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Students' Identification and Application of Models to Rationalize Organic Acid-Base Trends

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Abstract

Acid-base chemistry is an essential component of the undergraduate chemistry curriculum. Acid-base concepts are introduced in general chemistry and expanded on in organic chemistry, biochemistry, and other advanced chemistry courses. Through a mixed approach of surveys and think-aloud interviews, the proficiency of second-semester organic students in acid-base chemistry was measured. Students were given two questions, both requiring them to rank the acidity of three compounds and justify the ranking. The first question focused on substituted carboxylic acids, and the second question focused on substituted aromatic structures. Although most students were able to correctly rank both sets of molecules, the correctness of their justifications was structure-dependent. Students did better at justifying the acidity of the aromatic structures, but while they were more successful at ranking the acidity of the substituted carboxylic acid structures, students were largely unsuccessful at justifying the trend. Students often relied on memorization, attributing acidity to the presence of specific functional groups or substituents. Specific alternative conceptions observed in both surveys and interviews include the idea that resonance structures are always central in justifying properties for molecules that have π bonds, and that alkenes and alkynes have differing numbers of resonance structures given they have different bond orders. Finally, students had difficulty with identifying the most acidic proton and often selected sites based on content that could be memorized from lectures. Students were also asked to report their confidence in their answers on a 6-point Likert scale from 0–5, and statistically significant differences were observed between students who ranked compounds correctly versus incorrectly for both questions in the study. However, when comparing the correctness of the justifications, a statistical difference between reported confidence was only observed with the aromatic structures question. The substituted carboxylic acids question required the application of models and ideas that extended beyond memorization.

Keywords: Acid-Base Chemistry, Aromatic Molecules, Carboxylic Acids, Hybridization, Resonance, Inductive Effects, Alternate Conceptions, Confidence.

Introduction

As a central chemistry concept, acid-base chemistry is used to explain the structure and reactivity of organic, inorganic, and biological molecules, and is used to develop frameworks for qualitative and quantitative analyses. General or introductory chemistry courses introduce students to Brønsted-Lowry acid-base models and quantitative calculations involving pH, titrations, and buffers (ACS, 2015). There is an emphasis on the relationships between the magnitude of the K_a, acid strength, and conjugate base strength. On the other hand, Lewis acid-base theory and rationalizing acid-base trends using molecular structure are not discussed to the same extent in most introductory chemistry courses. However, these models are central to understanding organic chemistry concepts and are either revisited or introduced at the start of the organic sequence. Lewis acid-base theory and structural models provide insight not only into organic acidity and basicity, but also readily extend to explanations of related concepts like electrophilicity and nucleophilicity, and can even explain chemo- and regioselectivity in organic reactions. More than 85% of organic and biochemical reactions can be rationalized using acid-base concepts (Rossi, 2013; Stoyanovich, Gandhi, & Flynn, 2015). In the past two decades, chemical education research has predominantly focused on students' understanding of acid-base chemistry and potential pedagogical reforms in introductory chemistry (Cooper, Kouyoumdjian, & Underwood, 2016; Cox, Poehlmann, Ortega, & Lopez, 2018; Mercier, 2018). More recently though, research has been extended to assess students' understanding of acid-base chemistry in organic chemistry to identify alternative conceptions that persist from general chemistry or emerge as more sophisticated acid-base models are introduced (Bretz & McClary, 2014; Cartrette & Mayo, 2011; Duis, 2011; L. M. McClary & Bretz, 2012; L. T. McClary, V., 2011 ; Petterson et al., 2020; Schmidt-McCormack et al., 2019). The goal of this study is to assess students' use of models to rationalize acidity at the end of the second semester of organic chemistry (OC2). More broadly, the long-term goal of our studies is to identify and develop pedagogical reforms, particularly to address alternative conceptions early to provide students with stronger conceptual frameworks for future courses. One study (Bhattacharyya, 2006) noted the progression of alternative conceptions from undergraduate cohorts to chemistry graduate students, which illustrates the importance of addressing these issues.

Cartrette and Mayo (Cartrette & Mayo, 2011) outlined the relationship between students' understanding of the Brønsted-Lowry and Lewis acid-base models. Their findings supported that students relied on declarative knowledge to rationalize answers but were unable to extend this knowledge to solve complex problems. Much of organic chemistry requires using models to predict trends, which accounts for the challenges students generally note with organic chemistry. Research supports (Anderson & Bodner, 2008; Grove & Lowery Bretz, 2012) the idea that the transition from quantitative to qualitative thinking from general to organic chemistry requires students to have a deeper understanding of fundamental concepts, which explains why organic chemistry is generally regarded as a gatekeeper course. As noted (Bhattacharyya & Bodner, 2005; Grove & Lowery Bretz, 2012), with organic chemistry, rote memory does not reflect understanding and does not ensure success or mastery of the concepts. The challenges with using rote memory, particularly with acid-base concepts in the context of organic chemistry, have been noted in several studies. For example, students tend to associate acidity with specific functional groups (Bretz & McClary, 2014), rely on heuristics that seemingly support conclusions based on associations instead of more sophisticated explanations (L. McClary & Talanquer, 2011), depend on cues as a way to identify the appropriate strategy due to a lack of conceptual grouping (Petterson et al., 2020), and struggle to relate Brønsted-Lowry and Lewis acid-base models (Schmidt-McCormack et al., 2019). The latter observations support the reliance on rote memory to navigate problems and illustrate challenges students face in applying concepts and models.

