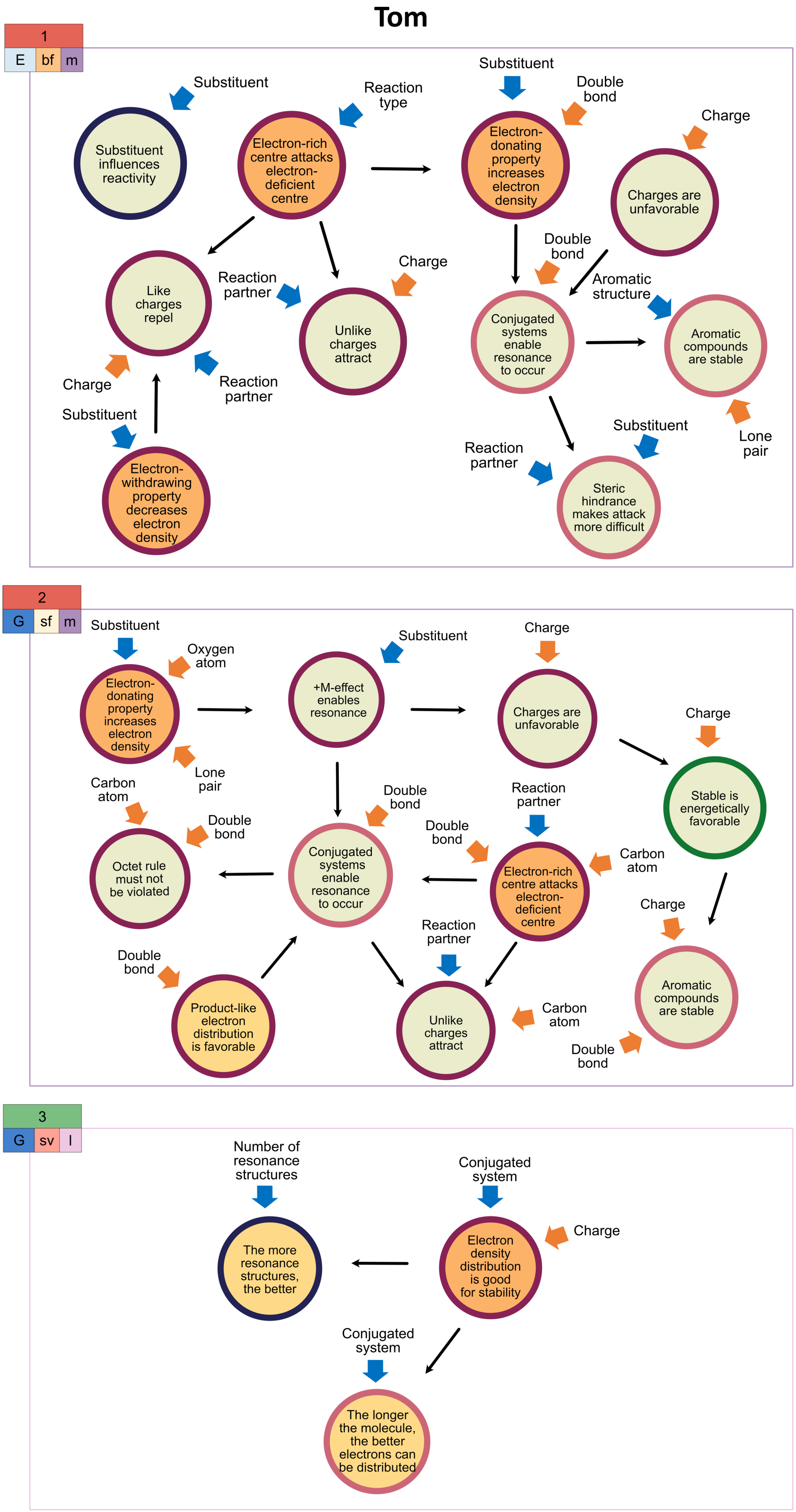


Figure 34. Tom's resource graphs for the different tasks.

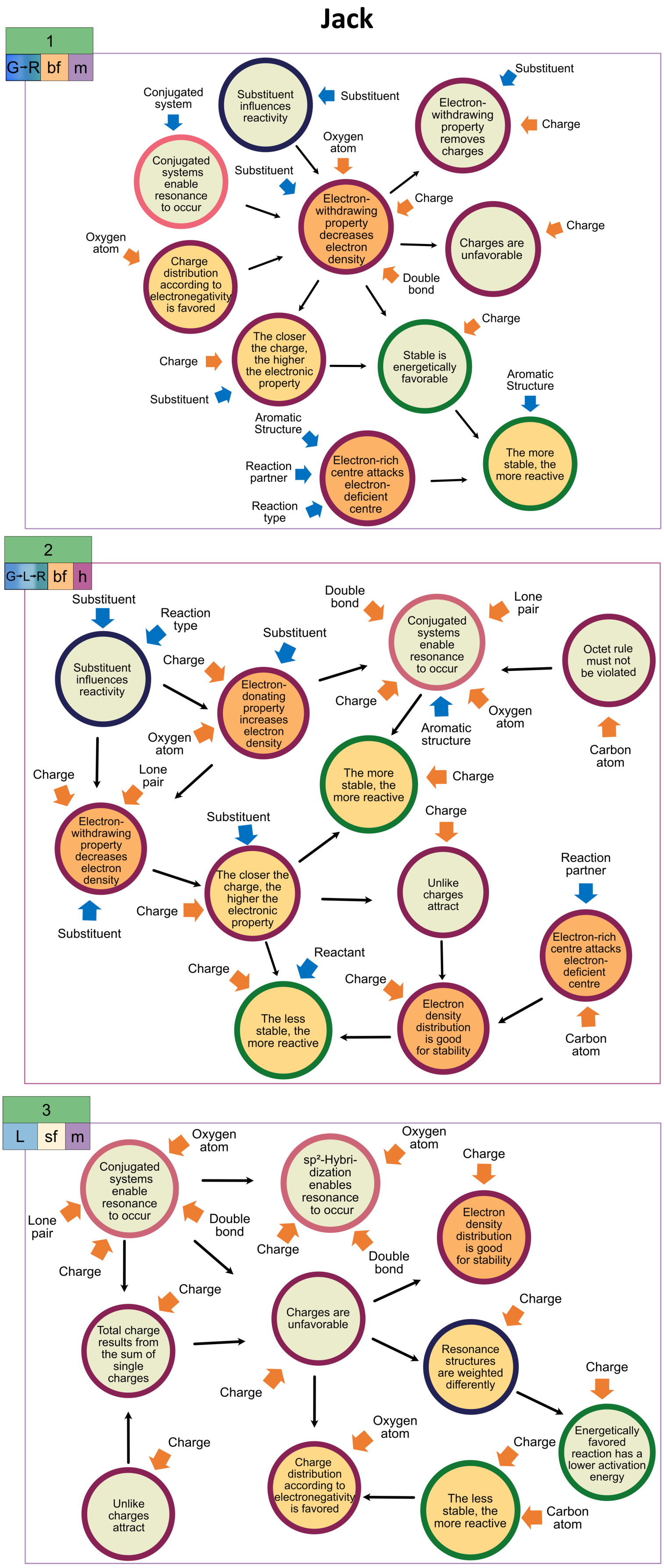


Figure 35. Jack's resource graphs for the different tasks.

Pascal

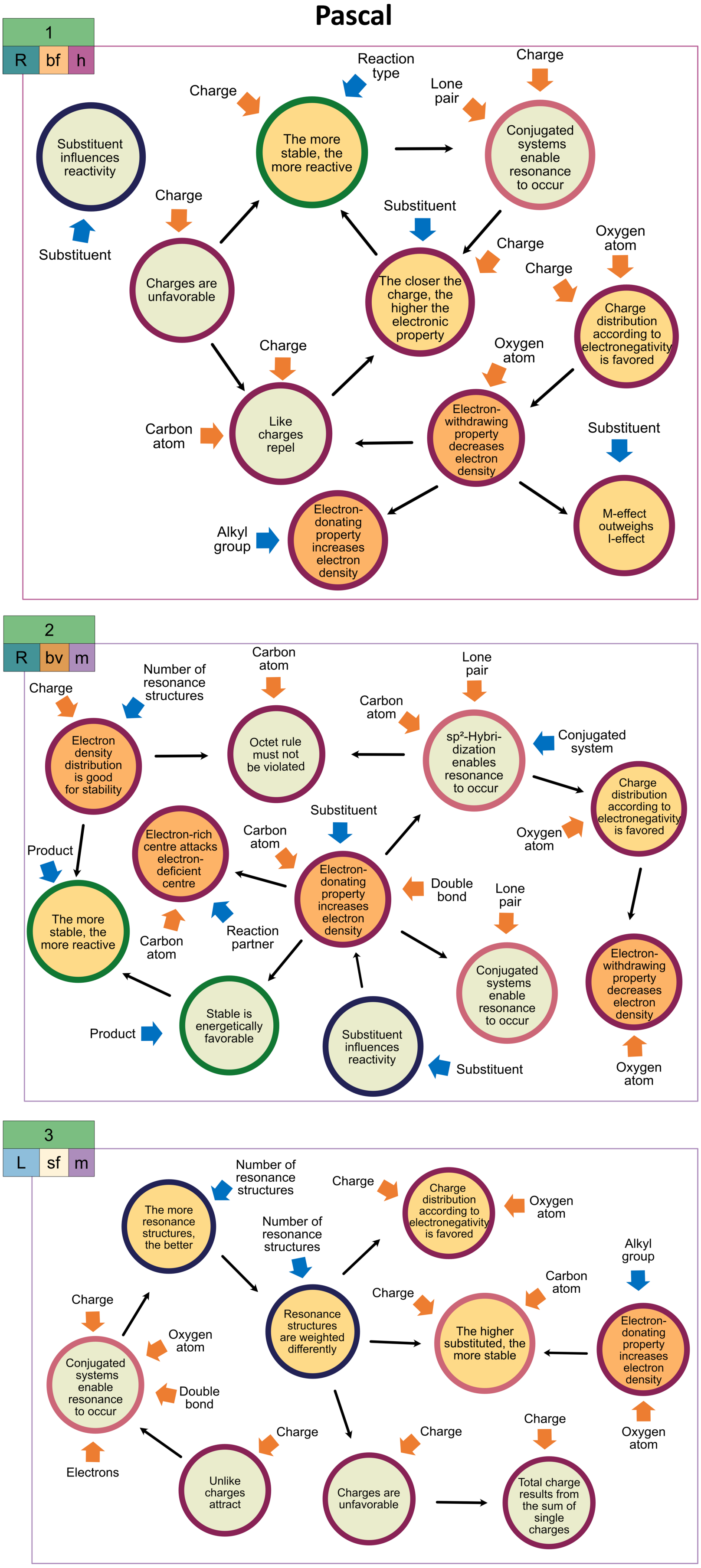


Figure 36. Pascal's resource graphs for the different tasks.

Charlotte

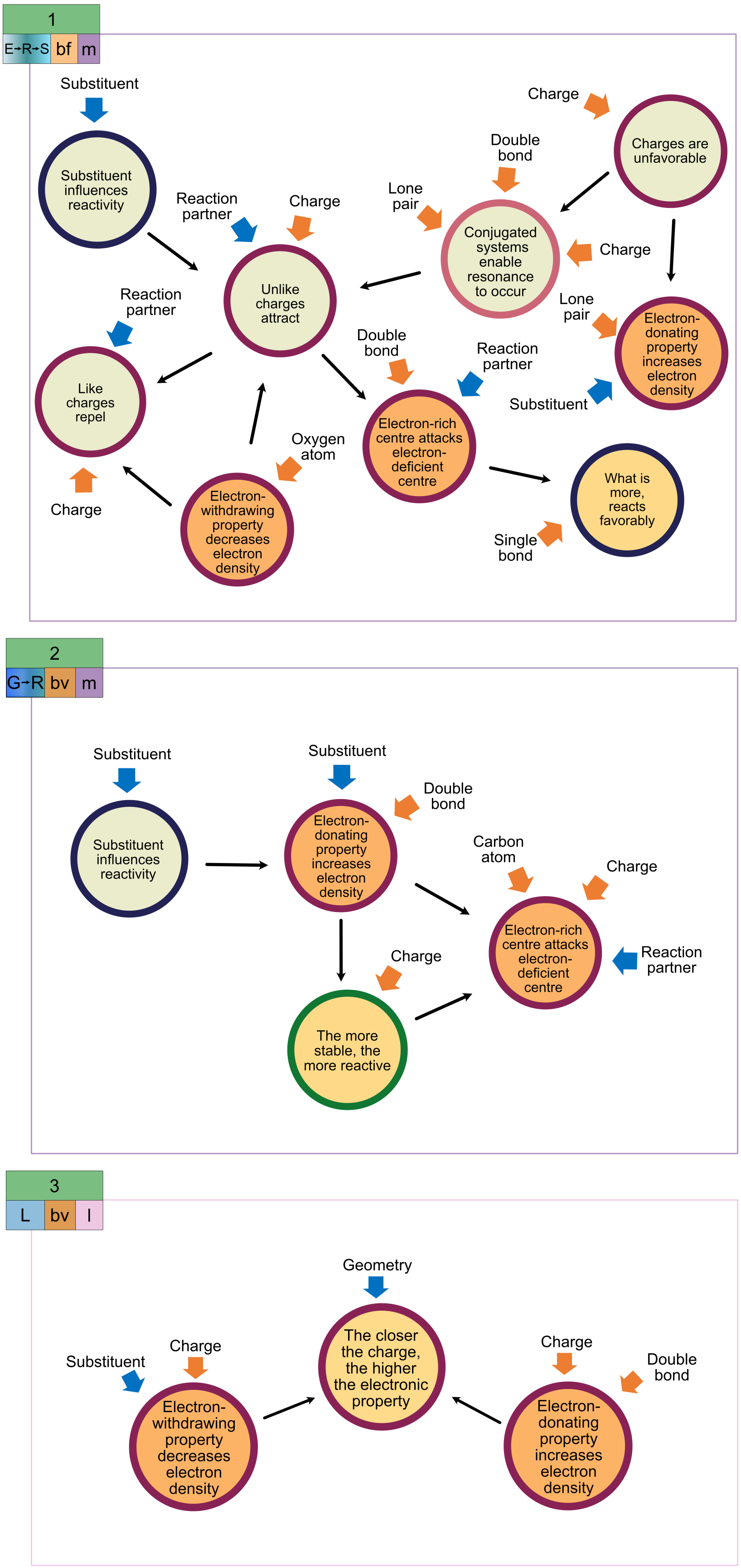


Figure 37. Charlotte's resource graphs for the different tasks.

