Ten essential delocalization learning outcomes: How well are they achieved?

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Abstract

OBJECTIVE: Delocalization (resonance) is a concept in organic chemistry that influences the chemical reactivity, activity, structure, and physical properties of molecules. However, the concept has proven challenging for students. The goal of the present study was to investigate to what extent ten essential delocalization learning outcomes (LOs) were achieved by students, how students use and reason about delocalization as well as the connections between the LOs. The goal is to discover where and how students may be struggling when answering delocalization-related exam questions and uncover potential barriers to learning delocalization.

METHODS: We analyzed students' responses (N = 3787) on twelve exam questions related to seven of the ten LOs for the degree of achievement, common errors, and scientific reasoning.

RESULTS: The achievement on the LOs was variable. We report types of errors and strategies used, the errors are primarily related to drawing resonance structures or the resonance. Six key findings emerged from the analysis: (1) the majority of answers had few (<10%) representational errors (2) in an implicit question where delocalization or inductive effect concepts could be used to justify a response, half the students used delocalization concepts, (3) delocalization was used in 10–20% of answers when relevant but not prompted or required, (4) strategies that helped students reason with the representations (*i.e.*, drawing out electrons or expanding a structure) were correlated with higher achievement of the LOs, (5) students' reasoning aligned with course expectations, and (6) students who achieved later LOs typically (60–95%) also achieved LO1 and LO2 (*Identify that electron delocalization is relevant, Draw resonance structures*).

CONCLUSIONS: The findings have implications on how students achieve the LOs and suggest ways educators can better support learners with the tools to achieve the LOs.

IMPLICATIONS: The findings from this work could be used to design and evaluate new teaching techniques or materials, including scaffolding concepts. Further investigations could lead to a deeper understanding of students' mental models and thought processes related to delocalization concepts.

KEYWORDS
Chemical education research, Organic chemistry, Resonance theory, Testing/Assessment, Qualitative analysis, Quantitative analysis

Introduction

Delocalization, or resonance, is an integral part of organic chemistry, affecting the structure, properties, activity, and reactivity of molecules and is present in most medicines, biological structures, materials, and other compounds. Educators have described that the subject of delocalization is difficult to learn and that students struggle with the concept.[1] Empirical studies have revealed several incorrect ideas about resonance, such as the view that resonance structures are alternating or that resonance structures exist as an equilibrium,[2,3] or may not even think to use delocalization and would have to be prompted to do so.[4–7] One intervention focused on building and exploring the representations in delocalization (*i.e.*, hybrid and resonance structures) showed improvement in students' conceptions of the resonance structures.[8] Similarly, students taught by an instructor who focused on the meaning and limitations of resonance structures had a higher conceptual understanding of resonance compared to students in a course setting that emphasized identifying/drawing only.[3]

We recently proposed ten essential learning outcomes (LOs) about delocalization that a student should be able to demonstrate by the end of an organic chemistry course sequence (Figure 1), which address concepts of structure, properties, and reactivity.[9] The LOs are based on interviews with faculty, textbook analyses, analyses of the knowledge and skills required in future courses, and past literature.[10]

The goal of this research was to investigate how the ten essential delocalization learning outcomes have been achieved on summative examinations by students in Organic Chemistry I and II courses at one institution. In doing so, we sought to connect existing literature of students' difficulties learning resonance concepts described above with the clearly defined expectations (intended LOs), working with a larger sample size. We also investigated their strategies and explored the ways in which students may be struggling in their learning, to uncover potential barriers to learning more advanced delocalization or chemistry concepts.

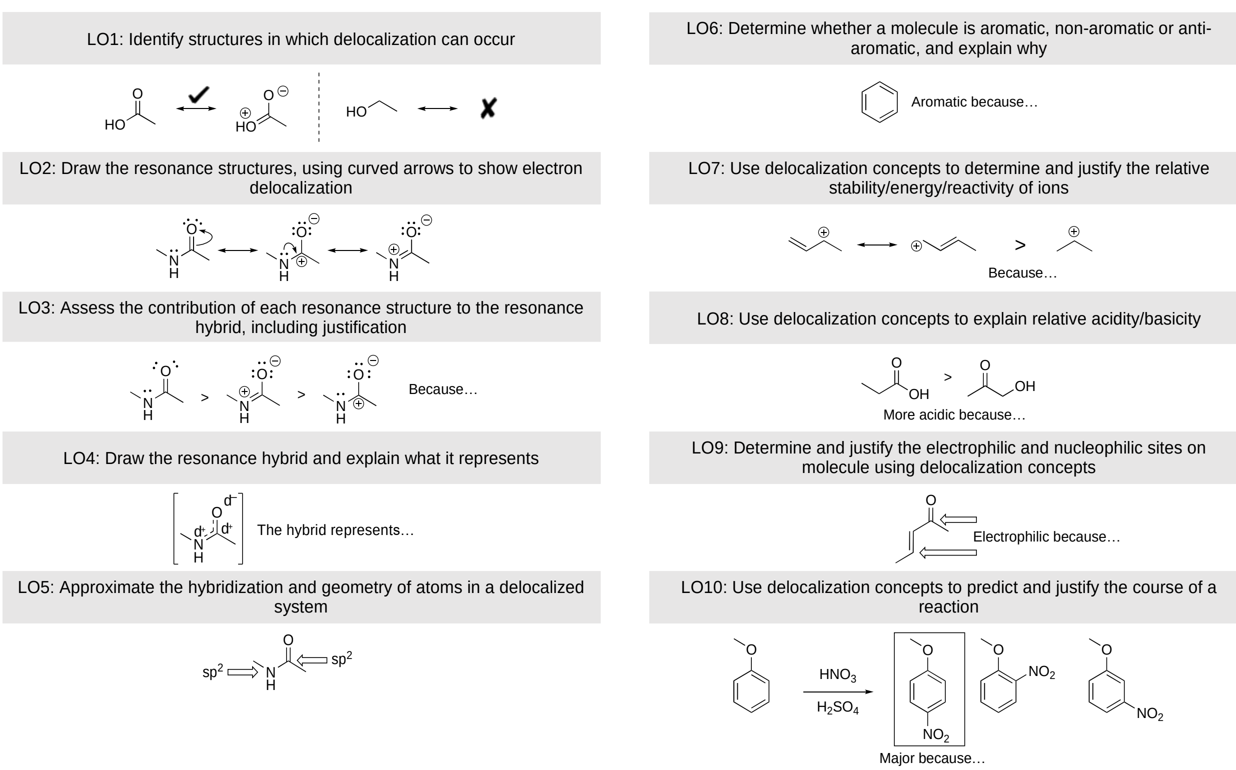


Figure 1. The ten essential LOs for delocalization. Reproduced from Carle and Flynn (2020).

Herein, we use the term delocalization to represent the concept, except when talking about resonance structures or the resonance hybrid, or when quoting question statements or students.

Research questions

We explored the following three research questions to achieve the project's goal:

RQ1: What is the relative achievement rate on the delocalization-related learning outcomes, as demonstrated by summative assessments?

RQ2: What are the common strategies and errors on delocalization-related exam responses?

RQ3: What is the sophistication of arguments for delocalization-related exam questions that require justification?

Theoretical frameworks

We used three frameworks: learning outcomes (described above), modern information processing theory, and a modes of reasoning framework.[11]

Modern information processing theory

This research is guided by modern information processing theory.[12–16] When faced with information, we process information in working memory, which is short-term and can only hold a limited amount of information. Memories are stored in long-term memory within an interconnected network, called schema, with links between the concepts.

Once in the long-term memory, information can be recalled if cued. A specific concept can activate a schema where all connected information can be accessed in the working memory. However, some information may not be recalled because of inference (*i.e.*, memories can interfere with the retrieval of other memories)[17] or poor encoding (*i.e.*, memories cannot be accessed because it was poorly encoded or the concept was not embedded in a schema).

People solve problems in the working memory by comparing information from their environment with information retrieved from their long-term memory. Four categories were identified as a potential barrier to solving a problem: (1) inability to recall, (2) inability to apply or understand, (3) poorly understood content, and (4) non-content-specific barriers.[18] The categories were common for learners memorizing declarative knowledge (*i.e.*, facts and data) without procedural knowledge (*i.e.*, skills and techniques).[19,20]

In this study, we examined delocalization concepts through the lens of IPT, specifically on how information is retrieved from long-term memory to use in working memory to solve a problem.

Reasoning framework

A scientific argument is used to persuade and justify a claim using evidence and reasoning.[21] The *claim* is the position being argued, or the principle that is trying to be conveyed. The *evidence* is the data that is used on which the claim is based.[22] The *warrant* is the relationship between the claim and the evidence and why the evidence backs the claim.

Several frameworks exist to qualify reasoning, such as Type I and Type II reasoning,[23,24] abstractness and abstraction,[25] rule-, case- and model-based reasoning,[26] modes of reasoning,[11] and mental models,[27] among others. Students may use a variety of reasoning techniques to answer questions.

To analyze the written responses of questions requiring a justification in this study, we used the modes of reasoning framework proposed by Sevian and Talanquer (2014). This framework has been used to determine modes of reasoning in several studies,[11,28–31] including similar studies that analyze students' written responses.[29–31] The framework described four modes of reasoning, two non-causal modes (descriptive and relational) and two causal modes (linear and multi-component).

In *descriptive* reasoning, concepts are provided without including causality.[11] For example, a statement simply stating "This proton is more acidic" would be considered descriptive because the statement simply states a fact, without any relationships or why that fact is true. *Relational* reasoning involves outlining a relationship between two concepts; however, the underlying reason for that relationship is not explained.[11] For example, a response stating: "The proton is more acidic because of resonance" would be considered relational because the response outlines the relationship between those two concepts without explaining why those concepts are used. Causal reasoning addresses the reasons **why** a phenomenon occurs[25,29,32–35] and implies a cause and effect relationship between components. In *linear causal* reasoning, the relationship between concepts is present and the reason is stated for why the concepts are important and how they relate to the claim.[11] For example, consider the statement "The proton is more acidic because resonance will better stabilize its conjugate base, and a more stable conjugate base means a stronger acid". In this statement, the reason is stated for why resonance is important—higher stability. In *multi-component causal* reasoning, multiple linear causal relationships are involved. This type of reasoning involves weighing multiple factors and explaining why each is important, often involving an analysis of why one factor is dominant.

Methods

Settings and course

Participants in the study were students in Organic Chemistry I or II courses at a large, research-intensive Canadian university. The University of Ottawa's Research Ethics Board approved this study as a secondary use of data (H03-15-18).