Longitudinal studies have illustrated that students' use of models in acid-base chemistry becomes more sophisticated over time (Crandell, Kouyoumdjian, Underwood, & Cooper, 2019). However, related studies measuring reported confidence indicate that students continue to overestimate their understanding of the acid-base concepts (L. M. McClary & Bretz, 2012). Our study also incorporates a confidence ranking question to assess students' awareness of their abilities in ranking and explaining acid-base trends. Given students' prior experience in at least two other chemistry courses, the question arises whether this experience may impact students' self-awareness of their conceptual understanding.

One of the key models used to explain acid-base trends is resonance. Recent research regarding resonance identified alternative conceptions regarding students' understanding of resonance, which illustrates further challenges in using resonance to explain acid-base trends. Students focus on drawing resonance structures, and while they may successfully draw structures, they struggle with interpreting their meaning and applying embedded information to explain structure and reactivity (Duis, 2011; Kim, Wright, & Miller, 2019; Xue & Stains, 2020). This study expands on the existing research by assessing students' abilities to identify when resonance is pertinent in explaining acid-base trends.

To account for students relying on heuristics to accurately rank compounds' acidities, our study asked participants to provide a 2-3 sentence explanation to accompany their ranking. The results of this study establish which alternative conceptions students hold regarding how hybridization and resonance acidity affect acid-base chemistry, quantify the prevalence of these alternative conceptions, and inform instructional interventions to improve students' awareness of the scope and limitations of various acid-base models. This study was guided by the three research questions below:

Research Questions

1. How do second-semester organic chemistry (OC2) students apply the concepts of hybridization, inductive effects, resonance, and conjugation to rationalize acid strength?
2. What alternative conceptions do students have regarding these concepts, and which are most deeply rooted?
3. How do students gauge their own understanding of organic chemistry concepts when determining acid strength?

Methods

Student Participants and Data Collection

These studies were performed at a large private southeastern research-intensive university. All students were informed of their rights as human research subjects, and students who did not consent to their responses being used for this study were omitted from data analysis. Only students residing in the United States and over 18 years of age were included in the study. All data were handled per the Institutional Review Board (Protocol #2021-0182); when identifiers were collected, the data were anonymized and not shown to professors until after final grades were posted.

These studies followed two cohorts of OC2 students, from different instructional terms, taking the course with different professors. Due to Covid-19 restrictions, the two cohorts of students experienced the course through different instruction media. Cohort A (N = 65) from the 2020 Fall semester experienced the course completely remotely, and the survey was distributed as a for-credit assignment. Cohort B (N = 30) during the 2021 Summer semester was a hybrid course, with some students attending in-person whereas others were completely remote; the survey was distributed as an encouraged review assignment for the final exam. For both cohorts, the surveys were distributed at the same point in time during the academic term, after the class covered enolate chemistry.

Aside from COVID-19 restrictions preventing control of the instruction medium, the study also did not control for students' past experience with chemistry (Advanced Placement, International Baccalaureate, introductory college-level general chemistry). Of note is the unique introductory chemistry curriculum at the institution studied; students typically take one semester of general chemistry, then two semesters of organic chemistry, before taking the second semester of general chemistry. The chemistry courses are not separated by students' intended major or pre-professional track. Lastly, not every section achieved high response rates (Cohort A 98%, Cohort B 50%).

Along with surveys, data were also collected using think-aloud interviews (Cartrette & Mayo, 2011; Petterson et al., 2020). The questions discussed in this work were a 15-minute component of one-hour-long interviews that were conducted over Zoom, and the problems were presented by the interviewer via the screen sharing function. The interviewer filled out the student participants' answers to the ranking questions, then referred to the recording and transcript for their explanations. The interviews were recorded, where OC2 student participants kept their video off and microphone on; all files were password-protected and transcribed to eliminate identifiers and protect anonymity. Following the interviews, the main researcher noted general observations for each, serving as a secondary data source along with the recording and transcript. Further analysis of data is described under Qualitative Analysis.