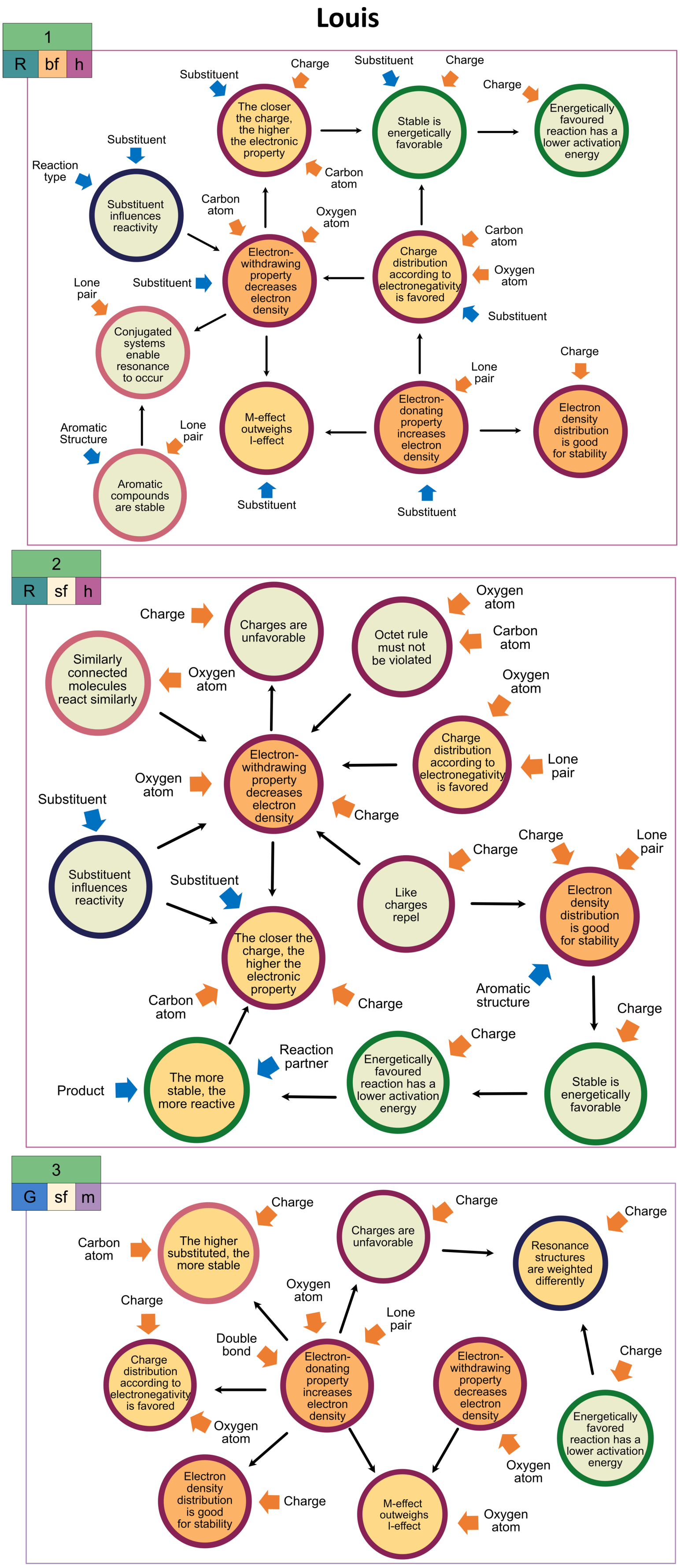


Figure 38. Louis' resource graphs for the different tasks.

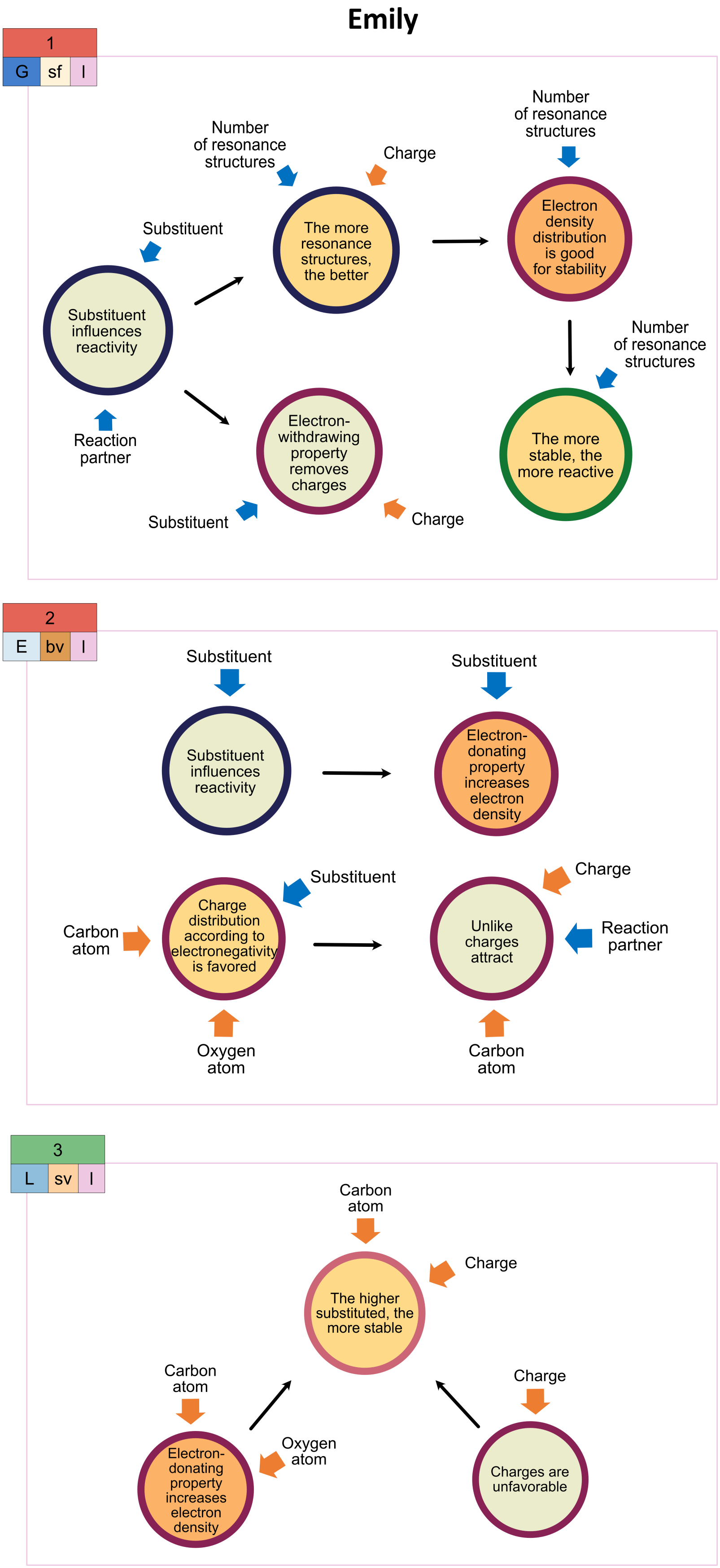


Figure 39. Emily's resource graphs for the different tasks.

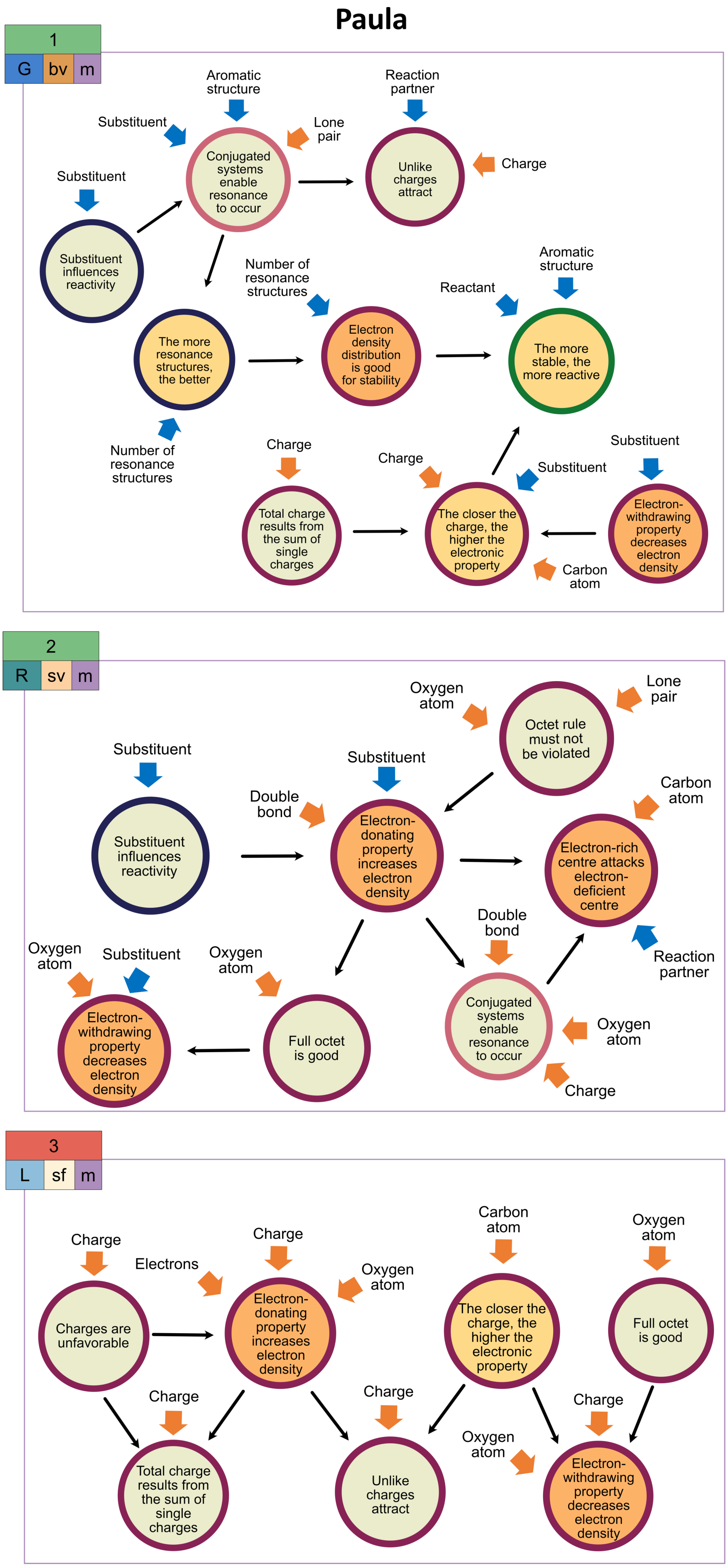


Figure 40. Paula's resource graphs for the different tasks.

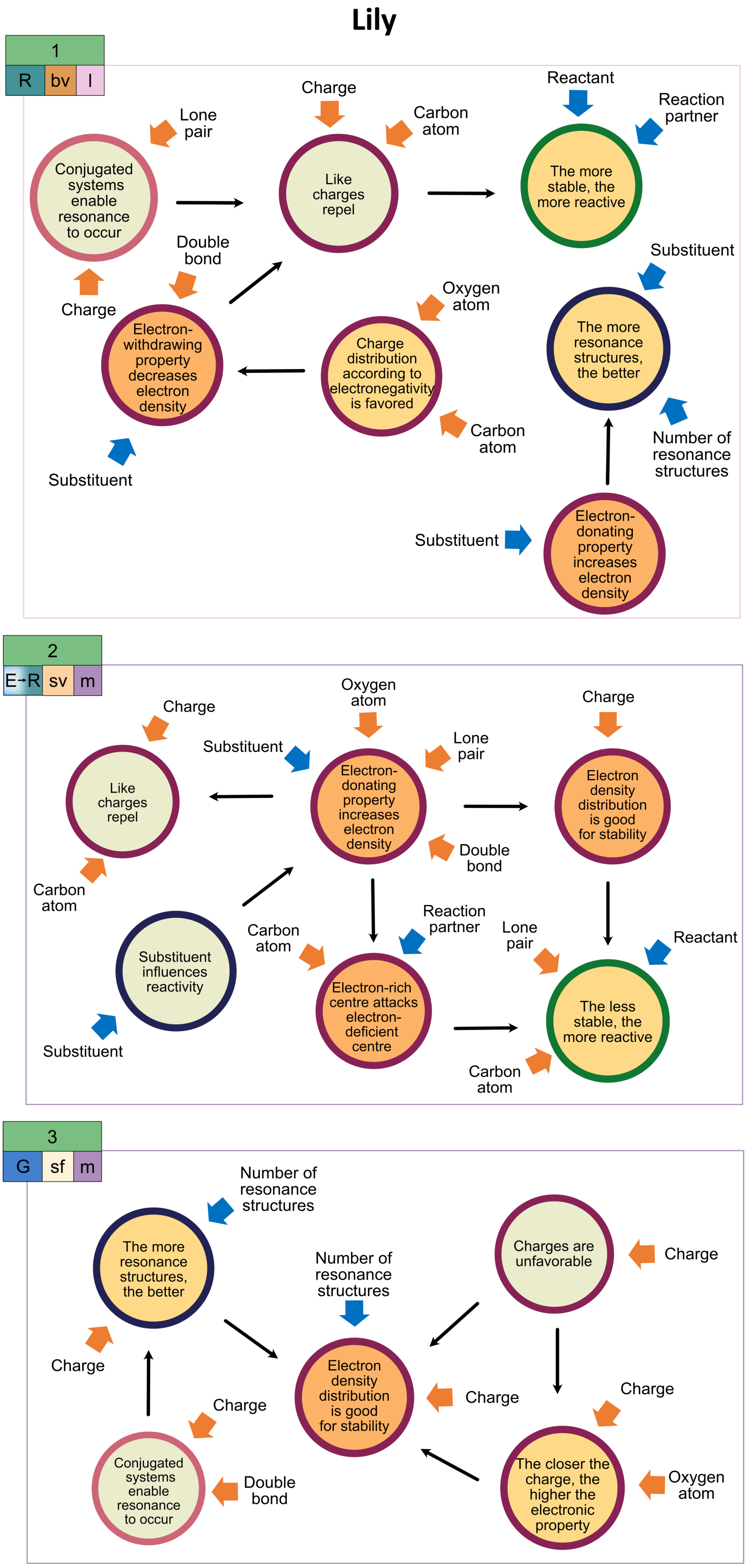


Figure 41. Lily's resource graphs for the different tasks.