Organic Chemistry I is offered in the winter semester of students' first year of studies, and Organic Chemistry II is offered in the summer and fall semesters. Both courses may be taken in either English or French and consist of two weekly lectures (1.5 hours each, mandatory, lecture or flipped format) and an optional tutorial session (1.5 hours, also called a recitation or discussion group). The Organic Chemistry I course has a required, associated laboratory section (3 hours biweekly). The Organic Chemistry II course has a laboratory course that runs concurrently and is only required for some programs (3 hours weekly). The organic chemistry courses use a principles and patterns of mechanisms curriculum; in that curriculum, the electron-pushing formalism is explicitly taught before deeper concepts of reactivity are addressed, reactions are taught in a gradient of difficulty and sections are organized by governing mechanism.[36–38]

Questions analyzed in this study

Twelves questions were selected (Figure 2) from exam questions in Organic Chemistry I and II courses as they represented the intended LOs identified in previous work.[9] The questions were chosen based on the available exam questions that aligned with delocalization LOs (Table 1). Several of the questions assessed multiple LOs (Questions 1,2,3,8) and each LO was assessed once, at least partially. LO2 (*Draw*) was assessed in three ways: explicitly (Question 1 and 12), implicitly (Question 2), and within a mechanism (Question 3 and Question 8). Explicit questions stated that resonance was required and was not embedded within a mechanism or context. Implicit questions are questions that do not state in the prompt that delocalization is required. Mechanistic question explicitly required delocalization within but within a mechanism.

Table 1. Selected questions aligned with the LOs.

	Organic Chemistry I	Organic Chemistry II
LO1 (Identify)	Q2 (Exam 2, N = 286)	No questions available
LO2 (Draw)	Q1 (Exam 1, N = 288) Q2 (Exam 2, N = 286) Q3 (Exam 2, N = 286)	Q8 (Exam 3, N = 296) Q12 (Exam 4, N = 389)
LO3 (Contribution)	Q1 (Exam 1, N = 288) Q3 (Exam 2, N = 286)[a]	No questions available
LO4 (Hybrid)	Q1 (Exam 1, N = 288)	Q12 (Exam 4, N = 73)[b]
LO5 (Hybridization)	Q1 (Exam 1, N = 288)[a]	No questions available
LO6 (Aromaticity)	Q5 (Exam 2, N = 286)[a]	Q7 (Exam 3, N = 296)[a]
LO7 (Stability)	Q4 (Exam 2, N = 286)[a]	Q6 (Exam 3, N = 296)[a]
LO8 (Acid/base)	Q2 (Exam 2, N = 286)	Q10 (Exam 4, N = 389)[a]
LO9 (E^+/Nu)	No questions available	Q11 (Exam 4, N = 389)[a]
LO10 (Reaction)	Q3 (Exam 2, N = 286)	Q9 (Exam 3, N = 296)[a] Q8 (Exam 3, N = 296)

[a]No justification was required in the question. [b] The LO was not required but some students drew the resonance hybrid, therefore we assessed LO4.

Organic Chemistry I

Exam 1, N = 284

Question 1

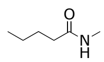
a. Draw all the resonance structures using the curved arrows to show electron movement.

b. Rank the resonance structures in order of contribution to the resonance hybrid and justify your answer.

c. Draw the resonance hybrid.

d. What is the hybridization of each of the following atoms?

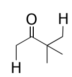
i. O
ii. N



Question 2

a.Circle the most acidic proton in the molecule below.

b. Explain your answer by making a comparison of the two possible conjugate bases.



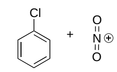
Exam 2, N = 288

Question 3

Consider the reaction of chlorobenzene with a nitronium ion (generated from HNO_3 and H_2SO_4).

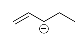
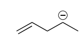
a. Draw the mechanism to explain the formation of the major product, including all resonance structures.

b. Circle the most important resonance structures.



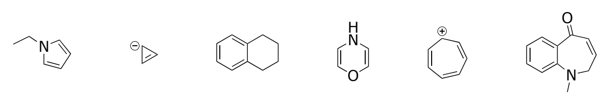
Question 4

Circle the most stable ion from the pair below.


Or


Question 5

For each of the following species, circle the aromatic ring(s) and underline the anti-aromatic rings(s) (do nothing with the non-aromatic rings).

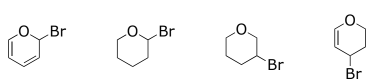


Organic Chemistry II

Exam 3, N = 269

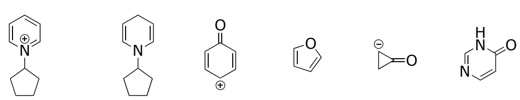
Question 6

Circle the compound that will undergo an S_N1 substitution most rapidly.



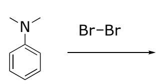
Question 7

Circle the aromatic compound(s) and underline the anitaromatic compound(s) from among the choices below.



Question 8

Give a mechanism and the major products of the following reaction, including resonance structure of the arenium.

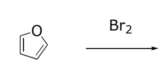


Question 9

Consider the reaction shown below between furan and Br_2.

a. Give the two products of the reaction shown below that have the formula C_4H_3BrO.

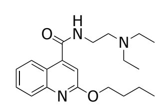
b. Circle the major product of the reaction.


Furan

Exam 4, N = 389

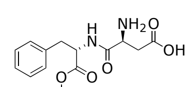
Question 10

Circle the most basic atom in cinchocaine, a long-acting local spinal anesthetic, shown below.



Question 11

Circle the most nucleophilic atom in aspartame, shown below.



Question 12

Draw the major resonance structures for the following compound. Include curved arrows to show the movement of electrons.

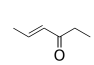


Figure 2. Twelve questions assessing ten LOs. Full answers can be found in the Supporting Information.

Coding scheme

We developed the coding scheme using inductive and deductive coding.[39] First, we compared students' answers to an expected answer and coded all strategies and errors encountered. After the first round of coding, the authors met and discussed the criteria required for a student to achieve a LO. The criteria came from inductive coding of the exam questions. The general criteria for LO achievement can be seen in Table 2, with the criteria in italics not being assessed in the question analyzed. Because many of the exam questions did not explicitly require students to justify their answers, we could not fully assess whether the full LOs have been achieved in all cases (refer to Table 2). If an answer contained justifications (even if not required) they were coded as fully achieved.

Table 2. General criteria for LO achievement

LO	General criteria to achieve the LO
LO1	Stated that delocalization can occur or drew resonance structures when not explicitly asked
LO2	Correctly drew the resonance structures, with the proper bonds and charges
	Correctly drew the curved arrows to show electron delocalization, *i.e.*, start at the source of electrons and finish are the correct position
	There is no change in the sigma bonds between resonance structures
	There are no extra or missing structures
LO3	Correctly identified the major contributor or correctly identified the order of contribution to the resonance hybrid
	Correctly used the evidence of charge and octet to justify their answers
LO4	Correctly drew the dashed bonds representing electron delocalization
	Correctly drew the partial charges (not full charge)
LO5	Correctly identified the hybridization of atoms in a delocalized system
	Justified the claim using a delocalization argument OR by drawing the resonance structures
LO6	Correctly labelled the cycles as aromatic, anti-aromatic and non-aromatic
	Justified the claim using a delocalization argument OR by drawing the resonance structures
LO7	Correctly identified the most stable structure
	Justified their answers by stating the cation is resonance stabilized OR by drawing the resonance structures
LO8	Correctly identified the most acidic proton or basic atom
	Justify the answer by stating that a conjugate base can be stabilized by resonance
LO9	Correctly identified the most nucleophilic atom (or electrophilic)
	Justify their answers by stating delocalization will lower nucleophilicity OR by drawing the resonance structures
LO10	Correctly identified the regioselectivity of a reaction

Justify their answers by stating delocalization will stabilize an intermediate OR by drawing the resonance structures of the intermediate

From the inductive coding, we formed categories for the types of strategies and errors found in answers. The types of errors were grouped into three categories: (1) electron-pushing formalism (EPF), (2) structures, or (3) formalism. EPF errors involved incorrectly using the electron-pushing formalism (curved arrows) to demonstrate electron delocalization. These types of errors have been documented in previous work[37,38] and include reversed arrows, arrows from charges/atoms, or extra/missing arrows. The arrows were considered correct if they represented the correct electron delocalization; if the structures were incorrect but the arrows were correct (*i.e.*, the following resonance structure was the results of the arrows), the arrows were labelled as correct. *Delocalization formalism* errors are related to specific symbols to demonstrate delocalization (e.g., double-headed arrow to indicate the relationship between the structures). *Structure* errors consisted of errors in drawing the resonance structures, including drawing the incorrect bonds or charges, as well as extra or missing structures.

For this research, the resonance hybrid was assessed from the resonance structures drawn in the question. Therefore, if an answer had incorrect resonance structures but the correct resonance hybrid for the structures drawn, they would be coded as having achieved LO4.

For some questions, responses would contain extra information explaining the work or using strategies. The strategies were coded and categorized as (1) visualizing electrons, (2) listing properties, (3) expanding implicit features, and (4) listing rules. *Visualizing electrons* involves trying to determine where the electrons can delocalize by drawing curved arrows or resonance structures. The *Listing properties* strategy was coded when the answer contained information about the structure such as hybridization or pK_a values. *Expanding implicit features* was reported in previous work[37] and means the response contains parts of the molecules that are not explicitly shown such as lone pairs of electrons or hydrogen atoms. *Listing rules* is a strategy where the rules to solve a problem are written down, for example the rules of aromaticity or acidity.

Question 1 required the student to justify their claim and so we analyzed their answer according to Toulmin's argumentation pattern.[22] To fully achieve the LO on Question 1, the answer had to have the correct claim (**A** > **C** > **B,** from Figure 5) and correctly relate resonance contributor rules to back their claim using the following six pieces of evidence: the presence of atoms with full/absent octets of electrons and number of charges. While there are six pieces of evidence, not all were required for the answer. The answer could state that all atoms have a full octet in structures **A** and **C**, but that structure **B** does not have full octets, making structure B the minor contributor. Then to differentiate between structures **A** and **C**, the number of charges could be used. Therefore, the evidence that structure **B** having two charges was not necessary to assign the contribution of each contributor to the resonance hybrid.

Two of the questions also required a justification and were coded according to their mode of reasoning presented in the theoretical framework (Table 3).[11]

Table 3. Criteria used to identify modes of reasoning in Question 1 and Question 2

Mode of reasoning	Description[11]	Criteria – Question 1	Criteria – Question 2
Descriptive	Salient entities in a system are identified.	Describes the octet (number of electrons on	Describes a proton as more acidic.

	Explicit properties are described. Explanation focused on surface features	an atom) and/or charge No link to contribution or hybrid No reason was given why octet/charge is used as an explanation	No link between acidity and other concepts No explanation why
Relational	Salient entities in a system are identified. Spatial or temporal relations between entities are identified. Correlations between properties and behaviors are established but not explained or justified.	Describes the octet/charge Links a resonance structure octet/charge to its contribution to the hybrid	Describes a proton as more acidic. Links concepts together (including delocalization)
Linear causal	Salient entities in a system are identified. Spatial or temporal organization of and connections between entities are identified. Relevant direct interactions between entities invoked. Proposed mechanisms involve linear cause-effect relationships and sequential chains of events.	Describes the octet/charge Links a resonance structure octet/charge to its contribution to the hybrid Explains WHY the octet/charge is relevant	Describes a proton as more acidic. Links concepts together (including delocalization) Explain that delocalization is used because it stabilizes on the conjugate base
Multi-component causal	Salient entities in a system are identified Spatial or temporal organization of and connections between entities are identified. Relevant interactions between entities are invoked. Effects of several variables are considered and weighed.	Describes the octet and charge Links a resonance structure octet and charge to its contribution to the hybrid Explains WHY the octet and charge are relevant Explain why one factor (octet) is more important to consider	Describes a proton as more acidic. Links concepts together (including delocalization) Uses resonance AND induction to explain their effects on the relative stability Explain why one factor (delocalization) is more important

Once we had developed the codebook, we re-coded the exams using a deductive approach. The coding book and expected answers can be found in the Supporting Information. Any statistical analyses were done using R; we used two tests: Chi-square to compared categorical data and *t*-tests to compare scores between two groups.