Development of Research Instruments

The question involving carboxylic acids with differentially hybridized carbon chains (Q1) was designed because no existing research has investigated how organic chemistry students rationalize a compound's acidity when both resonance effects and hybridization/inductive effects are simultaneously present. Including both concepts provides an effective way to probe whether students are merely memorizing trends, trying to apply a single model to several different situations, whether they can successfully parse through distractors, etc.

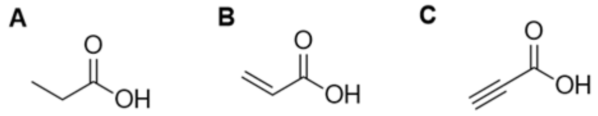
On the other hand, the question containing substituted phenols (Q2) was adapted from ACID I, designed by McClary and Bretz (Bretz & McClary, 2014; McClary & Bretz, 2012) We maintained two out of the three molecules as used in ACID I (*para*-methylphenol, *para*-nitrophenol), but modified the third molecule to *meta*-nitrophenol to specifically probe students' understanding of resonance versus inductive stabilization of negative charge. Q2 was used primarily as a calibration tool because student performance on ACID I has already been thoroughly analyzed (McClary & Bretz, 2012).

Each overarching question in the surveys and interviews included several sub-questions (*Figure 3.1.*): (a) a ranking of the three molecules from the most to least acidic, (b) an open-ended explanation question (no text limit, but instructions suggested that students write 2-3 sentences), (c) a confidence ranking question on a 6-point Likert scale from 0–5, adapted from Caleon and Subramaniam (Caleon & Subramaniam, 2010).

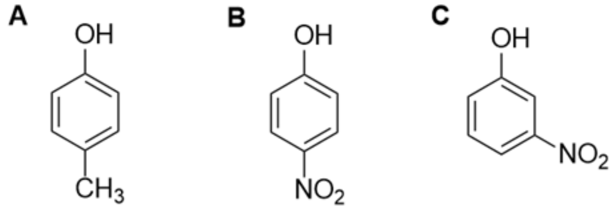
The interview only investigated Q1, since Q2 has already been thoroughly investigated (McClary & Bretz, 2012). The interview question was identical to Q1, only with more opportunities to probe the students' thought processes. Trial interviews were conducted with three chemistry majors, otherwise uninvolved with the study, who provided feedback regarding additional probing questions to ask, how to frame questions more effectively, and how to proceed with interview logistics.

Research Instruments

Q1: Hybridization Acidity



Q2: Aromatic Acidity



a) Rank the above molecules in order of acidity, with 1 being most acidic and 3 being least acidic.
   Molecule A
   Molecule B
   Molecule C

b) Please justify your ranking with relevant chemical reasoning. A 2-3 sentence explanation will suffice.

c) On a scale from 0-5, how confident are you in your answers to questions a) and b)? 0 = not confident at all, 5 = completely confident

Figure 3.1. Sets of structures used to probe students' understanding of hybridization, inductive effects, resonance, conjugation, and their relation to acid strength. Q1 was asked in both the surveys and interviews. Q2 was asked in only the surveys.

Data analysis

Qualitative analysis

Four researchers discussed then came to a consensus on the scoring criteria (*Table 3.1.*) to use for each survey/interview question. Together, the same researchers scored each student's explanations as correct, partially correct, or incorrect, following the scoring criteria. Furthermore, the explanations were coded both deductively and inductively; deductive codes were taken from the conclusions of the ACID I studies, whereas the inductive codes came directly from the students' survey responses. Three researchers independently reviewed the transcripts and audio/visual data from the interviews. All three researchers noted observations of (alternative) conceptions and performed an initial coding of responses as correct, partially correct, or incorrect. The research team then reconvened to discuss their findings to reach a consensus on the final coding results. These are presented in Sankey diagram format for the 10 OC2 students interviewed.

Table 3.1. Scoring Criteria for Rankings and Explanations

Question	Accuracy	Scoring Criteria
Q1 Ranking	Correct	C > B > A in acidity C, prop-2-ynoic acid, pK_a = 1.89 https://pubchem.ncbi.nlm.nih.gov/compound/Propiolic-acid B, prop-2-enoic acid, pK_a = 4.25 https://pubchem.ncbi.nlm.nih.gov/compound/Acrylic-acid A, propanoic acid, pK_a = 4.88 https://pubchem.ncbi.nlm.nih.gov/compound/Propionic-acid
	Incorrect	Not C > B > A ranking
Q1 Explanation	Correct	Carboxylic acid proton is deprotonated AND Increasing s-character of the carbon chains makes them more electronegative and inductively withdrawing, better stabilizing the conjugate base; trend needs to be applied across all three molecules
	Partial	Increased s-character/electronegativity/inductive effect of the carbon chain makes molecules more acidic, but only applies this to alkynes
	Incorrect	Wrong proton deprotonated AND/OR Only used resonance and/or conjugation to justify ranking AND/OR Incorrect chemistry (e.g., alkynes have more s-character, alkynes are electron-donating, etc.)
Q2 Ranking	Correct	B > C > A in acidity The reported pK_a values are provided as a reference (Liptak, Gross, Seybold, Feldgus, & Shields, 2002): B, *p*-nitrophenol, pK_a = 7.91 C, *m*-nitrophenol, pK_a = 8.13 A, *p*-methylphenol, pK_a = 10.26
	Incorrect	Not B > C > A ranking
Q2 Explanation	Correct	Para-EWG (electron-withdrawing group; nitro) stabilizes the conjugate base through resonance and inductive effects; meta-EWG stabilizes the conjugate base through inductive effects; para-EDG (electron-donating group; methyl) destabilizes the conjugate base through inductive effects OR Accurately compares p-EWG and m-EWG (resonance + induction versus induction), AND explains why EWGs stabilize and EDGs destabilize the conjugate base