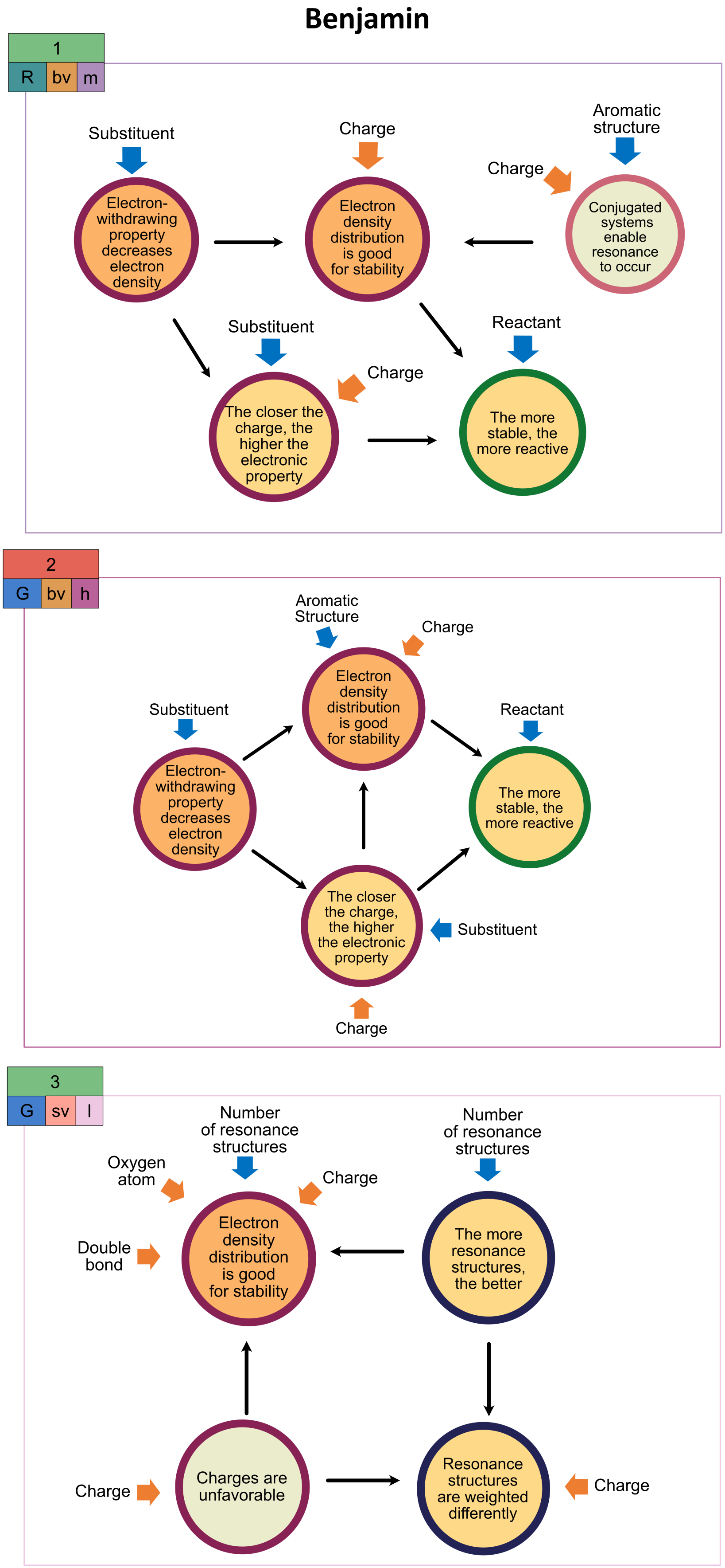


Figure 42. Benjamin’s resource graphs for the different tasks.

6.1.7 Students' Original Quotes and Their English Translation

In cases where students' original responses in German were grammatically incorrect (*e.g.*, word order or expression), they were translated into English in a grammatically correct way to facilitate reading flow. The translations were carefully reviewed (*i.e.*, compared to the interview video recordings) to ensure that they faithfully represent the original responses without changing their meaning. Pauses in students' utterances are indicated with […].

Text passage	German transcript	English translation of the transcript
Chapter 1 Figure 11 p. 19	**Oliver**: „*Na ja, das ist ja, also wenn es ja um Stabilität geht, dann schaut man sich ja eigentlich immer an, wie kann das, also wie beeinflussen die benachbarten Atome sozusagen diese Ladung. Und wenn diese Ladung halt gut ausgeglichen wird, dann ist es halt stabiler. Und ja, wenn das halt so eine richtige Formalladung ist, dann kann man eben halt auch mesomere Grenzstrukturen aufstellen.* […] *Und dass man es halt dann nochmal macht, diesmal wo der Sauerstoff mit einbezogen wird*."	**Oliver**: "*Well, when it comes to stability, you usually look at how the neighboring atoms influence the charge. And if the charge is well balanced, then the compound is more stable. As it's a formal charge, you can draw resonance structures.* […] *Then you'd draw it again, this time incorporating the oxygen* [atom]."
Chapter 1 Figure 15 p. 24	**Anna**: „*Aufgrund der Ethergruppe, das ist wieder Wissen, was ich aufgeschnappt habe, also in dieser Tabelle* […] *dass die Ethergruppen einen positiven M-Effekt haben und wenn ich mich nicht irre, einen minus I-Effekt* […]. *Ist wieder gelernt, dass der M-Effekt überwiegt, und deswegen kann ich Elektronen hier rein schieben* [zeigt auf positive Ladung] […] *dass quasi die Gesamtladung zählt, also dass die Gesamtladung gleich bleiben muss, das ist entscheidend.*"	**Anna**: "*Because of the ether group, that's knowledge I've picked up, so in this table,* […] *that ether groups have a positive M-effect and, if I'm not mistaken, a negative I-effect* […]. *I've learned that the mesomeric effect predominates, and that's why I can push electrons in here* [points toward positive charge] […] *so the total charge has to remain the same, that's essential.*"
Chapter 1 Figure 17 p. 26	**Anna**: „*Ich tendiere zu B, weil ich mir gedacht habe, dadurch, dass ich ja Elektronen hier reinschiebe* [bezieht sich auf reaktives Zentrum in A], *ist es möglich, dass hier an der Carbonylgruppe das delta positiv ist. Wenn ich, wenn der Benzolring, sage ich mal, seine Ladung theoretisch hier reinschieben kann* [bezieht sich auf reaktives Zentrum in A] *habe ich ja wieder eine geringe Reaktivität als wenn ich das in meta-Position habe.* […] *Ich überlege nochmal, Entschuldigung.* […] *Ich bleibe bei A.* […] *Dadurch, dass ich es mir nochmal aufgezeichnet habe* [bezieht sich auf mesomere Grenzformeln in A], *und nochmal darüber nachgedacht habe, habe ich mir überlegt, ok, gut, beide Wege,*	**Anna**: "*I think it is B because I thought that by pushing electrons here* [refers to reactive center in A], *it is possible that the delta positive charge is at the carbonyl group. If the benzene ring can push its charge here* [refers to reactive center in A], *I would have lower reactivity than if it were in the meta-position.* [...] *I'm reconsidering, sorry.* [...] *I'll stick with answer A.* [...] *By redrawing it* [resonance structures in reaction A] *and thinking about it again, I realized that both paths, A and B, show that it is possible to push electrons to this carbonyl group. The question now is, which of the two, they differ in the ether position, the ether group is in meta-position here* [in B] *and in para-position there* [in A] *to this carbonyl group.*

	sowohl A und B, zeigen, dass es möglich ist, dass ich Elektronen zu dieser Carbonyl-Gruppe schieben kann. Die Frage ist nur noch, welcher der beiden, also die unterscheiden sich ja in der Etherstellung, also die Ethergruppe ist ja einmal in meta [in B] *und einmal in para-Position* [in A] *zu dieser Carbonylgruppe. Jetzt ist die Frage, wie kann, welches kann quasi besser es aktivieren. Und da habe ich wieder zurück an die Aromaten gedacht und habe mir gedacht, wir haben hier eine aktivierende Gruppe, die steht meistens in para.*“	*Now the question is, which one can better activate it. And that's when I thought about the aromatics again and realized that we have an activating group, which is usually in the para-position.*”
Chapter 2 Figure 5 p. 11	**Audrey**: „*Jedenfalls hier kann es* [Doppelbindung] *halt nach oben klappen, dann sieht es so aus. Es kann aber auch, ich kann es jetzt quasi auch hier die andere Seite klappen.*“	**Audrey** “*Anyway, here it* [the double bond] *can just flip up, then it would look that this. But it can also, I can also flip to here to the other side.*”
Chapter 2 Figure 5 p. 11	**Ethan**: „*Und dann ja gut, dann habe ich jetzt hier die positive Ladung, okay, dann habe ich hier freie Elektronen, na dann gehen die jetzt da runter.*“	**Ethan**: “*And then, well, now I have the positive charge here, okay, and I have free electrons here, well then, they go down here now.*”
Chapter 2 Figure 5 p. 11	**Audrey**: „*Hier könnte die Elektronenbindung nach da klappen, die kann aber nicht nach außen klappen, weil außen wäre dann, glaube ich, instabil.*“	**Audrey**: “*Here, the electron pair could flip to there, but it can’t flip outside, because outside it would be unstable, I think.*”
Chapter 2 Figure 5 p. 11	**Luke**: „*Der kann nach unten klappen.* […] *Also es löst ja dann hier auch das Umklappen hier aus* [bezieht sich auf Doppelbindung]. *Und das freie Elektronenpaar ist ja nicht lokalisiert. Also würde ich wieder eigentlich so argumentieren, dass das ja nichts Statisches ist und ich habe hier nirgendwo dann in der Folge die Oktettregel verletzt oder zu viele Elektronen an einem Kohlenstoff- oder Sauerstoffatom.*“	**Luke**: “*It can flip down.* […] *It then also initiates the folding over here* [refers to the double bond]. […] *The free electron pair is not localized. So, I would argue again that this is nothing static and that I have neither violated the octet rule nor do I have too any electrons at a carbon or oxygen atom.*”
Chapter 2 Figure 10 p. 17	**Nina**: „*Ich mache jetzt einfach mal irgendwas* […]. *Ja, also theoretisch könnte es ja so sein, dass, ich weiß halt nicht, ob das irgendwie logisch ist, aber okay, grade hatte ich ja auch dann von dem Sauerstoff ja auch wieder so was umgeklappt und wenn ich das jetzt halt mal machen würde einfach mal so, dann hätte ich hier in dem Fall halt theoretisch sowas* [zeichnet mesomere Grenzformel in A]. *Und in dem anderen Fall* [bezieht sich auf Reaktion B], *wenn ich das genauso machen würde, so, wenn ich das jetzt einmal genauso mache,*	**Nina**: “*I’ll just do something now* […]. *Yes, so theoretically it could be like that, I don’t know if that’s logical somehow, but okay, just before, I also flipped something over from the oxygen, and if I would do that just like that now, then I would theoretically have something like that* [draws the resonance structure in A]. *And in the other case* [refers to reaction B], *if I did it the same way, then it would look something like this* [points to resonance structure in B]. *I don’t know if that’s right and if that helps me at all, but it’s somehow the only thing I can think of doing*

	dann würde das ja irgendwie so aussehen [zeigt auf mesomere Grenzformel in B]. *Weiß nicht, ob das richtig ist und ob mir das überhaupt irgendwas bringt, aber ist irgendwie das einzige, was mir grade so einfällt zu machen.* […] *Aber jetzt, ja, so mit dem, was aus den vorherigen Aufgaben irgendwie so hängen geblieben ist, müsste es eigentlich theoretisch so gehen.*“	*right now.* […] *But yes, with what has somehow stuck in my mind from the previous tasks, it should actually theoretically work like this.*”
Chapter 2 Figure 11 p. 17	**Catherine**: „*Wenn Sauerstoff zwei freie Elektronenpaare hat, dann geht man schon davon aus, dass es damit was machen kann beziehungsweise dass mesomere Grenzstrukturen entstehen können.*“	**Catherine**: “*If oxygen has two lone pairs, then it can be assumed that it does something with them, or that resonance structures can be formed.*”
Chapter 2 *Results and Discussion Section* p. 18	**Elizabeth**: „*Ich glaube freie Elektronenpaare sind auch einfach ein Indiz für mich dafür, dass man Mesomerie, machen kann und nicht nur Doppelbindungen, sondern halt auch freie Elektronenpaare.*“	**Elizabeth**: “*I guess lone pairs are also an indication for me that you can apply resonance, not only double bonds, but also lone pairs.*”
Chapter 2 Figure 12 p. 18	**Elizabeth**: „*Okay, wenn das nicht klappt, klappe ich die Doppelbindung hoch* [zeigt zum Sauerstoffatom], *sodass hier dann eine negative Ladung entsteht* [zeigt zum Sauerstoffatom] *und hier* [zeigt zum Kohlenstoffatom] *eine positive.*“	**Elizabeth**: “*Okay, if that does not work, I flip the double bond up* [refers to the oxygen atom] *so that there is a negative charge here* [refers to the oxygen atom] *and a positive charge here* [refers to the carbon atom].”
Chapter 2 Figure 13 p. 18	**Paula**: „*Also hier habe ich die positive Ladung* [zeigt auf Produkt in Reaktion A], *bin dann hier rüber geklappt* [meint Doppelbindung, bezieht ich auf neu gebildetes Carbeniumion] […] *dann sind halt hier die zwei* [freien Elektronenpaare vom Sauerstoffatom] *und dann klappt halt eine dann auch wieder rüber zur positiven Ladung und macht dann halt hier die nächste Doppelbindung und dadurch ist die positive Ladung am Sauerstoffatom* [bezieht sich auf zweite mesomere Grenzformel in A].“	**Paula**: “*So here, I have the positive charge* [points to the provided product in reaction A], *then I flipped* [the double bond] *over here* [refers to the newly created carbocation]. […] *Then, here are the two* [free electron pairs of the oxygen atom] *and then one of them flips over again to the positive charge and makes the next double bond, and thus, the positive charge is at the oxygen atom* [refers to the second structure in reaction A].”
Chapter 2 Figure 14 p. 19	**Phil**: „*Ich halt weiß, je weiter delokalisiert eben die positive Ladung ist, desto stabiler ist das Ganze* [Molekül]. *Und dann habe ich halt geguckt, also beim ersten kann natürlich die Doppelbindung hier umklappen, dass ich dann die positive Ladung zwei Kohlenstoffatome weiter habe* [zeigt auf erste mesomere Grenzformel in A]. *Und dann ist auch noch das Sauerstoffatom eingebunden und kann noch mal ein Elektronenpaar spenden* [zeigt auf	**Phil**: “*I know the more delocalized the positive charge is, the more stable the* [molecule] *is. And then I just looked, so in the first one, of course, the double bond can flip over here, so I have the positive charge two carbon atoms further* [refers to the first resonance structure in A]. *And then the oxygen atom is also involved and can give another pair of electrons* [refers to the second resonance structure in A]. *This means that I have basically distributed the positive charge*