Validity and reliability

We addressed content validity by asking three experts to align the exam questions with the LOs. The alignment of the experts closely matched that of the authors, except for Questions 2, 3, and 8 assessing LO2 (*Draw).* The content experts mentioned that those questions only partially assessed the LO, but over 80% of the exams contained resonance structures therefore we included those as assessing LO2 (*Draw)*. Similarly, none of the experts aligned Question 12 with LO4 (*Hybrid)* since as written the hybrid is not necessary; however, 20% of students drew the resonance hybrid, and so we decided to investigate it for those students only. The experts labelled the questions in the same way the authors did as partially and fully assessed each LO. In some cases, the experts mentioned that more LOs have been assessed. For example, all three experts indicated that Question 2 fully assessed LO7 (*Stability*) and LO8 (*Acid/base*) while the authors had only assigned the question to LO8.

To address inter-rater reliability,[40] another researcher coded 15% of the exams and we compared the codes. The percent agreement and Krippendorf α values were acceptable after the first round of coding for all questions except Questions 2, 3, 6, and 8, at >80% agreement and a Krippendorf α value above 0.7.[41] For those questions, the raters met and discussed until agreement on the coding scheme was reached on all aspects (*i.e.*, LO achievement, errors, arguments, strategies, and reasoning). A different subset of exams was then coded and compared; the percent agreement and the calculated Krippendorf α values were acceptable. All percent agreements and Krippendorf α values are listed in the supporting information (SI).

Results and discussion

Overall LO achievement

The responses showed varying achievement rates on the assessed questions and LOs (Figure 2).

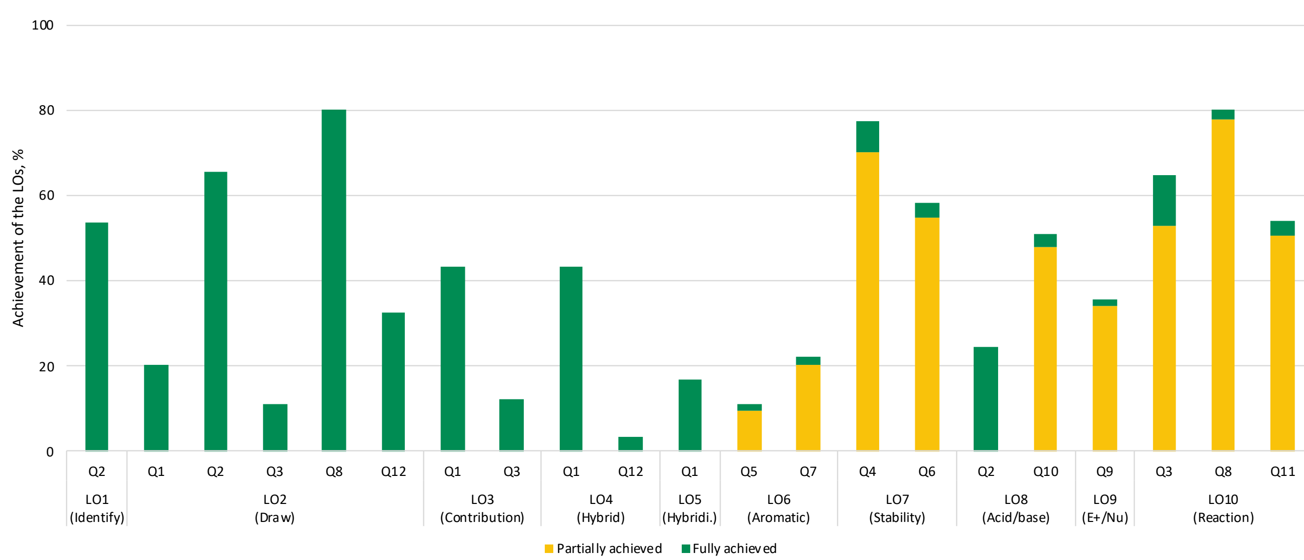


Figure 3. LO achievement across all questions. Green = completely achieved, with justification, Yellow = partially achieved, had the correct answer but no justifications. Justifications were not required for the answers seen as partially achieved.

LO1 (*Identify)*: Some students could not or chose not to use delocalization concepts

Overall, 63% of answers to Question 2 achieved LO1 (*Identify)* (Figure 3). 54% of the answers used delocalization concepts as the justification for their claim, 15% used inductive effects, and 9% used both factors. The exam question could be answered using delocalization, inductive effects, or hybridization in the justification (argument). Analyzing either factor indicates that the enolate is more stable of the two conjugate bases. Therefore, we do not know if students had the knowledge and skills to use delocalization and simply chose to analyze the question another way.

A few answers included delocalization, despite not being prompted. Questions 4–8 did not explicitly have delocalization in their prompts; however, a small percentage of answers either contained resonance structures or mentioned that delocalization could occur (Question 4 = 7%, Question 5 = 8%, Question 6 = 9%, Question 7 = 10%, Question 8 = 12%) (Figure 3). Some students explicitly reasoned using delocalization to answer questions related to the other LOs, such as using delocalization to explain aromaticity, base strength, and nucleophilic sites.

Half of the answers did not use delocalization concepts for Question 2, and approximately 10% of answers explicitly used the concept in Questions 4–8. Our previous work has shown that delocalization is introduced at the beginning of the first semester of an organic chemistry course and is not subsequently used in the course for a length of time (equivalent to a number of chapters); moreover, few practice questions represent LO1 (*Identify*).[9] Therefore, students may not realize that delocalization is a factor to consider in these problems. Previous work has shown that students did not frequently consider the delocalization of electrons within a mechanism.[4,5,42] LO1 (*Identify*) is a fundamental skill for the other LOs to be achieved in later organic problems where delocalization may not be explicitly required. Therefore, being able to determine where delocalization applies is important for learners. Making the learning outcomes explicit and providing opportunities for learners to practice this skill could help; learners likely need scaffolding (*e.g.*, explicit prompts to consider delocalization in their answers) initially.

LO2 (*Draw*): Varying level of achievement depending on question types, and when it was asked

LO2 (*Draw*) was addressed in five of the questions analyzed and was achieved in 13 – 65% of responses (Figure 4). These questions span the two-course levels, with Questions 1, 2, and 3 being from OCI, and Questions 8 and 12 being from OCII. We found that in OCI, more students achieved LO2 in an explicit question (Question 1) compared to both an implicit (Question 2) and mechanistic question (Question 3). In OCII, more students achieved LO2 on the mechanistic question (Question 8) than the explicit question (Question 12).

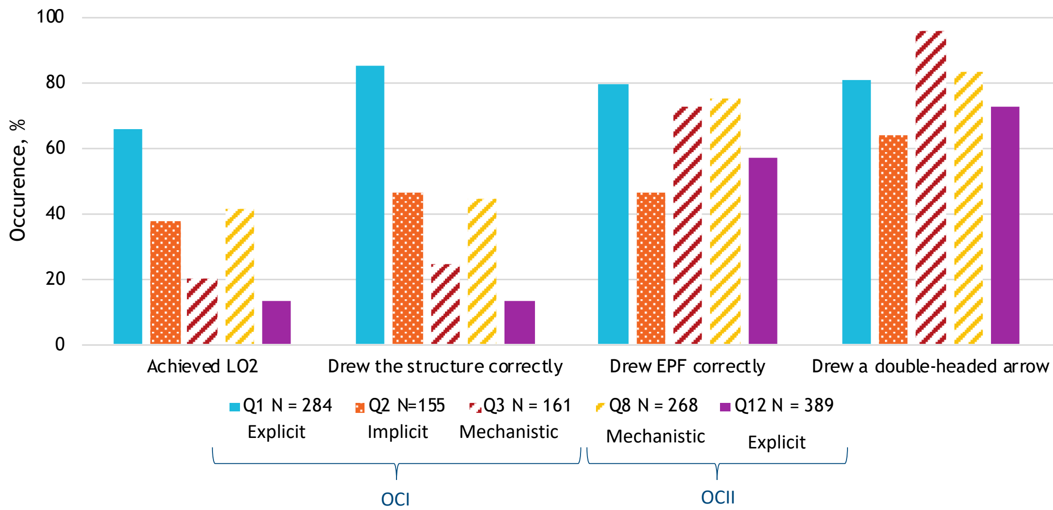


Figure 4. Achievement of criteria for LO2 for each of the questions that assess LO2. Filled bars represent explicit questions, the dotted filled bar represents the implicit question, and lined-filled bars represent the mechanistic questions.

Answers from OCII questions contained the correct electron pushing formalism more often than OCI. LO2 (*Draw*) was assessed in five questions and achieved to various degrees, depending on the type of question, timing of assessment, and the complexity. In OCI, most students (75%) achieved the LO in Question 1; this question explicitly asked for resonance structures and had the lowest complexity. Fewer students (40%) achieved the LO in Question 2; this question did not explicitly ask for resonance structures and the question had higher complexity as resonance concepts (or inductive effects) were needed to answer a larger question. The fewest students (18%) achieved the LO on Question 3; this question explicitly asked for resonance structures but in a later stage of the question and as part of a larger mechanism. Students may have the skills to achieved LO2 but may have difficulty using the skills when not explicitly required or in complex questions. In OCII, 32% of students correctly answered the explicit question (Question 12) but 80% of students correctly answered the mechanistic question (Question 8).

The most common errors related to the EPF were missing arrows (OCI) and incorrect arrows (OCII). In the explicit questions, there were very few answers without curved arrows, which is unsurprising since the prompt stated that curved arrows had to be drawn. The three not-explicit questions (Question 2,3,8) did not explicitly state that curved arrows were required and drawing resonance structures themselves do not require associated curved arrows. However, most students used EPF arrows despite not being explicitly asked (80% in Question 2, 87% in Question 3, 92% in Question 8), and in over 50% of missing arrow cases, answers contained no curved arrows at all. Students may not have drawn the curved arrows because they could not or because they chose not to.

In Question 12, however, 35% of answers contained an incorrect arrow (i.e., the arrow base or point did not start/point at the right location), an error seen in less than 5% of exams for the other LO2 (*Draw*) questions. This error was often found in conjunction with a structure error since many answers had impossible structures (33% of the answers contained both structure and EPF errors). The EPF arrows with these structures were considered incorrect since the electrons could not delocalize as indicated (*i.e.*, would have created a pentavalent carbon atom).

Many answers did not have all the expected structures. Different educators teach delocalization differently and may have different expectations of which resonance structures should be drawn. For our analysis, we used the expected answers (Figure 5), which were the structures provided in the course marking scheme; these would be aligned with the instructor's expectations of the students for that specific course. Other correct structures could be included (*e.g.*, **G** and **S**).