	zweite mesomere Grenzformel in A]. *Heißt, ich habe die positive Ladung im Grunde über diese drei Atome verteilt* […] *Weil bei der zweiten Grenzstruktur habe ich den Fall, dass die positive Ladung an einem benachbarten Kohlenstoff, also zum Sauerstoffatom benachbarten Kohlenstoffatom ist. Und das führt eben dazu, dass einfach ein Elektronenpaar vom Sauerstoff eben weiterklappen kann und eben diese Bindung bildet.* […] *Hier könnte jetzt einmal das* [Doppelbindung] *auch umklappen* […] *Ich habe zwar auch das Sauerstoffatom dabei, aber das kann halt seine Elektronenpaare nicht spenden, um die positive Ladung zu delokalisieren. Und bei B geht das eben nicht, weil ja die positive Ladung nur an den beiden Kohlenstoffatomen ist, die im Grunde zwei weiter sind vom Sauerstoff aus, also nicht an einem direkt benachbarten Atom. Deswegen wird es da für die weitere Delokalisierung eben nichts bringen, wenn noch ein Elektronenpaar vom Sauerstoff umklappt. Und es würde auch gar nicht gehen, weil dann wäre der Kohlenstoff fünfbindig, der hier.*“	*over these three atoms.* […] *In the second resonance structure, the positive charge is on a carbon atom neighboring the oxygen atom. And this leads to the fact that one pairs of electrons of the oxygen can simply flip over and form this bond.* […] *Here now* [the double bond] *could also flip over* [refers to the resonance structure in B] […] *I have the oxygen atom here, too, but it can't give its electron pairs to delocalize the positive charge. This is not possible in B because the positive charge is only at these two carbon atoms, which are basically two carbon atoms further from the oxygen, thus not at a directly neighboring atom. That's why it won't do any good for the further delocalization if another pair of electrons of the oxygen flips over. And it would not work at all because then, this carbon would be five-bonded.*”
Chapter 2 *Results and Discussion Section* p. 19	**Luke**: „*Dann habe ich überlegt. Was kann das Sauerstoffatom? Das Sauerstoffatom hat einmal einen Minus-I-Effekt, weswegen die positive Ladung intensiviert wird. Aber ich habe gedacht, dass ist gegenüber diesem Plus-M-Effekt auch zu vernachlässigen, weil das Elektronenpaar wieder reingegeben werden kann zur positiven Ladung und dann die positive Ladung hier hängt. Ich würde zwar sagen, dass ist nicht so energetisch günstig hier mit der positiven Ladung am Sauerstoff, aber es zeigt schon mal, dass die positive Ladung relativ gut verteilt werden kann.*“	**Luke**: “*Then I thought, what does the oxygen atom do? The oxygen atom has a negative inductive effect, which is why the positive charge is intensified. But I thought that it can be neglected given the positive resonance effect, because the electron pair can be pushed toward the positive charge, and then, the positive charge would be here. I would say that is energetically not so favorable here with the positive charge on the oxygen, but it shows that the positive charge can be distributed relatively well.*”
Chapter 3 Figure 3 p. 650	**Oliver**: „*Also eigentlich geht es ja nur, ob der Substituent jetzt ein ortho-, meta- oder para-dirigierend.* […] *Dort, wo die negative Ladung ist, dieses Produkt wird dann bevorzugt gebildet. Weil das ja ein Elektrophil ist. Das* Br^+.“	**Oliver**: “*Actually, it is only a question of whether the substituent is ortho-, meta-, or para-directing.* […] *Where there is a negative charge, this product will be formed preferentially because Br+ is an electrophile.*”
Chapter 3 Table 1 p. 651	**Charlotte**: „*Und dann dachte ich, ich gehe erstmal wieder zum Thema zurück, Mesomerie. Und hab dann halt gezeichnet, ok, was für Mesomerie Formeln gibt es überhaupt von diesem Molekül. Ich denke, dass das irgendwie halbwegs richtig war. Und da hab ich ja dann später auch wieder die Pfeile eingezeichnet* [zeigt auf	**Charlotte**: “*And then I thought, I'll go back to the topic, resonance. And I just drew, ok, what kind of resonance structures are there for this molecule. I think that this was somehow correct. Later, I drew in the arrows again* [referring to electron arrows in a structure] *just to see, where a positive charge in the ring is possible, because I know, the*

	Elektronenverschiebungspfeile in einer Struktur]. *Um zu sehen, ok, wo ist eine positive Ladung im Ring halt möglich, weil ich ja weiß, ok, im Ring wird die Substitution erfolgen oder am Ring. War dann halt der Gedanke, das Br minus, dahin anzudocken.*“	*substitution will take place at the ring. So, the idea was to dock the Br minus there.*”
Chapter 3 Table 1 p. 651	**Tiffany**: „*Es wäre halt die Geometrie. Also ich weiß, dass freie Elektronenpaare viel Raum einnehmen.* […] *Die liegen einfach nur näher, und dann wäre es vielleicht noch logisch, dass man sagt, es reagiert hier* [bezieht sich auf Reaktion A], *weil hier die Elektronendichte schon sehr hoch ist und dass dann so eine Addition stattfindet, wäre vielleicht unrealistischer verglichen zu hier, wo sie so ein bisschen weiter auseinandersteht.*“ **I**: „*Hängt das dann mit der Sterik zusammen?*“ **Tiffany**: „*Ich, ja, würde ich schon sagen, weil diese freien Elektronenpaare nehmen viel Platz ein. Das* [Sauerstoffatom in Reaktion A] *hat auch nochmal freie Elektronenpaare. Ich könnte mir vorstellen, dass das vielleicht auch noch was damit zu tun hat.*“	**Tiffany**: “*It would be the geometry. I know that lone pairs take up a lot of space.* [...] *They are just closer, it would be logical to say that it reacts here* [refers to reaction B], *because here* [refers to reaction A], *the electron density is already very high and when such an addition takes place, would perhaps be more unrealistic compared to here, where it is a bit further apart.*” **I**: “*Is that related to sterics, then?*” **Tiffany**: “*I, yes, I would say so, because the lone pairs take up a lot of space. There* [refers to oxygen atom in reaction A] *are also lone pairs again. I would imagine that might have something to do with that as well.*”
Chapter 3 Table 1 p. 651	**Jack**: „*Ja, es gibt gewisse ungünstige Positionen für positive Ladungen, in denen beispielsweise bei elektronenziehenden Gruppen, (.) wie Brom, ist ja auch, hat einen minus I-Effekt, aber einen plus M-Effekt, weil der plus M-Effekt eigentlich immer überwiegt, das heißt, wenn wir jetzt beispielsweise eine positive Ladung beim Brom haben, was in dem Fall glaube ich nicht der Fall sein kann sogar, wäre das eine ungünstige Situation bzw. wenn ich hier eine negative Ladung habe* [bezieht sich auf die Carbonylgruppe einer Struktur im Wheland-Komplex], *wäre das auch ziemlich ungünstig, weil ja der minus M- und minus I-Effekt hier eigentlich die Elektronen rauszieht, das heißt, diese partielle positive Ladung würde noch erweitert werden.* […] *Das heißt, die Begründung, warum es nach B verläuft, ist einfach, weil die positive Ladung am weitesten entfernt von der Gruppe ist und hier haben wir sie halt in der Nähe der Gruppe* [zeigt auf Carbonylgruppe], *was ungünstig für die Stabilität wäre.*“	**Jack**: “*Yes, there are certain unfavorable positions for positive charges, in which, for example, with electron-withdrawing groups, (.) bromine has a minus I-effect, but a plus M-effect, because the plus M-effect actually always predominates. That is, if we now have, for example, a positive charge with bromine, which in this case actually cannot be the case, that would be an unfavorable situation, or if I have a negative charge here* [refers to the carbonyl group in a structure of the Wheland complex], *that would also be quite unfavorable, because the minus M- and minus I-effect actually pull the electrons out here, that is, this partially positive charge would be increased.* [...] *The reason why it is B, is simply because the positive charge is farthest away from the group, and here, we have it just close to the group* [refers to carbonyl group], *which would be unfavorable regarding stability.*”

Chapter 3 Table 1 p. 651	**Jack**: „*Ich glaube, ich weiß, worauf die Aufgabe hinauswill, wenn ich mich nicht irre, wir können nämlich die negative Ladung einmal im Ring komplett rumschieben und das heißt, es ist konjugiert. Vielleicht, maybe, who knows.* […] *Das heißt, wir haben hier eine Stabilisierung, ja. Wir sind ja, so, theoretisch ist das ja eigentlich die Idee, dass man das hier ganze einmal rumschieben kann* [bezieht sich auf Reaktion A]*, also ist das vermutlich die stabilere und das Ganze wird beim anderen nicht der Fall sein* [bezieht sich auf Reaktion B].“	**Jack**: "*I think I know what the task is getting at, if I'm not mistaken, namely, we can push the negative charge around once in the ring completely and that means it's conjugated. Maybe, who knows.* [...] *That is, we have a stabilization here, yes. So, theoretically, that's actually the idea, that you can push this around here once* [refers to reaction A]*, so that is probably the more stable one and the whole thing will not be the case with the other one* [refers to reaction B]."
Chapter 3 Table 1 p. 651	**Nora**: „*Ich würde jetzt mal sagen, dass die A stabiler ist, weil hier eben diese mesomeren Grenzformel stabilisiert wird* [zeigt auf zweite mesomere Grenzformel in Reaktion A] *durch hier, den plus I-Effekt von dem Alkylrest. Und hier ist es halt eben so am Rand und da kommt quasi nichts mehr* [zeigt auf mesomere Grenzformel in B]*, deswegen, ja.* […] *Also hier geht es ja jetzt offensichtlich um das Produkt und dann habe ich einfach geguckt, wie kann ich die positive Ladung delokalisieren, habe die beiden/, also habe die mesomeren Grenzformeln davon gezeichnet und dann habe ich eben kurz überlegt und bin halt zu dem Schluss gekommen, dass das da die bestmögliche Verteilung ist* [zeigt auf zweite mesomere Grenzformel in A]. *Die positive Ladung kann dann am besten stabilisiert werden, weil an sich gibt es ja bei jedem zwei mesomere Grenzformeln. Aber hier oben, die* [zweite mesomere Grenzformel in A] *ist sozusagen, ich weiß nicht, am wertvollsten, weil es da eben am besten stabilisiert werden kann.* […] *Ähm, weil ich ja dann auch wieder diese positive Ladung am O habe, aber das ist nicht unbedingt stabil und deswegen dachte ich, dass es sinnvoller ist, wenn ich meine positive Ladung am C-Atom habe.*“	**Nora**: "*I would say that A is more stable, because here, this resonance structure is stabilized* [refers to the second resonance structure in A] *by the plus I-effect of the alkyl substituent. And here, it is just so at the end and there is nothing more* [refers to resonance structure in B]*, therefore, yes.* [...] *So here, it is obviously about the product, so I just looked how can I delocalize the positive charge, I drew the two/, so I drew the resonance structures of it and then I just briefly thought about it and came to the conclusion that this is the best possible distribution* [refers to the second resonance structure in A]. *The positive charge can then be best stabilized, because there are actually two resonance structures for each molecule. But up here, this one* [second resonance structure in A] *is, I don't know, the most valuable, because it can be stabilized best there.* [...] *Um, because then, I also have this positive charge on the O, but that's not necessarily stable and that's why I thought that it makes more sense if I have my positive charge on the C-atom.*"
Chapter 3 Figure 5 p. 653	**Benjamin**: „*Wir haben das OH Minus, das greift da an* [zeigt auf reaktives Zentrum], *es greift am liebsten da an, wo wir eine positive Ladung da stabilisieren können.* […] *Wo das* [Doppelbindung] *hier hochklappt, bildet sich hier eine partialpositive Ladung* [zeigt auf resultierendes Carbeniumion] *und diese partialpositive Ladung ist umso stabilisierter, je mehr sie mesomer im, unter anderem umso stabilisierter, je mehr*	**Benjamin**: "*We have the OH minus, which attacks there* [refers to reactive center], *it prefers to attack where we can stabilize a positive charge* [...] *This* [the double bond] *flips up, so a partial positive charge forms here* [points to the resulting carbocation]*, and this partial positive charge is more stable the more we can delocalize it, the more we can shift it in the ring or the more we can shift it overall in the molecule. And the ring is very capable of moving the positive charge here,*

	wir sie im Ring verschieben können oder je mehr wir sie insgesamt im Molekül verschieben können. Und der Ring ist hier halt sehr gut in der Lage dazu, die positive Ladung hier dann hierhin, dann hierhin [zeigt auf verschiedene Positionen der positiven Ladung in den mesomeren Grenzformeln] *beziehungsweise, wenn man den Substituenten hier hat* [bezieht sich auf Para-Position in A], *kann man sie auch noch auf das O schieben, was hier eine Stabilisierungsmöglichkeit mehr gibt* [bezieht sich auf Reaktion A] *als hier unten* [bezieht sich auf Reaktion A], *das heißt, hier oben ist der Übergangszustand stabiler* [in A], *das heißt meiner Meinung nach ist der nukleophile Angriff hier oben* [bezieht sich auf Reaktion A] *bevorzugt.*“	*then here, then here* [refers to different positions of the positive charge in the resonance structures], *or if you have the substituent here* [refers to para-position in A], *you can also shift it to the O*[xygen], *which provides an additional stabilization possibility* [refers to reaction A] *compared to down here* [refers to reaction B], *meaning the transition state is more stable up here* [in A], *so in my opinion, the nucleophilic attack up here* [refers to A] *is preferred.*”
Chapter 3 Figure 5 p. 653	**Benjamin**: „*Hier* [bezieht sich auf Reaktion A] *kriegen wir die positive Ladung irgendwie weiter ein bisschen, ein bisschen weiter verschoben als oben* […]. *Ich habe mir die Sachen erstmal aufgezeichnet, dann habe ich geschaut, ok, wie kriege ich die positive Ladung verschoben. Zwei mal eine Doppelbindung umgeklappt* [zeigt auf mesomere Grenzformeln in A und B], *ok, jeweils die ersten mesomeren Grenzstrukturen. Dann habe ich geschaut, ok, hier oben kann ich noch das freie Elektronenpaar vom O draufklappen, habe ich eine positive Ladung auf dem O, eine weitere Möglichkeit, das Ganze zu stabilisieren* […] *das heißt, ich habe hier nur zwei mesomere Grenzstrukturen* [in B], *hier oben habe ich drei mesomere Grenzstrukturen* [in A], *je mehr mesomere Grenzstrukturen, desto stabiler das Carbeniumion, desto sinnvoller ist es bei A das Ganze zu machen.*“	**Benjamin**: “*Here* [refers to reaction A], *we somehow manage to move the positive charge a bit further, a bit more than above.* [...] *I first drew the structures, then I looked at how to move the positive charge. I flipped the double bond twice* [refers to resonance structures in A and B], *okay, the first resonance structures in each case. Then I looked at it, okay, up here I can fold the lone pair of electrons from* [the] *O*[xygen], *I have a positive charge on O*[xygen], *another way to stabilize the whole molecule* [...] *meaning I have only two resonance structures here* [in B], *up here* [in A], *I have three resonance structures, the more resonance structures, the more stable the carbocation, the more reasonable it is to do the whole reaction with A.*”
Chapter 3 Figure 8 p. 655	**Claire**: „*Meine ersten Gedanken waren, dass ich auf jeden Fall erst die Mesomeriestruktur hinmale und da war ich mir aber in dem Moment nicht mehr ganz sicher, ob das* [Doppelbindung] *jetzt vom Sauerstoff runterklappt oder doch vom Ring nach oben klappt. Habe mich dann jetzt aber für den Sauerstoff entschieden, dass das runterklappt* […] *weil Brom, also hat da eine positive Ladung und damit eigentlich geschieht ein elektrophiler Angriff und dafür brauchen wir eh die negative Ladung, beziehungsweise dafür wäre ja gut, wenn eine negative Ladung am Ring wäre, damit das halt da gut angreifen kann.* […] *Und dann hatte ich mir*	**Claire**: “*My initial thoughts were that I definitely should first draw the resonance structure, but at that moment, I wasn't entirely sure anymore if it* [the double bond] *folds down from the oxygen or up from the ring. However, I have now decided on the oxygen folding down* […] *because bromine has a positive charge, indicating an electrophilic attack, and for that, we need a negative charge, or it would be good to have a negative charge on the ring so that it can attack effectively.* […] *Then, just to be sure, I drew the other form again to see if it would even make any sense. Just to check it myself, but I realized it doesn't make any sense; it cannot attack neither in the para nor the meta*

	sicherheitshalber die andere Form nochmal aufgezeichnet, um zu gucken, ob die denn überhaupt Sinn machen würde. Einfach um selber zu gucken, aber da habe ich gesehen, macht gar keinen Sinn, da kann das weder para noch meta angreifen und die positive Ladung ist da einfach nicht sinnvoll und bringt auch nicht viel. […] *Das war die Ringform, wo ich mir dann dachte, wenn hier das Brom angreift* [zeigt auf Struktur], *dann habe ich ja aus der vorherigen Position noch rechts und links Doppelbindungen* [zeigt auf das Produkt], *aber in meinem Produkt ist die Doppelbindung einmal oben und einmal beim Brom und da dachte ich, wie kriege ich die dahin, dass die dahinkommen?* […] *Generell optisch, einfach so, so von der Intuition her optisch finde ich, das macht einfach mehr Sinn, dass es para oder ortho angreift. Die Ladungen unterstützen meine Theorie.*“	*positions, and the positive charge doesn't make sense and doesn't contribute much.* […] *Regarding the ring form, I thought, if bromine attacks here* [points to a structure], *I would have double bonds on the right and left from the previous position* [refers to the depicted product], *but in my product, one double bond is above and one is near the bromine. I wondered, how can I get them to be there?* […] *In general, visually, from my intuition, I find it makes more sense that it attacks para or ortho. The charges support my theory.*”
Chapter 3 Figure 9 p. 656	**Jack**: „*Also, das ist eine Ketogruppe, Keto macht glaube ich, genau ortho oder para stabilisierend, aber in dem Fall* [in B] *ist das ja meta. Ok, also ich vermute, dass A mehr gebildet wird, aber das nur, weil auswendig gelernt hat, dass es diese Bindungen in ortho und para dirigieren. Ok, aber das kann man ja mal nachweisen, indem wir die einfach mal angreifen lassen* […] *Minus M-Effekt auf jeden Fall, das heißt, die positive Ladung muss da hoch gebracht werden* […] *Das Einzige, was es kann mesomer ziehen, so, wenn wir die hochklappen* [bezieht sich auf Doppelbindung des Ketons] *habe ich negative Ladung da oben, aber die positive kriege ich ja nicht weg* […] *Ich will ja eigentlich Ladungen neutralisieren, deshalb habe ich, halte ich das eigentlich nicht für ein Möglichkeit gehalten irgendwie. Sehr irritierend.*“	**Jack**: “*So, this is a ketone group. I believe keto groups stabilize in the ortho or para positions, but in this case* [B], *it's in the meta position. Okay, so my assumption is that A will be formed more, but that's just because I've memorized that these bonds direct in ortho and para positions. Okay, but we can verify that by letting them attack it.* […] *Minus M-effect, definitely, which means the positive charge needs to be brought up* […] *The only thing it can do is resonance, so when we flip it up* [refers to the double bond in the ketone group], *I have negative charge up there, but I can't get rid of the positive charge* […] *I actually want to neutralize charges, so I didn't really consider that as an option somehow. Very irritating.*”
Chapter 3 Figure 10 p. 657	**Claire**: „*Ich denke, dass durch den plus M- und minus I-Effekt, die positive Ladung bei der ersten Variante besser stabilisiert wird* […] *dass je instabiler, je besser, also je besser mesomer stabilisiert eine Verbindung ist, desto stabiler ist sie und desto weniger reaktiv ist sie.* […] *Weil je besser stabilisiert sie ist, deswegen eher würde sich hier die Ladung weiter verteilen* [zeigt auf reaktives Zentrum], *und wir brauchen ja hier die positive Ladung, damit das OH minus da angreift.* […] *Also der einzige Unterschied in den beiden Ausgangsverbindungen, das ist ja*	**Claire**: “*I think that due to the plus M- and minus I-effects, the positive charge in the first reaction is better stabilized, and* […] *the more unstable, the better; the more a compound is stabilized by resonance, the more stable and less reactive it is.* […] *Because the better it's stabilized, the more the charge would distribute here* [pointing to the reactive center], *and we need the positive charge there so that the OH minus attacks.* […] *So, the only difference between the two starting compounds is actually the ether. Therefore, I thought about what the difference in the reaction could be caused by*

	eigentlich die Gruppe, also der Ether. Und deswegen habe ich mir überlegt, was denn da der Unterschied oder was der Unterschied in der Reaktion ausmachen könnte durch die Ethergruppe. Die oder die Position, wo unser Nucleophil ja angreift ist ja dieselbe, daran ändert sich ja nichts, das heißt, das kann ja nur sein, dass da die Angriffsstärke irgendwie durch die Estergruppe verringert oder stärker wird. Und deswegen habe ich mir gedacht, dass es damit zusammenhängen könnte, dass die Gruppe je nachdem, wo die positive Ladung dann halt ist, die besser stabilisiert oder nicht. Und deswegen halt habe ich mir die Stabilitäten angeguckt, um halt herauszufinden, was passiert denn überhaupt mit der Ladung. […] *Also ich habe halt als erstes geguckt, wo denn unser Hydroxidion überhaupt angreifen würde.* […] *Einfach, um selber so herauszufinden, also einfach, um einen Überblick zu haben, wo greift es an? Oder was könnte da überhaupt passieren? Was muss passieren, damit es da angreifen kann?*“	*the ether group. The position where our nucleophile attacks is the same, that doesn't change, which means the attacking strength can only be influenced by the ether group, making it either decrease or increase. That's why I thought it could be related to how well the group stabilizes the positive charge, depending on its location. So, I looked at the stabilities to figure out what happens to the charge* […] *First, I checked where our hydroxide ion would attack.* […] *Just to have an overview of where it attacks or what could happen there. What needs to happen for it to attack there?*”
Chapter 3 Figure 11 p. 658	**Charlotte**: „*Ich habe hier* [Produkt B] *erstmal gedacht, dass das richtig wäre, weil es kompakter ist und der Einfluss auf die positive* [Ladung]*, näher ist, also sterisch jetzt einfach. Und dann dachte ich, okay, es hat einen negativen I-Effekt* […] *würde ich A sagen, weil das* [zeigt auf mesomere Grenzformel] *habe ich nicht hinbekommen und das funktioniert irgendwie, sage ich jetzt mal, deswegen sage ich A* […] *weil der Teil, also der negativ polare Teil* [zeigt auf Sauerstoffatom in Produkt A] *entfernter zum Carbeniumion liegt, als bei B und der positive Einfluss der C Doppelbindung* [zeigt auf Doppelbindung in Produkt A] *auf das Carbeniumion, also der positive I-Effekt dadurch irgendwie sich entfalten kann, oder eine Wirkung hat und damit das Carbeniumion stabilisiert* […] *weil meine Begründung beruht ja eigentlich nur auf den I-Effekten und der Polarität im Molekül, aber ich habe die mesomeren Formeln jetzt auch nicht in meiner Argumentation bezogen.* […] *Da bin ich mir halt auch, also da kann ich halt auch nichts dazu sagen, weil selbst das, was ich richtig gezeichnet habe, gefühlstechnisch, ich weiß nicht was mir das jetzt sagt* […] *weil ja jetzt entsteht eine positive Ladung am O* [bezieht sich auf mesomere Grenzformel] *ich weiß nicht, ob das gut ist?*“	**Charlotte**: “*I initially thought that this* [Product B] *would be correct because it is more compact, and the influence on the positive* [charge] *is closer, so, sterically. And then I thought, okay, it has a negative I-effect.* [...] *I would say A because this* [refers to resonance structure]*, it did not work out, and this somehow works, that's why I say A* [...] *because the part with negative polarity* [pointing to oxygen atom in product A]*, is farther away from the carbocation than in B, and the positive influence of the C double bond* [pointing to the double bond in product A] *on the carbocation, the positive I-effect can somehow unfold, thereby stabilizing the carbocation.* [...] *Because my reasoning is actually based only on the I-effects and the polarity in the molecule, but I haven't considered the resonance structures in my argumentation.* [...] *I am not sure, I can't say anything about that because even what I have correctly drawn, I don't know what that tells me now.* [...] *now, a positive charge at O* [refers to resonance structure]*, I don't know if that is good?*”

Chapter 3 Figure 12 p. 659	**Lucas**: „*Ja, deswegen würde ich sagen, der Sauerstoff da* [bezieht sich auf Methoxy-Gruppe] *ist nicht so in die Mesomerie eingebunden wie der andere, und deswegen ist eben die mesomere Grenzstruktur, bei der hier eine positive Ladung vorliegt im Fall A besser stabilisiert als in Fall B. Und deswegen würde ich sagen, in Verbindung A erfolgt der Angriff bevorzugt.* […] *Lass mich noch kurz überlegen.* […] *Ja, also ich habe ja wie gesagt bei beiden die positiven Ladungen.* […] *So, und dann ist ab dem Punkt, wo das hier hochklappt und ich hier die positive Ladung habe* [zeigt auf aromatischen Rest]*, kann ja was anderes passieren. Heißt, diese positive Ladung hier kann stabilisiert werden durch einmal das Elektronenpaar von hier und einmal durch das, also von hier. So. Genau, und hier ist es halt nur durch dieses Elektronenpaar.* […] *Weil das vom Sauerstoff unten nicht hochklappen kann.* […] *Ja, also ich meine, bevorzugt findet der Angriff ja statt, wenn das Ganze im Grunde so aussieht: Ich habe hier eine positive Ladung* [bezieht sich auf Kohlenstoffatom an der Estergruppe]. […] *Also ich habe, klar, in dem Fall jetzt mehr mesomere Grenzstrukturen* [bezieht sich auf Reaktion A]*, aber die im Grunde auf dem Zustand basieren, dass eben hier die Doppelbindung ist* [bezieht sich auf Kohlenstoffatom an der Estergruppe] *und eben keine positive Ladung an dem Kohlenstoffatom. Was ja eigentlich ideal wäre für den Angriff von der OH-Minus-Gruppe. Ja, doch, ich glaube, ich würde* [lachend] *erst mal meine Lösung hier umentscheiden, weil in dem Fall, wo ich hier das Elektronenpaar noch mit eingebunden habe* [zeigt auf Sauerstoffatom in der Methoxygruppe]*, ist die positive Ladung ja noch mal weiter übers Molekül verteilt als im anderen Fall. Und ich will die aber eigentlich nicht weiter übers Molekül verteilt haben, ich will die ja, genau, hier haben* [bezieht sich auf Kohlenstoffatom an der Estergruppe in Reaktion B]*, wo dann eben der Angriff stattfinden soll nucleophil.*“	**Lucas**: “*Yes, that's why I would say the oxygen here* [refers to the methoxy group] *is not as involved in resonance as the other one, and that's why the resonance structure with a positive charge present is better stabilized in case A than in case B. So, I would say in compound A, the attack is preferred.* [...] *Let me think for a moment.* [...] *Yes, as I said, in both cases, there are positive charges.* […] *So, from the point where this moves up and I have the positive charge here* [points to the aromatic ring]*, something else can happen. This means that this positive charge here can be stabilized by the lone pair from here and also from here. Yes, and here, it's only through this lone pair.* [...] *Because the one from the oxygen below cannot move up.* [...] *Yes, so I mean, the attack is preferred when the whole thing looks like this: I have a positive charge here* [refers to the carbon atom of the ester group]. [...] *Well, in this case, I have more resonance structures* [refers to reaction A]*, but they are mostly based on the state where the double bond is here* [refers to the carbon atom of the ester group] *and there is no positive charge on the carbon atom. Which would actually be ideal for the attack from the OH-minus group. Yes, I think I would* [laughing] *reconsider my solution here because, in the case where I involved the lone pair here* [refers to the oxygen atom of the methoxy group]*, the positive charge is spread further over the molecule than in the other case. And I don't actually want it spread further over the molecule; I want it right here* [points to the carbon atom of the ester group in product B]*, where the nucleophilic attack should occur.*”
Chapter 3 Figure 13 p. 660	**Emily**: „*Ich habe halt immer geschaut, wohin die positive Ladung sich bewegt. Ja, und dann habe ich überlegt, praktisch, wo es dann eigentlich mehr Grenzstrukturen gibt und da ist es dann stabiler und da würde das dann bevorzugt gebildet werden.* […] *Also, also das Plus, das wandert ja, und wenn es dann mehr Grenzformeln gibt, also da, wo es mehr gibt, dann wird das*	**Emily**: “*I always looked where the positive charge moves to. And then I thought, practically, if there are actually more resonance structures, and it would be more stable there, and that's where it would be preferentially formed.* [...] *So, yeah, the plus, it moves, and if there are more resonance structures. So, if there are more, it will be formed preferentially.* [...] *So, it* [the