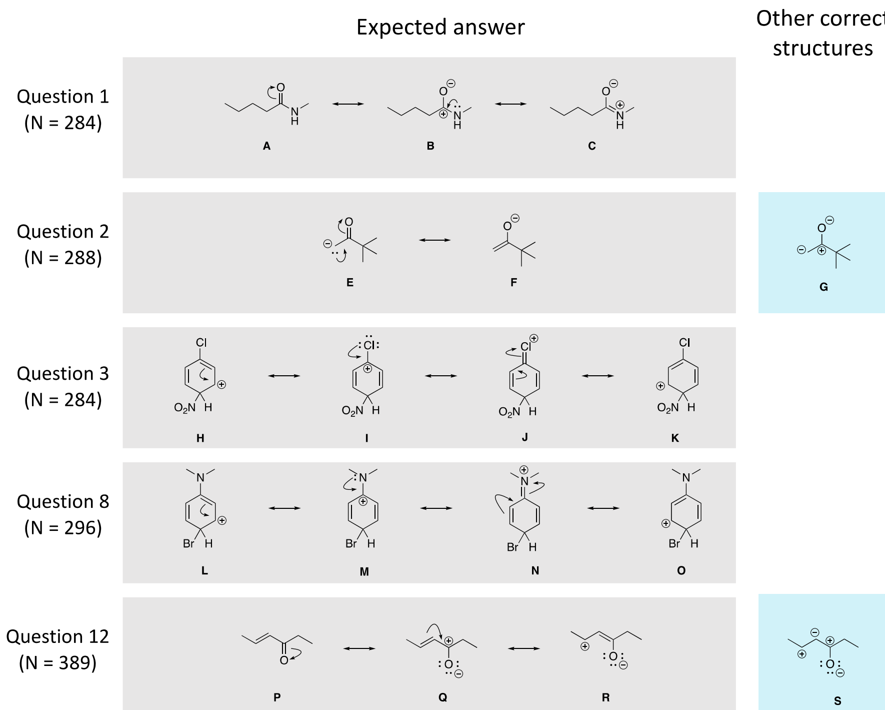


Figure 5. The expected resonance structures for the five questions related to LO2 (*Draw*).

For Question 1, 90% of the answers contained all three correct structures, and 2% omitted structure **B**. For the implicit Question 2, which has only two major resonance structures, 23% of students drew structure **E** as the product of the acid–base reaction; however, many did not draw **F** despite mentioning in their written answer that resonance stabilized the conjugate base. Without at least seeing a drawing of the other resonance forms, we cannot tell if students knew how resonance was involved in the molecule.

In Question 3, 60% of the answers did not include resonance structure **J**. This structure is the highest contributor to the resonance hybrid (since all atoms have a filled octet). One factor for missing this structure could be that the electrons come from outside of the ring; however, only 20% of the answers were similar in Question 8 (*i.e.*, omitting structure **N**). The different functional groups attached to the rings may have made it easier for students to cue delocalization of electrons from a nitrogen atom (with a lone pair) compared to a chlorine atom.

While answers to Question 8 showed structure **N** in their answer, 17% of answers omitted structure **L/O.** 21% of the answers drew the lone pair on the nitrogen delocalizing into the ring as part of the nucleophilic attack.

In Question 12 (OCII), structure **Q** was omitted in 78% of answers. A quarter of the answers used two curved arrows to arrive at structure **R**, bypassing structure **Q** (Figure 6). Structures **N** and **Q** are minor contributors to the hybrid and could be why structures were omitted. The questions did not ask for a specific number of resonance structures, so omitting a structure (especially a minor one) could be expected. Although the minor structure is important to identifying electrophilic and nucleophilic sites (LO9), it could be deemed unimportant when showing electron delocalization. For educational purposes, clear communication is needed regarding the purpose of the question (*e.g.*, draw the resonance structures that reveal they main electrophilic sites in the molecule), the specific expectations (*e.g.*, draw the four most important resonance structures for the following molecule), or other relevant information.

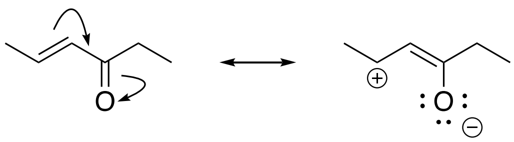


Figure 6. Resonance structures for Question 12, missing two minor contributors.

Impossible structure errors related to the application of delocalization concepts in OCII. Two types of structure errors were more prevalent in OCII than OCI; drawing impossible structures and drawing an incorrect reaction (Figure 7). Only 4% of answers in Question 1 contained these structure-related errors but 40% of exams in Question 12 contained these errors. A few answers contained a reaction (7%) in OCII and a negligible (<1%) amount in OCI. These errors were also minimal (<5%) in the mechanistic questions. The students were different in each of the courses and we have not analyzed how various sections of the courses have been taught, so we cannot make claims about the students' gains or losses in knowledge from one course to another.

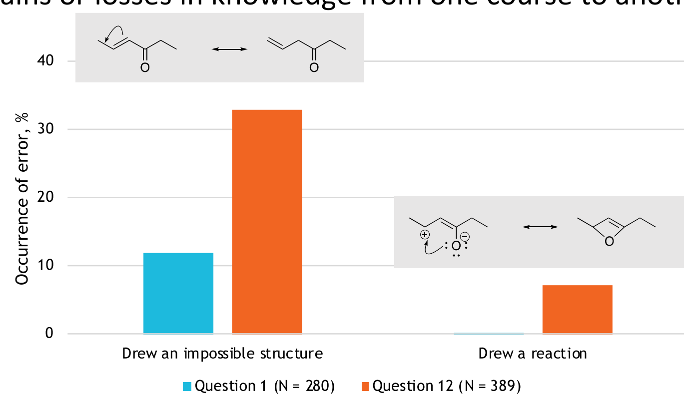


Figure 7. Comparison of errors in drawing the resonance structures.

Most students' answers had the correct double-headed arrow to show the relationship between resonance structures: 82% for Question 1, 85% for Question 2, 99% for Question 3, 84% for Question 8 and 72% for Question 12. The remaining answers included reaction arrows (*i.e.*, one-directional), equilibrium arrows, or nothing.

LO2 (*Draw)* achievement seemed dependent on how the resonance structures were prompted. In OCI, students were more successful on explicit questions. Drawing resonance structures is typically taught at the beginning of the organic chemistry course sequence and would therefore be expected in the OCI final exam. There is typically a gap between chapters that use and practice delocalization, which could lead to poor recall of the subject matter or poor application of the concept.[18] However, OCII students were more successful than OCI students when drawing resonance structures within a mechanism. Electrophilic aromatic substitutions are taught at the end of OCI,[36] meaning that students in the OCI cohort had less practice using delocalization within a reaction mechanism and OCII students would have had more opportunities to practice, both using delocalization within a mechanism and using the curved arrows to draw mechanism. In Question 3 (OCI) more than half the answers did not contain resonance structures. Many of these answers had incorrect mechanisms indicating that to achieve LO2 (*Draw*) within a reaction, prior skill with the EPF and reactivity is needed.

Of the three main types of errors (structure, EPF, and delocalization formalism), structure errors were most common – especially in OCII. The delocalization formalism errors were minimal; 3–20% of answers contained a formalism error. EPF errors were also minimal for Question 1 (<20%) but were high for the other questions, especially Question 2 (64%) and Question 12 (43%). Both questions with high EPF errors also contained a high amount of structure errors (Question 2: 46%, Question 12: 13%). For Question 2, many students drew reversed arrows and had the wrong charge. In Question 12, over 35% of students drew impossible structures, with incorrect use of the EPF.

Several answers did not include all the expected structures seen in Figure 5 (Question 1: 3%, Question 2: 11%, Question 3: 62%, Question 8: 28%, Question 12: 77%). Omitting minor resonance structures may be appropriate, depending on the context (*e.g.*, need for solving a given problem) and expectations (*e.g.*, course expectations), which need to be clearly communicated.

Impossible structures were seen in the OCII explicit question (Question 12).[3,10] This error, along with the reaction error, may indicate that students struggled to answer the questions and that they may not have recalled information about delocalization or known to use their knowledge. Previous work identified a gap in practiced questions related to delocalization spanning several (10–14) chapters.[9] This lack of practice questions may have led students to not understand how to answer the questions.

Most students in OCI (90%) used the correct delocalization formalism (i.e., double headed arrow), with fewer in OCII (78%). In Question 12, 20% of students used the equilibrium arrows, similar to previous work.[2,3,8] Using the correct arrow may not indicate that students conceptualize what the structures represent but simply that it is used to denote resonance structures. One of the main representational issues reported in the literature is the alternate conception that resonance structures are alternating or in equilibrium.[2–5,8] The exam analysis could not show any indication on whether the students conceptualized that resonance structures are not real or alternating.

In most questions, the EPF was used correctly: Question 1 (80%), Question 2 (83%), Question 3 (>99%) and Question 8 (81%). Question 12 (48%) contained more incorrect arrows than the other questions, which was linked with the impossible structure error.

LO3 (*Contribution)*: Students usually gave the correct contribution order, but often lacked the justification

LO3 (*Contribution)* was fully achieved in Question 1 by 44% of the students and partially achieved in Question 3 by 10% (Figure 3); both questions came from OCI exams. Question 3, did not require a justification, therefore only the students' circling of the major contributor could be assessed.

Most justifications contained the essential evidence to reason about their claim. Two other pieces of evidence were found in the exams: 5% of answers mentioned the stability of the resonance structure, and 10% mentioned the electronegativity of the oxygen atom.

Six pieces of information could be leveraged as evidence to support the claim; atoms' octets on all three structures and the charge on all three structures; 21% of answers contained all six pieces of evidence. However, not all the evidence was required to justify the correct claim and 46% of answers contained enough evidence to back up their claim. Choosing to use some of the evidence shows that students were able to identify the key information required to solve the problem.

Most answers (88%) had a descriptive type of reasoning in which the answer just described the resonance structures without backing (Figure 8). A few answers (8%) had relational reasoning in which the answers explicitly said that the charges and octet made a resonance structure the major/minor contributor. Only three answers were causal; these three answers mentioned that charges and that lacking octets destabilized molecules. The causal answers also outlined a relationship between the stability of resonance structure and their contribution to the hybrid. These results differ from previous literature that showed mostly relational/linear reasoning.[31,34] However, the predominantly descriptive response format matched how the topic was taught in the OCI course; therefore, providing a descriptive argument was appropriate and expected in this case.

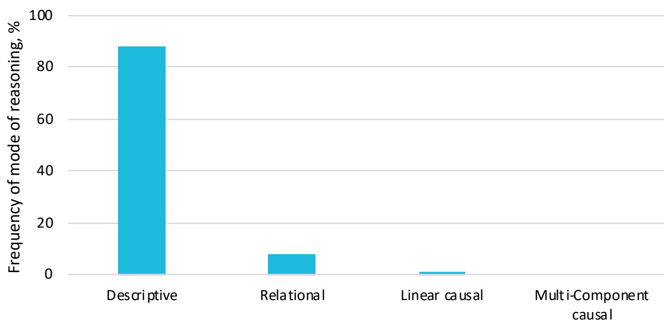


Figure 8. Modes of reasoning identified in answers to Question 1 (N = 280).