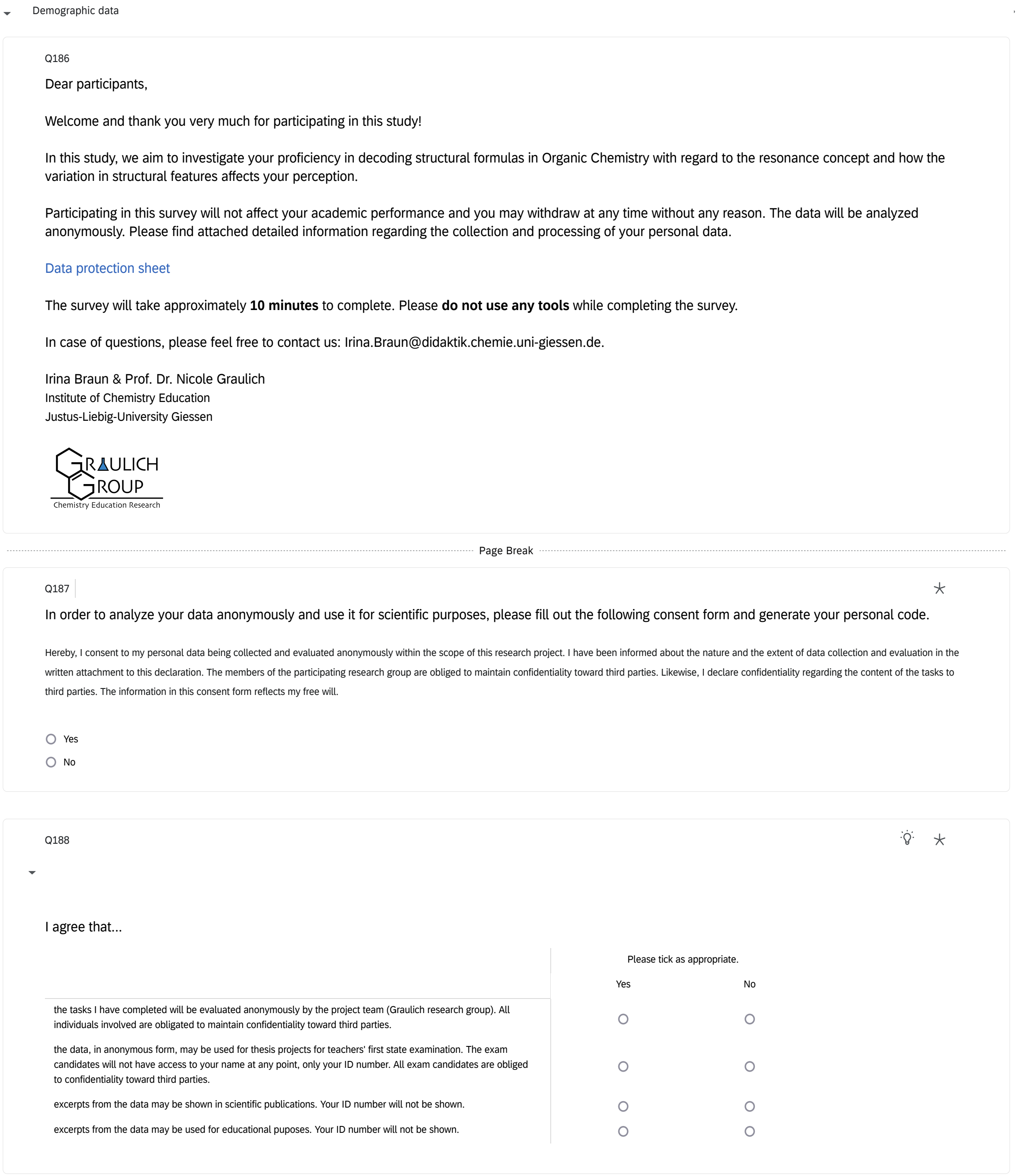
	bevorzugter gebildet. […] *Also der* [Substituent] *hat dann ein, einen M-Effekt und, also das hängt praktisch von dem Substituenten hier ab, wo es dann im Endeffekt angreift, also durch den Substituenten das, also, weil die positive Ladung daneben ist, gibt es ja diese weitere Grenzformel, weil der dann auch mit einbezogen werden kann.*“	substituent] *has a M-effect, and, well, it depends practically on the substituent here, where it attacks in the end, so, well, because here, the positive charge is next to the substituent, it can be also included, thus, there is this additional resonance structure.*”
Chapter 3 Figure 13 p. 660	**Alina**: „*Also ich weiß, dass bei der elektrophilen Substitution die Stellung am aromatischen Ring durch den ersten Substituenten beeinflusst wird, und zwar je nachdem, an welcher Stelle im mesomeren System eben Ladungen auftreten. Dementsprechend weiß ich, das ist ein Minus M-Substituenten, den erkenne ich an der Doppelbindung in Alpha-Stellung. Also zeichne ich das Ausgangsmolekül und begründe mit dem. Also habe ich das Typische von einem Minus M-Substituenten gemacht, habe das Elektronpaar heraus klappen lassen.* […] *Dadurch entsteht die positive Ladung an Kohlenstoffatomen, weil denen ein Elektron weggezogen wurde* [zeigt auf Sauerstoffatom]. *Eine negative Ladung weniger, heißt eine positive bleibt übrig. Für die erste Grenzstruktur habe ich dann die anderen zwei Elektronen einfach da gelassen, wo sie sind. Und dann habe ich im mesomeren System gearbeitet. Dann weiß ich, ich will die Ladung hier beseitigen* [zeigt auf Kohlenstoffatom]. […] *Dadurch entsteht die zweite positive Ladung und Ortho-Position und die kann ich wieder beseitigen, indem ich eben oben die Doppelbindung wieder runter klappe* […]. *Und da das oben nur eine Carbonylgruppe ist, gibt es auch oben keine mesomeren Grenzstrukturen mehr, die man vergessen könnte. Also bin ich durch.* […] *Ich habe Ladungen generiert im Ring und* […] *ich habe mein Br Plus. Das ist ein Plus und ein Plus. Ich weiß, gleich geladene Ladungen stoßen sich ab. Das heißt, ich habe also drei Positionen, die einfach blockiert sind.*“	**Alina**: “*I know that in electrophilic aromatic substitutions, the position is influenced by the first substituent, depending on where in the conjugated system the charges are. I know this is a minus M-substituent, I recognize it by the double bond in the alpha position. So, I draw the starting molecule and justify it with that. I've done the typical thing for a minus M-substituent, the lone pair shifts out.* […] *As a result, positive charges are on carbon atoms because an electron was pulled away* [points to oxygen atom] *from them. One negative charge less means one positive charge remains. For the first resonance structure, the two electrons remain at their position. Then I worked within the conjugated system. I want to eliminate the charge here* [pointing to carbon atom]. [...] *Therefore, the second positive charge gets to the ortho position, and I can eliminate it again by folding down the double bond from above.* […] *And since there's only a carbonyl group above, there are no more additional resonance structures up there that I could forget. So, I'm done.* [...] *I've generated charges in the ring, and* […] *I have my Br plus. That's a plus and a plus. I know that like-charged charges repel each other. That means I have three positions that are simply blocked.*”

6.1.8 Overview of Students’ Pseudonyms Used in Chapters 2 and 3

Student	**Chapter 2**	**Chapter 3**
1	Amanda	Amanda
2	Nora	Nora
3	Alina	Alina
4	Catherine	Tiffany
5	Audrey	Audrey
6	Anna	Anna
7	Paula	Claire
8	Liam	Liam
9	Mary	Mary
10	Oliver	Oliver
11	Phil	Lucas
12	Ethan	Ethan
13	Tom	Tom
14	Jack	Jack
15	Pascal	Pascal
16	Elizabeth	Charlotte
17	Luke	Louis
18	*excluded*	Emily
19	Nina	Paula
20	Lily	Lily
21	Benjamin	Benjamin

6.2 Supporting Information Study 2

6.2.1 Original Survey Designed and Used with *Qualtrics* Including the Consent Form and Demographic Questionnaire



Demographic data

Q186

Dear participants,

Welcome and thank you very much for participating in this study!

In this study, we aim to investigate your proficiency in decoding structural formulas in Organic Chemistry with regard to the resonance concept and how the variation in structural features affects your perception.

Participating in this survey will not affect your academic performance and you may withdraw at any time without any reason. The data will be analyzed anonymously. Please find attached detailed information regarding the collection and processing of your personal data.

Data protection sheet

The survey will take approximately **10 minutes** to complete. Please **do not use any tools** while completing the survey.

In case of questions, please feel free to contact us: Irina.Braun@didaktik.chemie.uni-giessen.de.

Irina Braun & Prof. Dr. Nicole Graulich
Institute of Chemistry Education
Justus-Liebig-University Giessen

GRAULICH GROUP
Chemistry Education Research

Page Break

Q187 *

In order to analyze your data anonymously and use it for scientific purposes, please fill out the following consent form and generate your personal code.

Hereby, I consent to my personal data being collected and evaluated anonymously within the scope of this research project. I have been informed about the nature and the extent of data collection and evaluation in the written attachment to this declaration. The members of the participating research group are obliged to maintain confidentiality toward third parties. Likewise, I declare confidentiality regarding the content of the tasks to third parties. The information in this consent form reflects my free will.

○ Yes
○ No

Q188 *

I agree that...

	Please tick as appropriate. Yes	 No
the tasks I have completed will be evaluated anonymously by the project team (Graulich research group). All individuals involved are obligated to maintain confidentiality toward third parties.	○	○
the data, in anonymous form, may be used for thesis projects for teachers' first state examination. The exam candidates will not have access to your name at any point, only your ID number. All exam candidates are obliged to confidentiality toward third parties.	○	○
excerpts from the data may be shown in scientific publications. Your ID number will not be shown.	○	○
excerpts from the data may be used for educational puposes. Your ID number will not be shown.	○	○

Frage 1

Which gender do you identify with?

○ Female
○ Male
○ Diverse
○ Prefer not to say

Frage 2

Display this question

If Um Ihre Daten anonymisiert auswerten und für wissenschaftliche Zwecke nutzen zu können, füllen Sie b Yes Is Selected

How old are you?

Page Break

Frage 4

What is your field of study in Chemistry?

○ Chemistry (please specify if major or minor)
○ Food Chemistry
○ Materials Science
○ Teaching degree (Chemistry)
○ Other (please enter):

Page Break

Q200

How far are you in your studies?

○ First semester
○ Second semester
○ Third semester
○ Fourth semester
○ Fifth semester
○ Sixth semester
○ Seventh semester
○ Eighth Semester
○ Ninth semester
○ Tenth semester
○ Other (please enter):

Self-assessment of prior knowledge

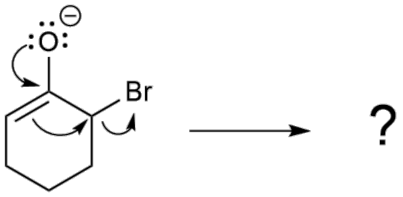
Please, self-assess your competencies in chemistry in terms of the following aspects.

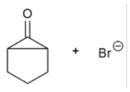
	I feel confident about it.	I feel rather confident about it.	I feel somewhat confident about it.	I feel rather unconfident about it.	I feel unconfident about it.
I can draw curved electron arrows (*e.g.*, in organic mechanisms) correctly.	○	○	○	○	○
I can identify whether resonance is possible in a molecule.	○	○	○	○	○
I can assess the thermodynamic stability of molecules based on their structural formulas.	○	○	○	○	○
I can define the resonance concept.	○	○	○	○	○
I can determine the hybridization of atoms.	○	○	○	○	○
I can estimate the geometry in molecules based on hybridization.	○	○	○	○	○
I can determine whether a molecule is aromatic.	○	○	○	○	○
I can assess the influence of electron delocalization on the stability of a molecule.	○	○	○	○	○
I can estimate the acid or base strength of molecules.	○	○	○	○	○
I can assess the influence of electron delocalization on the reactivity of a compound (*e.g.*, determining electrophilic sites).	○	○	○	○	○

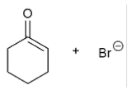
Prior knowledge tasks

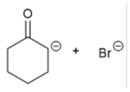
V1

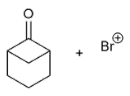
Select the correct product resulting from the depicted reaction step.



○ 

○ 

○ 

○ 

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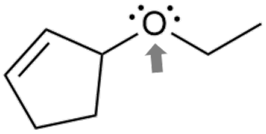
V2

Determine the hybridization of the labeled atom.



○ sp

○ sp2

○ sp3

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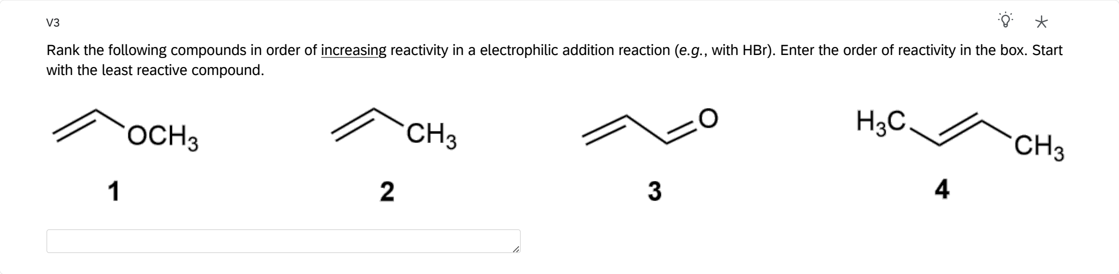

V3

Rank the following compounds in order of increasing reactivity in a electrophilic addition reaction (*e.g.*, with HBr). Enter the order of reactivity in the box. Start with the least reactive compound.

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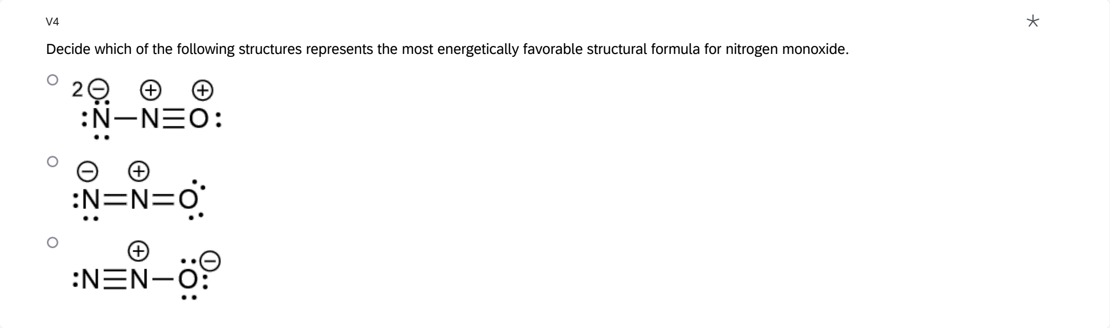

V4

Decide which of the following structures represents the most energetically favorable structural formula for nitrogen monoxide.

○

○

○

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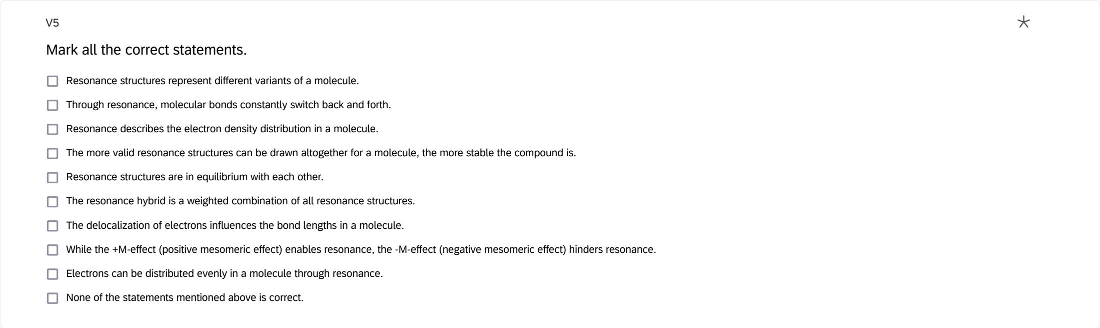
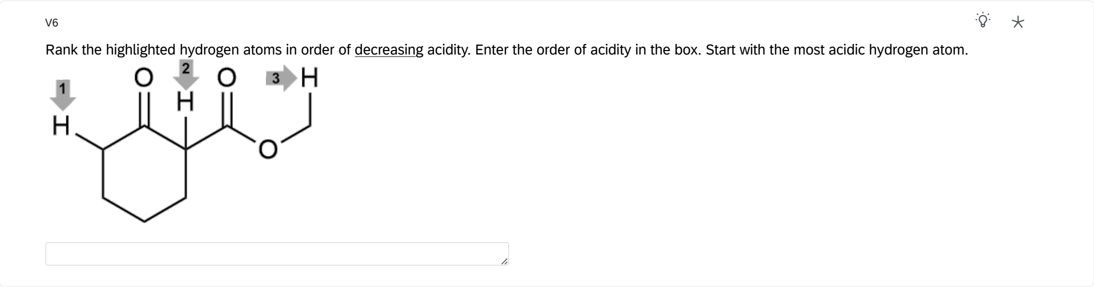


V5

Mark all the correct statements.

☐ Resonance structures represent different variants of a molecule.
☐ Through resonance, molecular bonds constantly switch back and forth.
☐ Resonance describes the electron density distribution in a molecule.
☐ The more valid resonance structures can be drawn altogether for a molecule, the more stable the compound is.
☐ Resonance structures are in equilibrium with each other.
☐ The resonance hybrid is a weighted combination of all resonance structures.
☐ The delocalization of electrons influences the bond lengths in a molecule.
☐ While the +M-effect (positive mesomeric effect) enables resonance, the -M-effect (negative mesomeric effect) hinders resonance.
☐ Electrons can be distributed evenly in a molecule through resonance.
☐ None of the statements mentioned above is correct.

Page Break



V6

Rank the highlighted hydrogen atoms in order of decreasing acidity. Enter the order of acidity in the box. Start with the most acidic hydrogen atom.

Page Break

V7

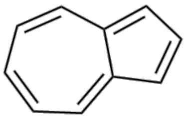
Indicate the geometry of the following molecule.

○ Trigonal pyramidal
○ Trigonal planar
○ Bent
○ Linear

Page Break

V8

Indicate whether the following planar molecule is an aromatic compound.



○ Yes

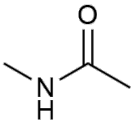
○ Unsure

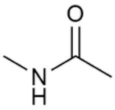
○ No

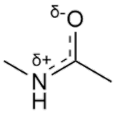
Page Break

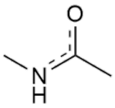
V9

Which of the following representations of the resonance hybrid best represents the electron distribution in the depicted carboxylic acid amide?



○ 

○ 

○ 

○ None of these options is correct.

Page Break

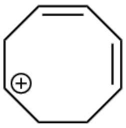
Q20

In the following, you will be shown 37 different molecules. For all molecules, the following task applies:

Decide, as intuitively as possible, whether the <u>charge</u> in the molecules can be thermodynamically stabilized via resonance.

Struktur 3

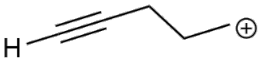
S3



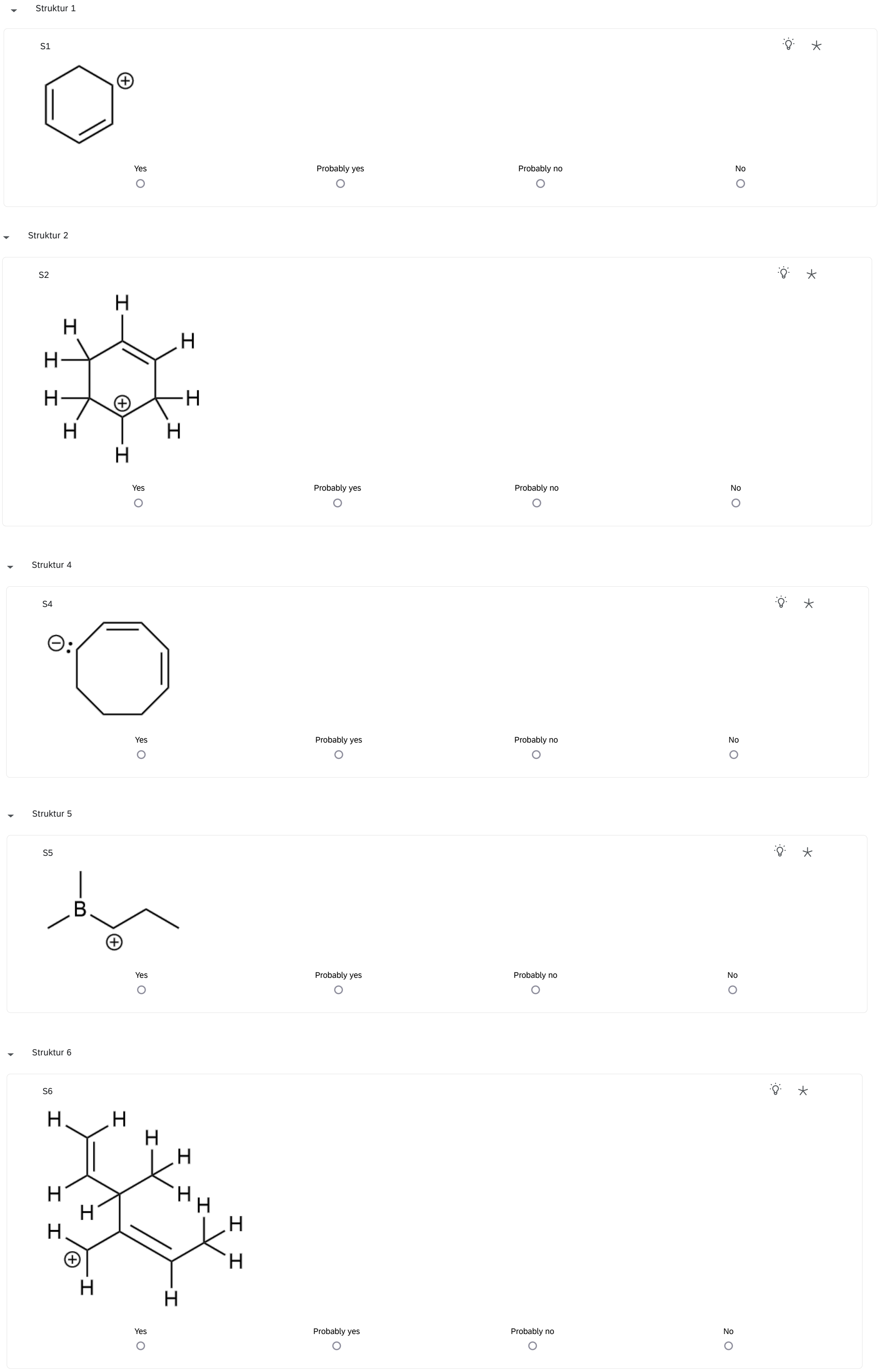
Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 14

S14



Yes	Probably yes	Probably no	No
○	○	○	○



Struktur 1

S1

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 2

S2

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 4

S4

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 5

S5

Yes	Probably yes	Probably no	No
○	○	○	○

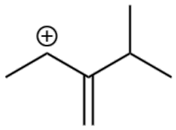
Struktur 6

S6

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 7

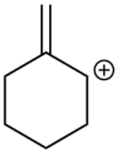
S7



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 8

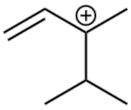
S8



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 11

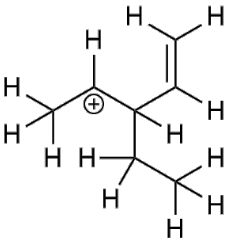
S11



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 12

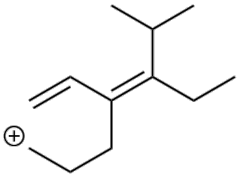
S12



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 13

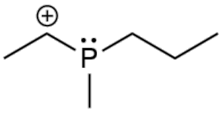
S13



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 18

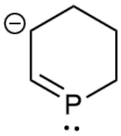
S18



Yes	Probably yes	Probaly no	No
○	○	○	○

Struktur 19

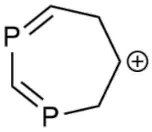
S19



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 20

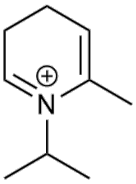
S20



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 25

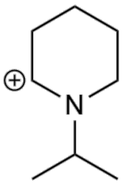
S25



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 26

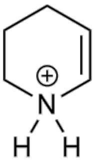
S26



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 27

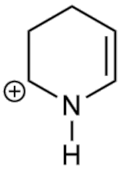
S27



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 28

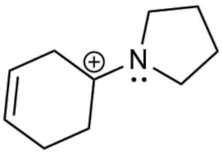
S28



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 29

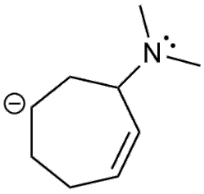
S29



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 30

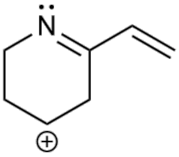
S30



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 31

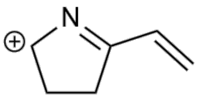
S31



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 32

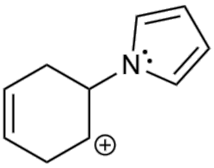
S32



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 33

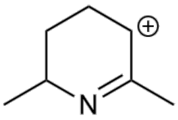
S33



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 34

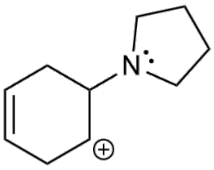
S34



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 35

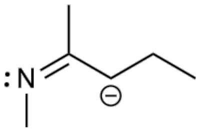
S35



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 36

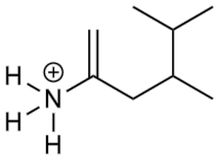
S36



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 37

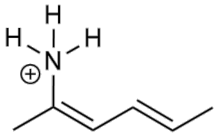
S37



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 38

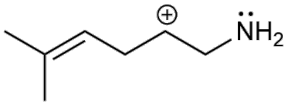
S38



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 40

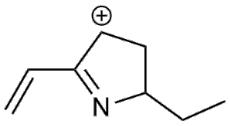
S40



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 41

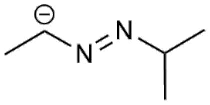
S41



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 42

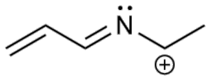
S42



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 43

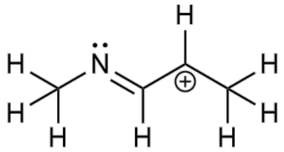
S43



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 44

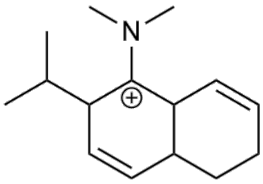
S44



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 45

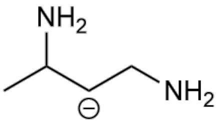
S45



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 46

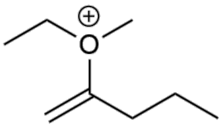
S46



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 47

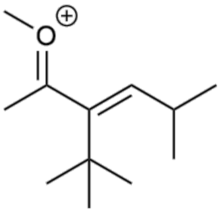
S47



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 48

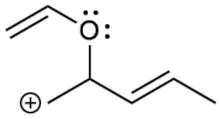
S48



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 49

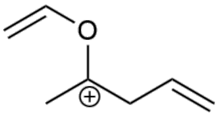
S49



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 50

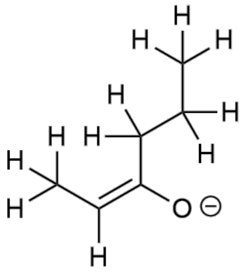
S50



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 51

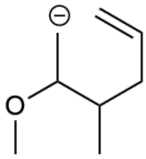
S51



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 52

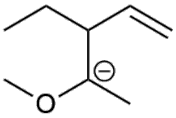
S52



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 53

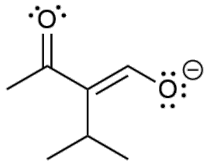
S53



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 54

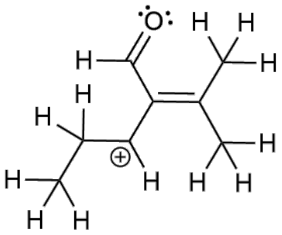
S54



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 55

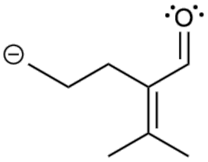
S55



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 56

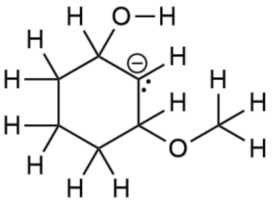
S56



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 57

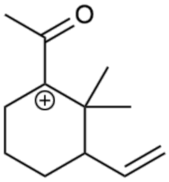
S57



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 58

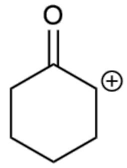
S58



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 59

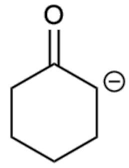
S59



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 60

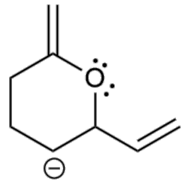
S60



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 61

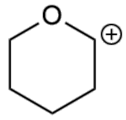
S61



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 62

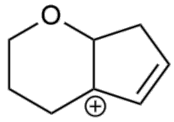
S62



Yes	Probably yes	Probably no	No
○	○	○	○

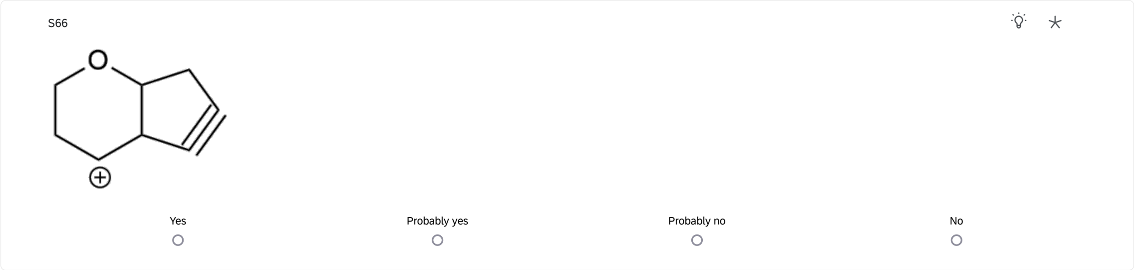
Struktur 64

S64



Yes	Probably yes	Probably no	No
○	○	○	○

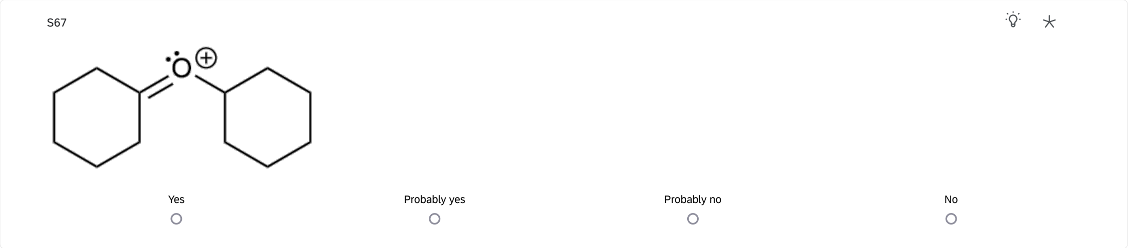
Struktur 66



S66

Yes	Probably yes	Probably no	No
○	○	○	○

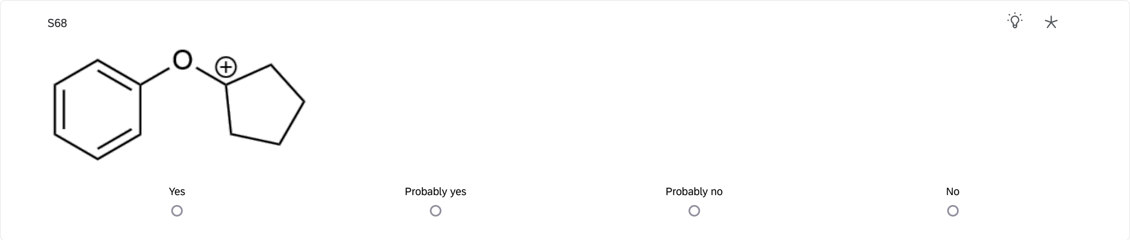
Struktur 67



S67

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 68



S68

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 69

S69

Yes	Probably yes	Probably no	No
○	○	○	○

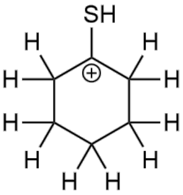
Struktur 70

S70

Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 71

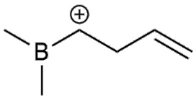
S71



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 72

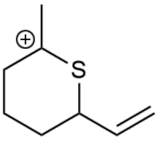
S72



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 73

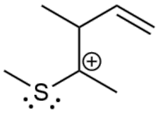
S73



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 74

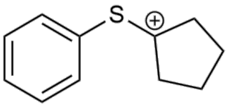
S74



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 75

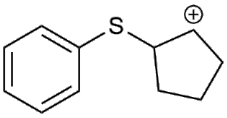
S75



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 76

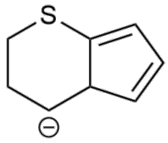
S76



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 77

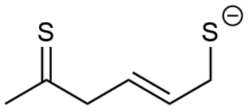
S77



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 78

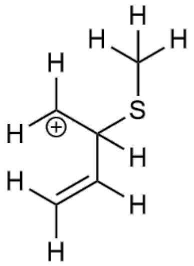
S78



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 79

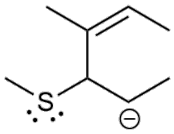
S79



Yes	Probably yes	Probably no	No
○	○	○	○

Strukur 80

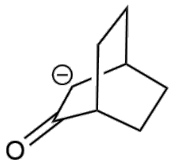
S80



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 81

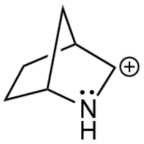
S81



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 83

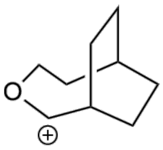
S83 *



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 86

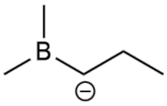
S86 *



Yes	Probably yes	Probably no	No
○	○	○	○

Struktur 88

S88 *



Yes	Probably yes	Probably no	No
○	○	○	○

Perceived cognitive load and feedback

Block 81

Q210

Regarding your decisions on resonance stabilization in the second part of this survey, please indicate the extent to which you agree with the following statements *(1 = strongly disagree, 7 = strongly agree)*.