Success on LO3 could be related to success on LO2 (*Draw*), as only 21 students demonstrated achieving the LO in Question 3. The low success rate was related to LO2 (*Draw*), since many answers did not contain all the resonance structures, with 60% of the answers not containing the major resonance contributor. In the exams that contained structure **I**, 55% selected the correct major contributor.

LO3 (*Contribution*) was well achieved; however, the most common error in Question 3 (45% of answers that contained the major structure) involved stating that a structure containing atoms without a full octet of electrons would be the major contributor, in line with previous work.[10] The achievement of the LO is also dependent on LO2 (*Draw)* since in Question 3 many answers did not contain the major contributor, and therefore could not select as the major contributor.

We wondered whether students would apply the concept of stability or contribution to the resonance hybrid in their answers. In this study, only 5% of the answers included "stability" when reasoning about contribution to the hybrid. Stability (a physical property) cannot be assigned to a structure that does not exist; instead, the expression "contribution to the resonance hybrid" can be used.[4] Using the word stability may contribute to the alternate conception that structures are real or alternating.[4] Students may still have used stability or believe stability is the key factor, without writing it down. Because students primarily used descriptive reasoning and listed the octet and charges, we do not know their mental models of delocalization. A prompt explicitly asking for causal reasoning or that asks students to describe their mental model of resonance structures could provide more information on students' mental models.

LO4 (*Hybrid)*: Half of the answers showed the correct hybrid structure

51% of the students successfully achieved LO4 for Question 1 (Figure 3). Question 12 did not explicitly ask for the students to draw the resonance hybrid but 19% of students included the hybrid in their answer. However, less than 50% of those answers had a correct resonance hybrid. We identified three categories of errors, related to the structure. The errors were categorized as bonds, partial charges and formalism errors.

There were few errors drawing dashed bonds (<16%). Bond drawing errors were the least common for both Question 1 and 12; 90% of responses had the bonds drawn correctly on the resonance hybrid structure, and 84% for Question 12.

The most common error was in drawing partial charges (49%), in which students either primarily drew full charges or incorrect partial charges. The main error was a missing partial charge (Question 1 = 16%, Question 12 = 32%) or an incorrect partial charge (*i.e.*, a positive charge instead of a negative charge) (Question 1 = 12%, Question 12 = 6%). The missing partial charge error was only coded if the answer contained the resonance structure that had the charge on it. These errors would arise from mapping the information of the resonance structures onto the hybrid. While most students successfully mapped the dashed bonds, the charges contained more errors.

The most common formalism error was labelling the hybrid as a transition state (Question 1 = 12% and Question 12 = 16%) was the hybrid being labelled as a transition state.

Achieving LO2 greatly increased the likelihood of achieving LO4. Achieving LO4 (*Hybrid)* was correlated with the success of LO2 (*Draw),* χ^2 (1, N = 280) = 31.55, $p < 0.001$, $\phi = 0.451$; 97% of the students who achieved LO4 also achieved LO2. In contrast, only 2% achieved LO4 without also achieving LO2 (Figure 9). We omitted the formalism errors for both LOs (LO2: double-headed arrow, LO4: symbol outside the bracket) because the formalism error of either would not affect the translation between representations.

Figure 9. Connection between achievement of LO2 and LO4 in Question 1.

LO4 (*Hybrid*) was achieved by 51% of students in Question 1. The most common error was a partial charge error, previous work reported that the dashed bonds errors were the most prevalent error[10] or that students would draw the major/minor contributor (53%).[3] A link between instruction and skills drawing the hybrid has been reported,[3,8] and our context may have contributed to the results obtained. The variance between previous work and our analysis could be related to the alignment on how the LOs have been intended and enacted. When teaching delocalization, a focus on the representation itself, explicitly demonstrating what information the representation provides has been shown to help students with the skills to use delocalization.[3,8]

Many students (15%) drew the correct hybrid (*i.e.*, bonds and partial charges), yet used the wrong formalism. The formalism of the hybrid is important to communicate what the structure represents; however, it does not represent whether students conceptualize the resonance hybrid. Formalism will help in communications and as such is important to teach but will not affect students understanding of the hybrid.

LO5 (*Hybridization)*: Answer had the correct hybridization for the oxygen atom was but not the nitrogen atom

Question 1, part d asked students to label the hybridization of the oxygen and nitrogen atoms of an amide. Only 16% of students successfully labelled hybridization of both atoms (Figure 3). The oxygen was correctly identified as sp^2-hybridized by 64% of the students, while only 31% correctly identified the nitrogen amide as sp^2-hybridized (Figure 10). The nitrogen atom was most labelled as sp^3-hybridized (57%). Answers of “between sp^2- and sp^3-hybridized” would be have been accepted for either atom, although no students provided that answer.

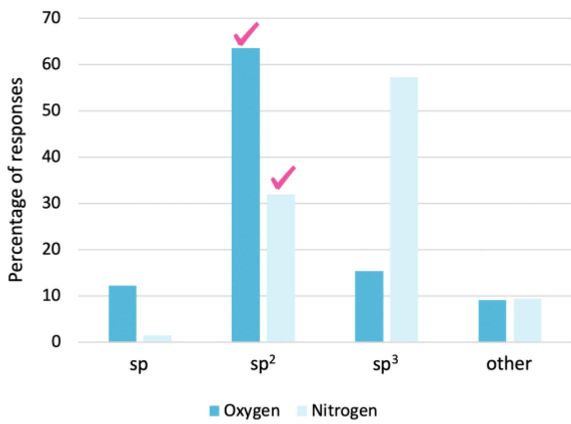


Figure 10. Hybridization labels for Question 1, part d (N = 284). The “other” category represents answers that are not represented by the three other levels, such as s or p designations.

LO5 (*Hybridization*) was achieved by few students. Students were more successful in assigning the hybridization of the oxygen atom than the nitrogen atom. We do not know the reasoning behind those labelling since the students were not required to justify their answers. However, the results suggest that students used the structure of the first resonance structure (major contributor) to decide on the atoms’ hybridization, rather than the more accurate hybrid structure.

LO6 (*Aromaticity*): Answers containing a strategy (including delocalization) were more successful than not

For LO6 (*Aromaticity*), 11% of students successfully labelled all eight cycles in Question 4 (OCI), while in Question 6 (OCII), 22% successfully labelled all the cycles (Figure 3). In both questions, >50% had at least six of the eight cycles correctly identified.

Common structures, such as benzene, cyclohexane, and cyclopentane, were most often identified correctly. None of the cycles were constantly labelled wrong, with the cycle being labelled incorrectly the most was still labelled currently in 44% of the answers (Figure 11). Looking at the amount of correctly labelled structures we saw that most students (over 50%) correctly labelled six or more structures. In Question 5, the most common score was 6 (1 point per correctly labelled cycle), while for Question 7 a perfect score was the most common (35% of the answers).

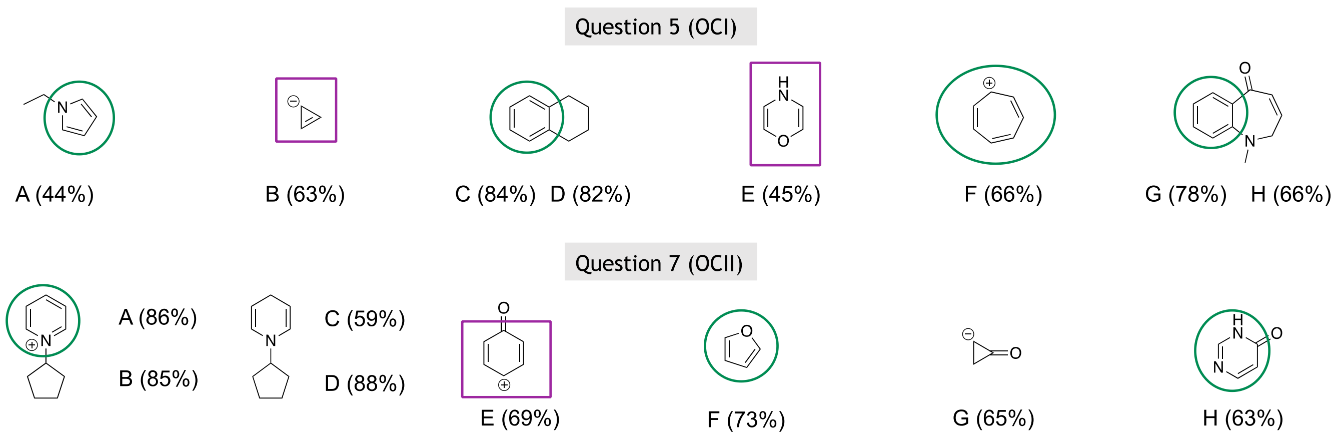


Figure 11. Answers given for Q5 (OCI, N = 288) and Q7 (OCII, N = 299). Cycles that are circled in green are aromatic, cycles that are squared in purple are anti-aromatic, and the remainders are non-aromatic. The percentage below or next to each cycle is the percentage of answers with that cycle correctly labelled.

Answers that contained explicitly drawn electrons, listed properties, and/or expanded structures also had higher scores. While the questions did not require justification, strategies were found in 63% of the answers in Question 5 and 78% of the answers in Question 7. For both questions, answers containing a strategy were more successful. In Question 5, the average score for an answer with a strategy was significantly higher (M = 5.7, SD = 1.68) than answers with no strategies (M = 4.5, SD = 1.80), $t(136) = 3.56$, $p = 0.0005$. Similarly for Question 7 the scores were higher for answers with a strategy (M = 6.1, SD = 1.94) than those without (M = 5.3, SD = 1.70), $t(231) = 3.14$, $p = 0.001$.

The most-used strategy for both OCI and OCII students was expanding the structure, 62% and 73% respectively. Students who used the visualizing electrons strategy, listing properties strategy and/or expanding the structure, had on average higher success in labelling the structures than students listing rules (Figure 12). For Question 5, listing rule by itself (M = 4.5, SD = 1.85) had no significant difference from using no strategy (M = 4.5, SD = 1.80), $t(45) = 1.82$, $p = 0.171$. The same trend was seen for Question 7, where using rules alone (M = 4.6, SD = 1.42) had no significant difference with using no strategy (M = 5.3, SD = 1.70), $t(48) = 0.91$, $p = 0.363$. But using at least one other strategy increased the average score (Question 5 = 5.27, Question 7 = 6.14).

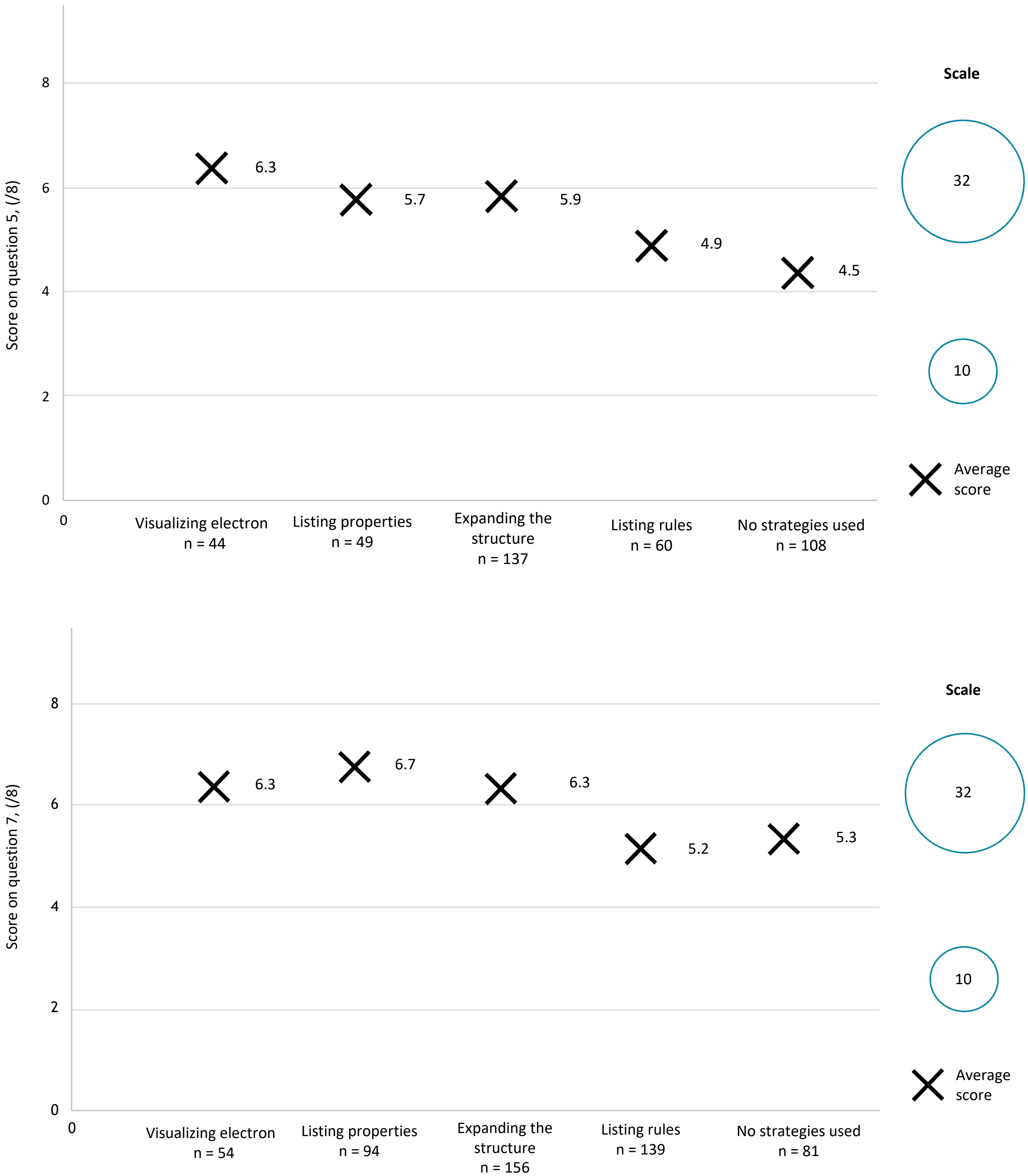


Figure 12. Distribution of students' scores depending on whether they used a strategy on Question 5, N = 288 (top) and Question 7, N = 296 (bottom).

Strategies differed depending on the ring type. The least number of strategies were used when determining common rings (*i.e.*, benzene, cyclohexane and cyclopentane). The low number of strategies could be due to students' familiarity with those rings since at least 82% of students labelled these correctly.

All three strategies (visualizing electrons, listing properties, and expanding the structures) were used on the three types of cycles. Listing properties (hybridization) was used more often (11%) to explain that a ring was non-aromatic (Figure 13). In Question 7, 79%, of answers that used the list properties strategy used it to label a sp^3-hybridized atom to show it was nonaromatic, while 64% of answers did so in Question 5. Students drew electrons in more often when determining if a cycle was aromatic or anti-aromatic, which was not surprising since deciding on aromaticity involves identifying the electrons involved.

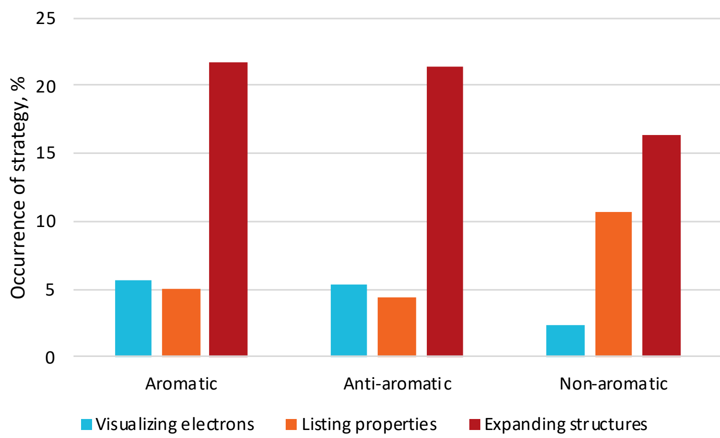


Figure 13. Strategies used based on type of ring.

LO6 (*Aromaticity*) was mostly achieved by students since they correctly labelled six of eight more than half the time. Previous work in a different context found that students seem to struggle to conceptualize aromaticity,[43] believing that any cyclic structure was aromatic.[44] In the current context, the results show that students can recognize aromaticity, which may be related to the alignment of the LOs with course instructions.

Answers containing strategies of expanding the structure, visualizing electrons, and listing properties tended to have higher scores (Question 5: 5.9, Question 7: 6.4) than those that did not use those strategies (Question 5: 4.5, Question 7: 5.3). Using these strategies, students extracted additional information from the representation. Drawing the implicit information encoded in the feature can reduce cognitive load.[45,46] Similar strategies have been connected with success in previous work[37,47] and can be taught explicitly.[38] However, listing rules showed no significant difference with using no strategies. Listing rules may result in rote memorization of defined rules, as opposed to applying concepts to extract information from the representation. Promoting and teaching the use of strategies that extract implicit information from the structures, while applying it to LO6 (*Aromaticity)* has the potential to equip learners with tools to succeed on delocalization questions.

LO7 (*Stability*): Using delocalization as a justification was connected with higher success

LO7 was assessed in Questions 2, 4 and 6 which was fully achieved between 7% and 14% of the time and between 59% and 78% of the time (Figure 3). Question 2 will be discussed in the next section, LO8 (*Acid/base*), since the two LOs are interconnected.

Question 4 required students to circle the most stable ion in a pair; one ion was stabilized by delocalization the other was not. 78% of students partially achieved this LO (no justification was requested); however, 14% of students added explanations or extra drawings to their answers. 7% of the students drew resonance structures or mentioned that one ion was resonance stabilized. All of the answers that invoked delocalization chose the correct ion, except one.

For Question 6, students had to choose which starting material would undergo an S_N1 reaction mechanism; the correct answer included the most stable carbocation that was stabilized by delocalization. Answers were correct 59% of the time. For this question, 10% of answers invoked delocalization as an extra explanation; of those, 90% identified the correct answer. The other strategies were rarely present in these answers (<5%).

LO7 (*Stability*) was well achieved; while no reasoning was required, some answers included information about delocalization. The answers that invoked delocalization (Question 4: 7%, Question 6: 10%) typically had the correct answer (Question 4: 95%, Question 6: 90%), which is aligned with previous work that showed participants seem to realize that resonance was more important in determining relative stability.[4,5] Therefore, LO1 (*Identify)* may be a building block that helps achieve LO7 (*Stability*).

LO8 (*Acid/base*): Answers included some causality and uses of strategies

LO8 (*Acid/base)* was achieved fully by 50% of the students (Question 2). This LO was also assessed in Question 9 but did not require a justification. In that question, 51% of students correctly selected the most basic atom (Figure 3). Like LO7, some students demonstrated the use of delocalization to answer the questions, for those students 48% had the correct answer.

In a multivariate acid/base question, half of the answers were correct, but it is unknown how they arrived at their claim. Question 10 required students to select the most basic atom in a molecule, and 51% of the answers correctly selected the nitrogen atom that could not participate in delocalization (Figure 14). This problem is multivariate since multiple factors can affect the basicity of the atoms. Students had to determine which basic atom was least stable and to do this they must consider delocalization, hybridization, electronegativity, and inductive effects. Alternatively, they could use pK_a values. Some may also have answered using heuristics or a memorized rule (*e.g.*, nitrogen is a base). Most of the students (87%) chose a nitrogen atom over an oxygen atom showing that students knew that nitrogen atoms were more basic than oxygen atoms. Without asking for explanations, we do not know the reasons for their choices.

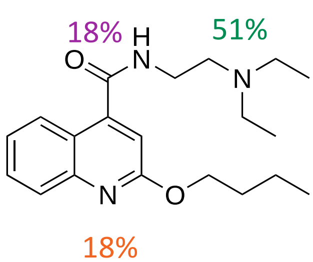


Figure 14. Percentage of students who circled each site in Question 10.

Answer with strategies other than listing rules and properties had higher success rates. The questions did not require justification, but many students (33%) used a strategy to answer the questions. Figure 15 shows the percentage of students who used a specific strategy, and how many of those obtained the correct answer. As with LO6 (*Aromaticity*) answers with expanded structures and visualizing electrons were more often correct, χ^2 (1, N = 389) = 32.34, $p < 0.001$, $\phi = 0.21$.

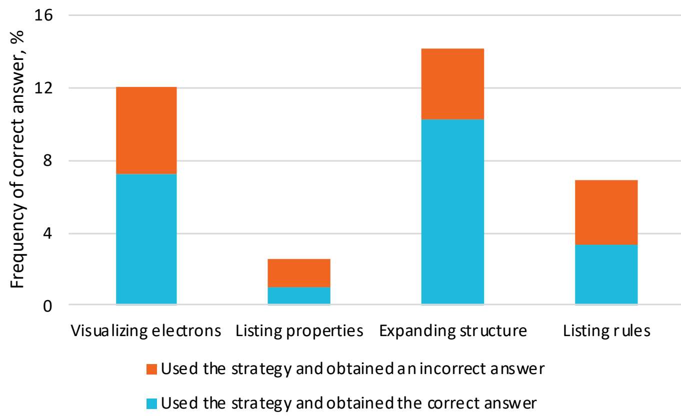


Figure 15. Frequency of correct answers for Question 10 (LO8) for answers with strategies and break down per strategy.

The most common answer with the correct claim used delocalization as evidence. Most answers (72%) had the correct claim—the proton they circled in part a of the question.

The evidence used for their claim could include resonance, induction, or proximity (*i.e.*, similar to induction, but only stating "close to oxygen"). 92% of the student that used resonance as evidence also had the correct claim (Figure 16) while 67% of the answers that used induction had the correct claim.

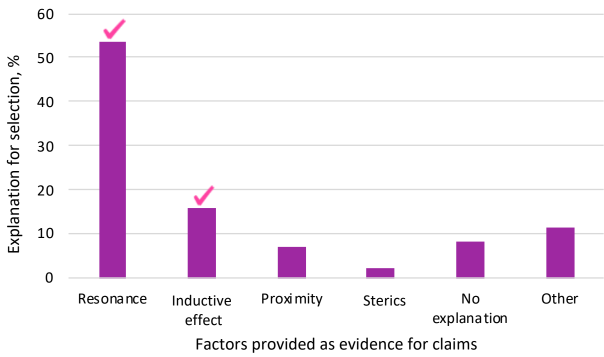


Figure 16. Question 2 (acid–base): Evidence used to justify the claim (N = 280).