	1	2	3	4	5	6	7
Overall, solving the task (*i.e.*, recognizing resonance in the different molecules) was difficult for me.	○	○	○	○	○	○	○
I am confident that I have correctly solved the tasks.	○	○	○	○	○	○	○
I put much effort into solving the task.	○	○	○	○	○	○	○
The molecules were very complex.	○	○	○	○	○	○	○
The problem-solving process was very complex.	○	○	○	○	○	○	○
The display of the molecules was inconvenient for identifying resonance.	○	○	○	○	○	○	○
It was exhausting to find the important information within the molecules.	○	○	○	○	○	○	○

Block 80

Q201

Did your task solving approach change during the survey completion? If yes, please describe.

Q202

Do you have any additional comments, suggestions, or feedback?

Block 78

Q211

You reached the end of the survey. Please take a screen shot of this completion page. You can upload the screen shot in your online assignment to earn points.

Here is your ID number for this survey: **${e://Field/Random%20ID}**

End of Survey

We thank you for your time spent taking this survey.

Your response has been recorded.

6.2.2 Items Included in the Cluster Analysis in Chapter 4

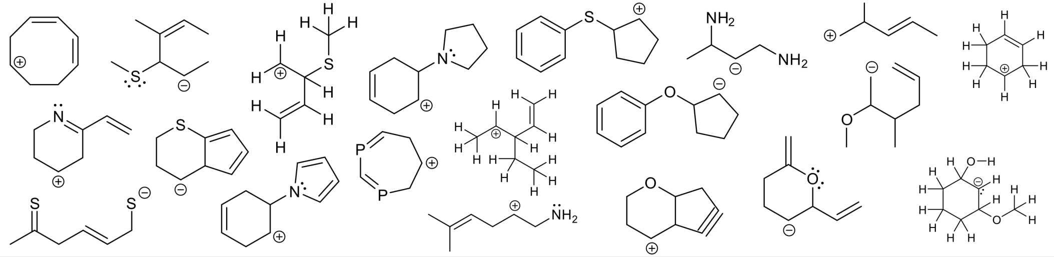
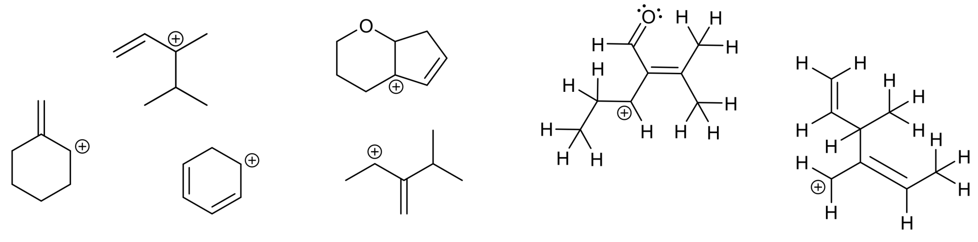
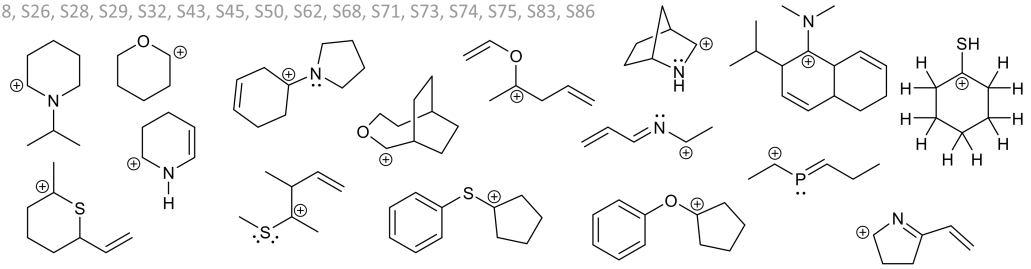
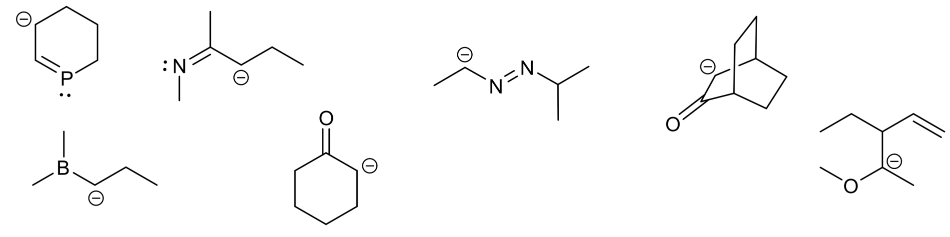
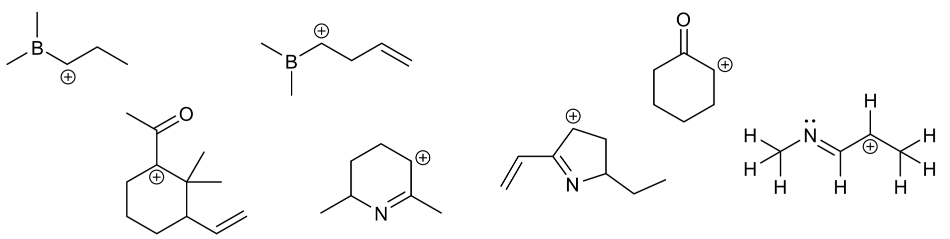
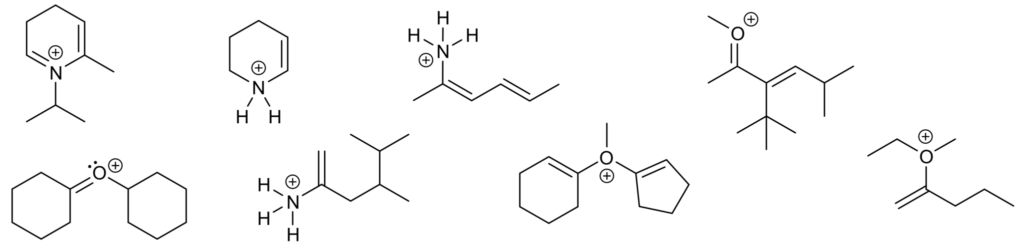
β-position of charge (20 items)	S2, S3, S12, S20, S31, S33, S35, S40, S46, S49, S52, S57, S61, S66, S69, S76, S77, S78, S79, S80 
Carbon atoms & positive charge (7 items)	S1, S6, S7, S8, S11, S55, S64 
Hetero atom & positive charge (16 items)	S18, S26, S28, S29, S32, S43, S45, S50, S62, S68, S71, S73, S74, S75, S83, S86 
Hetero atom & negative charge (7 items)	S19, S36, S42, S53, S60, S81, S88 
Hetero atom & positive charge & implicit considerations (7 items)	S5, S34, S41, S44, S58, S59, S72 
Positive charge on hetero atom (8 items)	S25, S27, S37, S38, S47, S48, S67, S70 

Figure 43. Overview of the items included in the quantitative data analysis presented in Chapter 4.

6.2.3 Items Included in the Quantitative Data Analysis in Chapter 5

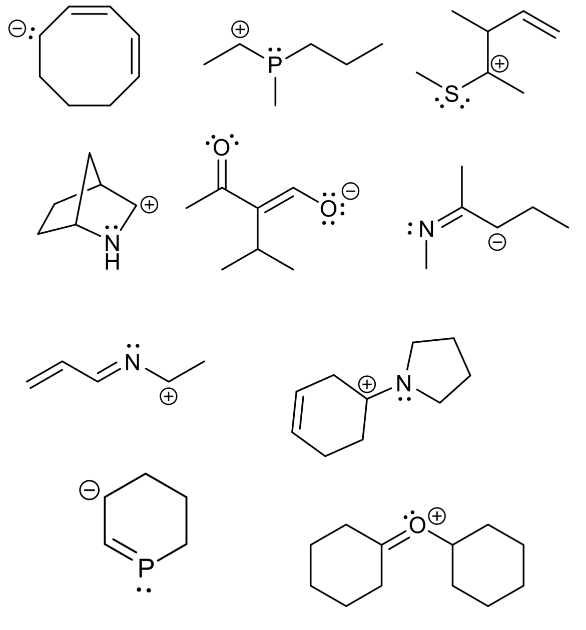
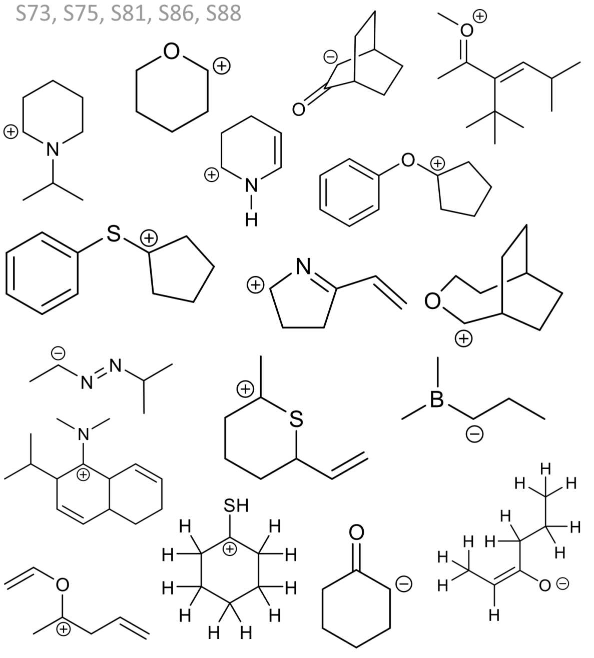
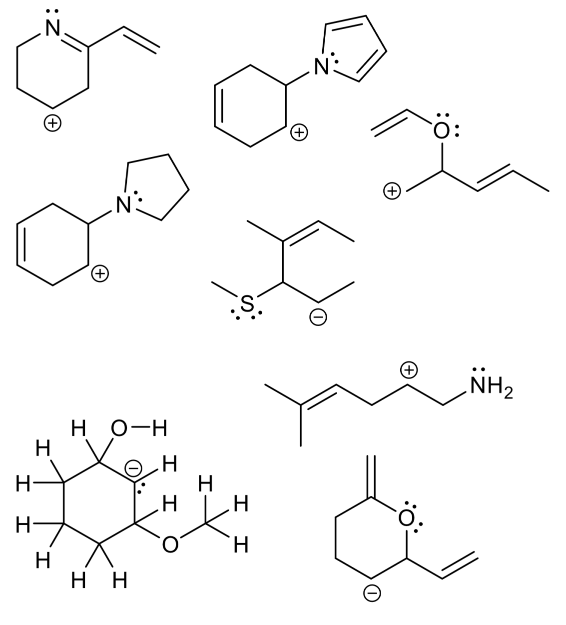
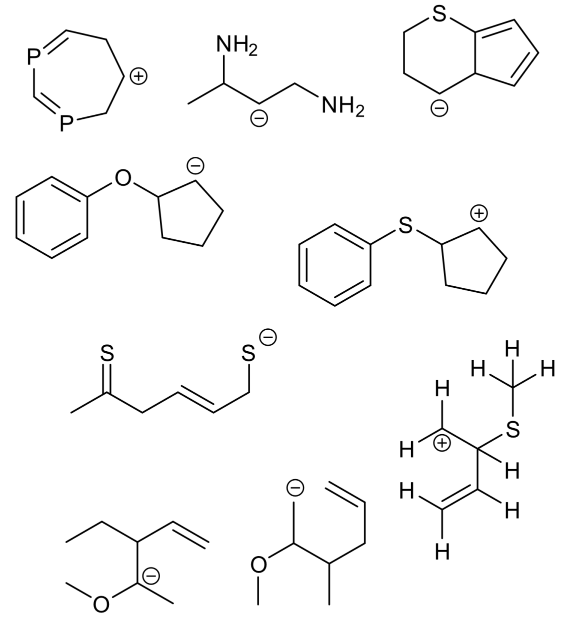
Indication of **l**one **p**airs **w**ith possibility of **r**esonance stabilization **LPwR** (10 items)	**N**o Indication of **l**one **p**airs **w**ith possibility of **r**esonance stabilization **nLPwR** (17 items)
S4, S18, S19, S29, S36, S43, S54, S67, S74, S83 	S26, S28, S32, S42, S45, S48, S50, S51, S60, S62, S68, S71, S73, S75, S81, S86, S88 
Indication of **l**one **p**airs **w**ith **n**o possibility of **r**esonance stabilization **LPwnR** (8 items)	**N**o Indication of **l**one **p**airs **w**ith **n**o possibility of **r**esonance stabilization **nLPwnR** (9 items)
S31, S33, S35, S40, S49, S57, S61, S80 	S20, S46, S52, S53, S69, S76, S77, S78, S79 

Figure 44. Overview of the items included in the quantitative data analysis presented in Chapter 5.

7. Acknowledgements

Abschließend möchte ich mich herzlich bei allen bedanken, die mich während meiner Promotion begleitet, unterstützt und die letzten Jahre so zu einer bereichernden und wertvollen Zeit gemacht haben.

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Ich danke euch von Herzen für die gemeinsame Zeit in der DC. Ob auf AG-Ausflügen, auf Konferenzen oder in den Mittagspausen – wir haben viel gelacht, diskutiert, uns wissenschaftlich ausgetauscht und eine tolle Zeit gehabt. Ich konnte immer auf euch und eure Unterstützung zählen. Ihr seid wirklich tolle Kolleg:innen und werdet mir fehlen.

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Den Studierenden, die an meinen Forschungsstudien teilgenommen haben

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Ich erkläre: Ich habe die vorgelegte Dissertation selbstständig und ohne unerlaubte fremde Hilfe und nur mit den Hilfen angefertigt, die ich in der Dissertation angegeben habe. Alle Textstellen, die wörtlich oder sinngemäß aus veröffentlichten Schriften entnommen sind, und alle Angaben, die auf mündlichen Auskünften beruhen, sind als solche kenntlich gemacht. Ich stimme einer evtl. Überprüfung meiner Dissertation durch eine Antiplagiat-Software zu. Bei den von mir durchgeführten und in der Dissertation erwähnten Untersuchungen habe ich die Grundsätze guter wissenschaftlicher Praxis, wie sie in der „Satzung der Justus-Liebig-Universität Gießen zur Sicherung guter wissenschaftlicher Praxis“ niedergelegt sind, eingehalten.

Ort, Datum	Unterschrift