The chemistry concepts used to justify the answers represent the evidence for the claims. Four concepts were expected to obtain the correct answer, and they were also the four most commonly mentioned concepts: acid strength (69%), relative stability of the conjugate base (64%), relative base strength (54%) and one or more of resonance (55%), inductive effects (21%), and electronegativity (26%). Other concepts include charge (34%), proximity (27%), electrons (35%), and others (21%).

Approximately half the answers had causal reasoning. 82% of the answers showed links between concepts. Links were determined if the two concepts were connected via linking words (*e.g.*, but, therefore, as such, for example, because) or symbols (*e.g.*, =, <, >). Some answers (34%) had the appropriate links between all four concepts (*i.e.*, acid strength, conjugate base strength, conjugate base stability, and one or more of resonance, inductive effects, or electronegativity) (Figure 17) but others lacked one of the concept or links.

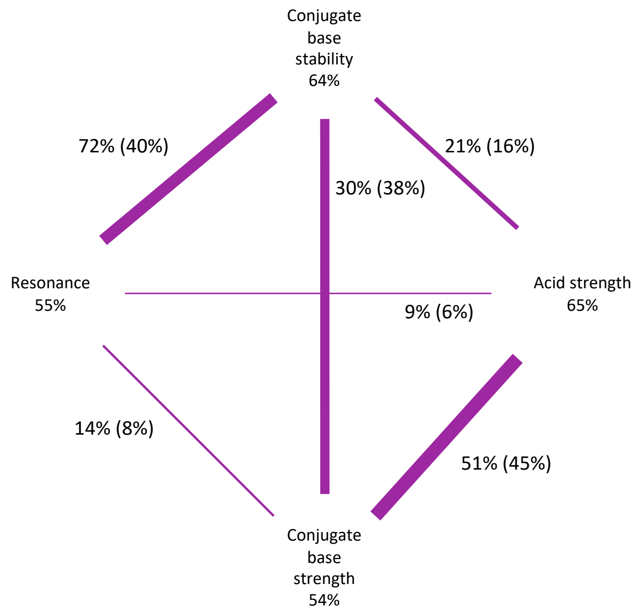


Figure 17. Percentage of answers with links between concepts (n = 155). The percentage in parentheses is out of all answers, including those who did not identify resonance (N = 286).

Table 4. Examples of modes of reasoning for Question 3.

Mode of reasoning	Example
Descriptive	"The first conjugate base has the negative charge on the oxygen, also has resonance structures with the oxygen" Exam 227
Relational	"[A] is the most acidic proton because the conjugate base is stabilized by resonance, while the other conjugate base is not" Exam 275
Linear causal	"The hydrogen attached to the first carbon is the more acidic proton in the molecules, this can be seen in the conjugate base has resonance, where the alternate conjugate base does not. The molecule with the more resonance forms a more stable conjugate base, which in turns comes from a stronger acid. Therefore, the hydrogen attached to the first carbon is the more acidic proton." Exam 134
Multi-component causal	"[A] is the most acidic proton because the conjugate base that would be formed if this proton was removed is more stable (weaker) compared to the C.B. [conjugate base] if the other proton was removed. The more stable C.B. would produce a stronger acid. The first C.B. is more stable since it has resonance structures that help stabilize electrons of the negatively charges carbon atom. It also has a stronger inductive effect that pull more [electron] density from the negative charge to stabilize the basic carbon." Exam 19

To be coded as causal, a response had to describe the relationship between an acid and its conjugate base (*e.g.*, the stronger the acid, the weaker its conjugate base) **and** explain how resonance (or induction) affects the relative stability of the conjugate bases. Examples can be seen in the linear and multi-component causal rows of Table 4. The effect of resonance or induction on the conjugate base needed to be shown and the argument needed to outline why that relationship was relevant. 38% of the answers had a causal answer (linear or multi-component causal), which explained how resonance (or other factors) stabilizes one conjugate base more than the other, making the originating acid stronger (Figure 18).

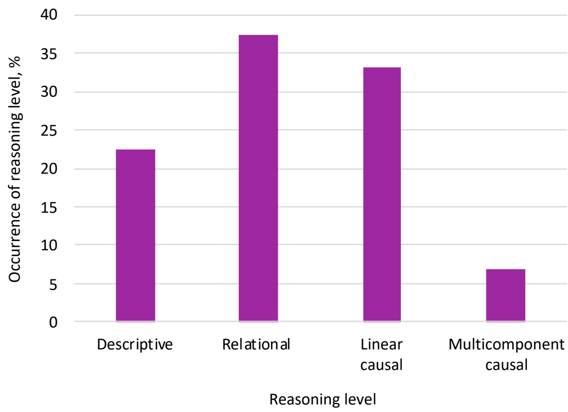


Figure 18. Modes of reasoning for Question 2 (acid/base). (N = 286).

LO8 (*Acid/base)* was achieved by half of the students in a multivariate problem that did not require reasoning, and by 34% of students when a written causal answered was expected. This LO builds on both LO1(*Identify)* and LO7 (*Stability),* and the causal link between the three LOs was seen in 38% of the answers containing delocalization.

The answers that demonstrated causal reasoning explained why resonance was used as evidence in their answers. However, many other answers did not explain why delocalization was invoked. This absence may be because the students could not or chose not to. Clearly articulating expectations to students or using reasoning scaffold[48] could promote more causal reasoning.

Question 2 mode of reasoning was similar to previous work that showed a prevalent relational/linear mode of reasoning.[31,34] The questions analyzed in this study and the previous study were similar as they both required students to compare two (or three) components and decide (claim) which is stronger (more likely for mechanism question) using evidence. This format has provided similar results in all three questions within our context. This work showed few (22%) descriptive answers and few (7%) multi-component causal answers, with most of the answers being relational (37%) and linear (33%).

LO9 (E^+/*Nu*): Half the students identified the most nucleophilic atom

The learning outcome was assessed in Question 10, required students to circle the most nucleophilic atom in a molecule, and was achieved by 53% of students (Figure 3). Students had to identify the atom that would have the highest electron density (*i.e.*, unable to delocalize its electrons) to identify the most nucleophilic atom (Figure 19). Most students identified that the nitrogen atom was more nucleophilic than the oxygens, however many selected the amide nitrogen. The questions did not require justification, some students (20%) used a strategy to answer the questions. We compared the frequency of correct answers between students who used the expanding structure and visualizing electrons strategies and did not use strategies (or listed ruled) and found a significant but negligible difference, χ^2 (1, N = 389) = 27.01, $p < 0.001$, $\phi = 0.061$.

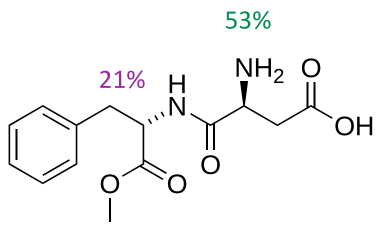


Figure 19. Common answers for Question 10. The correct answer is in green.

LO9 (*E+/Nu)* was achieved by half the students and answers that explicitly contained delocalization or strategies did not have higher scores than those without. Multiple factors were involved and therefore students may have chosen not to draw or use delocalization specifically. However, multiple studies report that students often have difficulties identifying electrophiles and nucleophiles,[49,50] and so we cannot say if students had difficulty with delocalization or identifying nucleophiles and electrophiles.

LO10 (*Reaction*): The assessments chosen did not fully assess the LO

LO10 (*Reaction*) was achieved by almost 60% of the students in Question 3 (OCI) and by 80% in Question 8 in OCII (Figure 3). Both questions asked for an electrophilic aromatic substitution (EAS) and to draw the resonance structures of the arenium ion. Question 10 also assessed LO10 regarding the bromination of a furan. This question only partially assessed the LO but was partially achieved by 54% of students.

Electrophilic aromatic substitutions could be answered using directing groups. The results showed that 65% of all students successfully identified the *para* or *ortho* isomer as being the major contributor to the resonance hybrid in Question 3, and 82% in Question 8. However, students may have simply memorized the rules for directing groups (*i.e.*, that chlorine is an *ortho*/*para* director) and not used delocalization in their reasoning. Most students who drew resonance structures correctly identified the *ortho* and/or *para* disubstituted benzene as being the major product (89% for Question 3, and 98% for Question 8).

Answer that mentioned delocalization or directing groups were successful in choosing the major product in OCI. Some of the answers (28% OCI and 30% OCII) used words to explain their claims (Figure 20). OCI students who used extra words to describe their answers were successful in identifying the final major product, however students in OCII were less successful. We saw no difference between what concept was invoked (*i.e.*, resonance vs use of directing groups) in both questions.

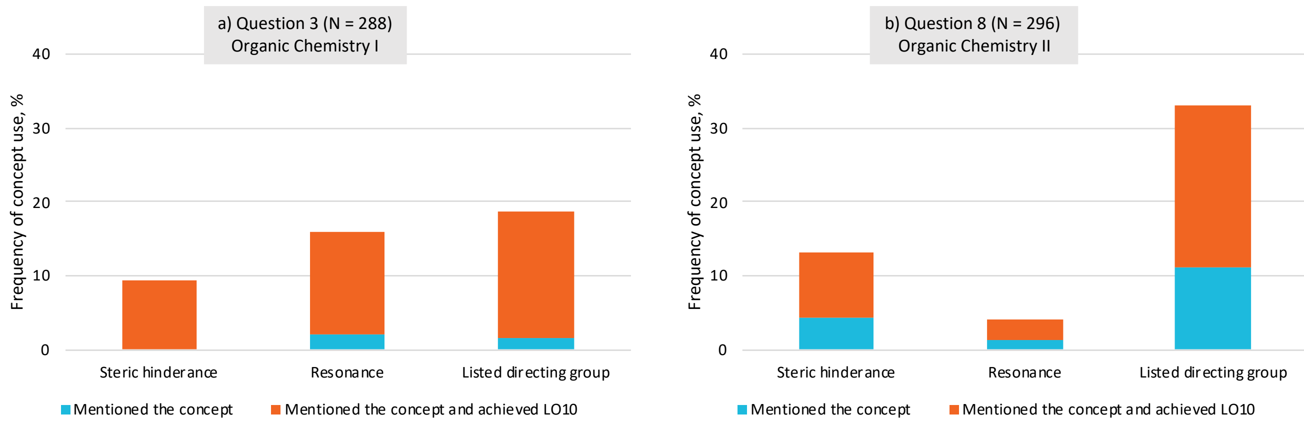


Figure 20. Frequency of students mentioned a concept when not explicitly asked. (a) Question 3, OCI, N = 288, (b) Question 8, OCII, N = 296. Orange: used the concept and achieved the LO, blue: mentioned the concept but did not achieve the LO.

Similarly, Question 9 asked students to draw the two products of the addition of bromine to furan, in which 67% of the answers had the correct products. Among those, the students were asked to identify the major product. The intermediate leading to the major product is best stabilized by delocalization, has the lowest transition state leading to its formation, and is therefore favored. Of the students who drew both isomers (67%), 53% selected the correct major product.

Although no justification was required, 13% of students either mentioned delocalization or drew resonance structures as part of their answers. There was no correlation between mentioning delocalization or drawing resonance structures and success on the question.

Students obtained the correct answer on the electrophilic aromatic substitution questions, unfortunately we cannot say if it was due to their skills using delocalization or memorizing directing groups. Therefore, more work would need to be done to identify the degree to which students are achieving this LO in different contexts. A scaffolded prompt that would explicitly require students to explain why a specific product is formed could potentially address the LO. The answers in Question 3 that contained a reference to delocalization were mostly successful, which was also seen in a previous study.[5] However, for Question 8 half of the answers mentioning resonance were successful.

Overall key findings

Along with findings related to each LO, five other key findings emerged from our data: (1) answers had few representational errors, (2) students either did not recall information about delocalization or chose not to use it, (3) delocalization was used between 10-20% of the time when not prompted for LO6-10 (*Aromaticity, Stability, Acid/base, E⁺/Nu, Reaction*), (4) students' reasoning aligned with course expectations, and (5) many LOs built on each other.

Answers had few representational errors. Few representational errors were found in the present context despite previous reports of students struggling with the representation of delocalization.[2,3] The few errors about the representations itself (e.g., incorrectly drawing the dashed bonds in the resonance hybrid) were minimal and mostly related to the resonance hybrid, which differs from previous work that showed that few students identified the resonance hybrid correctly (3%) while more than half the students (53%) identified a major or minor contributor.[3] In the current work, drawing the resonance structures was connected with higher success drawing the resonance hybrid, demonstrating the skill to translate information from one representation (resonance structures) to another (resonance hybrid) in a similar context.

Over 35% of the Question 12 answers contained at least one pentavalent carbon. This type of error could be representational since the students did not fully extract the information from the Lewis structure. In another study at the same institution, few students drew pentavalent carbons while answering questions that directly address the electron-pushing formalism and reaction mechanisms,[37,51] so this error could be related to the Lewis representation of delocalization specifically.

Strategies that helped students reason with the representations were correlated with higher achievement of the LOs. Using strategies that involved cognitive offloading of the representation (*e.g.*, visualizing electrons, listing properties, and expanding the structure) led to the achievement of LO6 *(Aromaticity*), LO7 *(Stability*), and LO9 (*E*$^{+}$*/Nu*). These strategies involve interacting with and using implicit information from the representation, and then using that information to solve the problem at hand. The use of those strategies indicates that students reasoned beyond surface features to understand the information decoded in the representation.

Students either struggle to recall information about delocalization or chose not to use delocalization concepts. In Question 2, LO1 (*Identify*) was achieved by only 54% (the question could correctly be answered in alternative ways) and delocalization was mentioned in roughly 10% of the answers in Questions 4–8. Previous work has shown that students did not frequently consider the delocalization of electrons within a mechanism.[4,5,42] The inability to recall information on delocalization would give cause for concern since without being able to identify delocalization when not explicitly told the other LOs could be impacted. Therefore, for the other LOs to be achieved in later organic problems (*e.g.*, organic synthesis, exploring mechanisms), being able to determine where delocalization applies is important. However, we do not know if this absence of delocalization information was because students chose not to mention delocalization or because they could not. Scaffolding the students to use delocalization could provide them with the skills to use delocalization in different contexts.

Some students are using delocalization strategies when not prompted (~10%). Delocalization was invoked by some students in all the non-explicit questions (Question 2: 54%, Question 4: 7%, Question 5: 7%, Question 6: 13%, Question 7: 10%, Question 9: 12%, Question 10: 7%, Question 11: 3%), so the prompts did cue some of the students to explicitly show delocalization. More students may have known how to use delocalization but chose not to. Answers that explicitly showed delocalization were typically successful.

Similarly, the resonance hybrid was in 19% of the answers to Question 12; the hybrid shows different information than the resonance structures and may help cue students to that information required for solving the problem. External representations have been reported to both help extract necessary information or distract from extracting the information.[46,52] Therefore, drawing the hybrid may have been a sense-making device to help answer the questions by helping students reason with the representation. Alternatively, students may have drawn it in hopes of getting part-marks on a summative assessment. In both cases, the question about delocalization cued the students to draw the hybrid.

Students' reasoning aligned with expectations for the question and course. Students' reasoning varied between the questions, which is most likely related to the question itself, courses expectations, and how the concepts were taught, including explanations, problem sets, and previous assessments.

For Question 1, most students used a descriptive mode of reasoning and gave their answer in a tabulated/list format, while in Question 2 more answers used relational and linear causal reasoning. Previous work analyzed two comparison questions (one comparing mechanisms and the other comparing bases) similar to Question 2 and showed students typically used relational to linear causal reasoning in their responses,[31,34] similar to our results for Question 2. Question 1 showed predominantly descriptive reasoning, which was aligned with more rule-based reasoning where the application of rules is used to explain or draw a structure.[53] This type of reasoning was aligned with the expectations of the course for that type of question (*i.e.*, ranking resonance structures).

The learning outcomes are interconnected. Some LOs build on earlier ones. For example, students who did not identify that delocalization could occur, also could not achieve any other LO within the question. Students who achieved LO2 (*Draw)* had a higher likelihood of achieving LO4 (*Hybrid*) and LO3 (*Contribution*) and LO10 (*Reaction)*, demonstrating that the LOs are interconnected. Similarly, answers that explicitly achieved LO1 (*Identify*) were typically successful in achieving LO6 (*Aromaticity),* LO7 (*Stability*), LO8 (*Acid/base*), LO9 (*E^+/Nu*), and LO10 (*Reaction*). This interconnection shows that having a strong base knowledge (LO1/LO2) relates to higher success on the other LOs.

Conclusion

This work investigated how ten-essential delocalization LOs were achieved on exams, including strategy use and common errors. The degree of achievement of the LOs was highly varied. Errors were primarily related to drawing the resonance structures and most often related to impossible structures. Answers that contained strategies that involved drawing information from the representation (*i.e.*, drawing out electrons, listing properties, and expanding the structures) were typically successful; however, listing rules was a strategy that was less correlated with successful answers. Two questions assessed reasoning and Question 2 (comparing relative acidity of protons) had a similar distribution of modes of reasoning as previously reported comparison questions in the literature[31,34] and aligned with the course expectations and context. However, students' reasoning to explain the relative contribution of resonance structures to the resonance hybrid was primarily descriptive (87%), aligned with how this analysis type is typically taught,[9] the expected answer, and the course setting.

Answers contained few representational errors (*e.g.*, errors in translating between resonance structures and the hybrid). The biggest representation error was seen in Question 12, where 35% of students drew a pentavalent carbon. Since this error was minimal (<2%) in previous studies assessing EPF and mechanisms,[37,51] this error could be related to the Lewis representation of delocalization specifically.

Approximately 10–20% of students used delocalization when not prompted and 19% of students used the resonance hybrid in a question that did not ask for it, potentially as a sense-making device. Similarly, when answering questions about LO6–10 that did not require justification, roughly 10% of students mentioned delocalization. In Question 2, students could use delocalization or inductive effect concepts to justify relative basicity; half of students used delocalization concepts. The other half give a variety of answers, which could indicate a preference for using another concept (inductive effects), an inability to recognize the relevance of delocalization for that context, or other reasons. Questions with explicit scaffolds or clearly stated expectations about which concepts to use could help students successfully use delocalization concepts for these questions.

Achieving LO1 (*Identify*) and LO2 (*Draw*) has led to higher success on the others LOs. In many cases, the LO1 and LO2 are part of the prior knowledge required for the latter LOs, and unsurprisingly the first two LOs would affect how students achieve the LOs.

These findings align with the context of our university and curriculum[36] and how the LOs have been intended and enacted.[9]

Limitations

We did not analyze in-depth how the concepts were taught. Therefore, alignment and links between student success, specific instruction, and other learning opportunities could not be assessed within the boundaries of our study. This investigation was limited by the exams and questions available, which came from a single course section. Many of the questions did not explicitly ask for justification or explanation, meaning many of the LOs could not be assessed fully and some may be overrepresented. The LOs could also be assessed in other ways.

Implications for research

This study analyzed students' written responses on exams, which allowed us to explore their reasoning and the chemical concepts they leveraged. Further investigation (*e.g.*, interviews) would be required to explore students' mental models of delocalization and why they used or did not use delocalization concepts in answering questions. Students who gave descriptive answers to some questions may have been able to give more sophisticated answers but did not choose to because of time constraints or believe it was not needed (*e.g.*, Question 1);[34] their decisions could be explored in further research.

Students sometimes did not apply delocalization concepts when it was appropriate or expected to do so; however, we do not know why (*e.g.*, could not recall, chose not to). Students sometimes struggled in questions that required the connection of delocalization with other concepts. This relationship could be investigated further to determine why students did not identify that resonance was relevant, and how the link between delocalization and other concepts affects students' overall organic chemistry skills.

Analyzing students' responses to each LO revealed unique errors and strategies but a more in-depth analysis could provide insight into students' thought processes. A further series of questions and various prompts could provide insight into how students approach delocalization-related questions. While we outlined the strategies used, we do not know why students chose or thought to employ them. The use of these strategies could be further investigated.

Implications for teaching

The findings from this work could be used to inform the design and evaluation of new teaching techniques or materials. The LOs are a basis for teaching the concept of resonance that can guide instructors in their teaching and assessments. Instruction should be aligned with the desired type of reasoning (*e.g.*, relational, causal), including the taught, practiced, and assessed portions of a course or program. Some LOs were connected to being able to achieve later LOs. These links could be used to design a learning progression for the subject of delocalization, which would help align the concepts within curricula.[54]

Some students did not recall or apply information about delocalization concepts. Therefore, formative assessment or practice of the concept could benefit students. Problems in which delocalization is implicit, explicit, or mechanistic would provide students opportunities to practice the skills.

OCI students achieved LO2 more than OCII students on the explicit delocalization questions. Constantly re-enforcing the concept, and giving students practice throughout their studies could help mitigate the results. Similarly, providing formative assessments during the course sequence could help identify students' skills using delocalization and identify areas needed for review.

Answers containing certain strategies, visualizing electrons delocalization, using properties, and expanding the structures, had correct answer more than those who did not. These strategies could be scaffolded for students. Listing rules was not connected with more successful answers, and as such moving toward more causal reasoning while teaching could provide the students with the skills to reason about delocalization and use delocalization concepts.

Students have the skills to use delocalization in multiple contexts. Using more practice questions, making expectations explicit, scaffolding the concept, and promoting rezoning and strategies could provide the students the tolls to use the concept.

Supporting Information

The SI contains background information on the LOs, the coding scheme, expected answers for each question, and inter-rater reliability data.

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Note

The authors declare no competing financial interest.

Acknowledgements

We thank Nicolas Streja for his work on the inter-rater reliability. MSC thanks the Social Sciences and Humanities Research Council of Canada for funding through a Canadian Graduate Scholarship – Doctoral (CGS-D).

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