Table 3.1. continued

	Partial	Accurately states EWGs decrease and EDGs increase electron density in the conjugate base and resulting effect on acidity, BUT does not compare p-EWG and m-EWG (resonance + induction versus induction) OR Accurately compares p-EWG and m-EWG (resonance + induction versus induction), BUT does not discuss effect of EDGs on electron density and conjugate base stability OR Discusses all three substituents, BUT does not explain that m-EWG cannot resonance stabilize
	Incorrect	Wrong proton deprotonated AND/OR Incorrect chemistry (e.g., EWGs increase electron density, nitro group is an EDG, etc.) AND/OR Does not discuss anything listed in "Partial"

Quantitative analysis

Data from the surveys were first tested for normality. Visual inspection of a histogram of student confidence (Likert scale) versus a normal Gaussian curve and calculations of skewness and kurtosis suggested the data were normally distributed. However, the Shapiro-Wilk test suggested otherwise ($p \approx 10^{-6}$), thus nonparametric tests were used for all statistical comparisons to be most accurate.

The survey data from the two OC2 sections were compared to investigate statistically significant differences in accuracy (*Table 3.2.*) and mean confidence. Based on two-tailed Fisher's Exact tests for accuracy, and Mann-Whitney U tests for confidence (*Table 3.2.*), no statistically significant differences were found between the two OC2 sections, thus the survey results were aggregated. The aggregated confidence data were then compared in several ways: based on ranking accuracy, explanation accuracy, and both ranking and explanation accuracy. The one-way Kruskal-Wallis test was used to make multiple group comparisons, and the Mann-Whitney U test was used to make pairwise comparisons. A p-value of 0.05 or less was considered statistically significant for all tests performed. All visualizations and statistical calculations discussed above were performed in R.

Table 3.2. Statistical Comparisons and p-Values Between Survey Cohorts

Question	Comparison	p-Value (Fisher's Exact or Mann-Whitney U Test)
Q1	Ranking Accuracy	0.14
	Explanation Accuracy	0.19
	Confidence	0.69
Q2	Ranking Accuracy	1.00
	Explanation Accuracy	0.52
	Confidence	0.50

Results and discussion

The objective of the research study was to gauge students' abilities in acid-base chemistry at the end of the second semester of organic chemistry. The chemical structures assessed in the study are shown below. Throughout the discussion, the substituted carboxylic acid structures in Q1 will be referred to as the "hybridization structures" because these structures differ with respect to the hybridization of the alkyl, alkenyl, and alkynyl substituents. The substituted aromatic structures in Q2 will be referred to as the "aromatic structures." These compounds are especially pertinent because a central focus in OC2 includes a discussion of the structure and reactivity of carboxylic acids and aromatic molecules. The surveys consisted of two parts per structure: (a) ranking structures based on their acidity, (b) explaining their rationale for the proposed ranking, with the explanation providing insight into students' reasoning to identify alternative conceptions and propose interventions. For both the ranking and explanation items, students reported confidence in their responses on a scale of 0–5, with 0 being the lowest and 5 being the highest confidence. The Dunning-Kruger effect suggests that students tend to overestimate their abilities, which has been observed in the context of organic acid-base chemistry (L. M. McClary & Bretz, 2012). Therefore, the confidence data was collected to gauge students' awareness of their understanding after three semesters of chemistry (including general chemistry and first-semester organic chemistry). Data presented will focus on students' confidence, ranking accuracy, and correctness of their explanations. Statistical comparisons between confidence, based on student performance, will be reported to measure students' abilities to gauge their understanding, with the acknowledgment that higher confidence does not imply greater performance.

Q1: Hybridization Acidity

Figure 3.2. compares students' reported confidence with their performance in ranking the acidity of the hybridization structures. Students who correctly ranked the acidity reported statistically higher confidence ($p = 0.0053$) than those who did not, which is counter to the findings by McClary and Bretz (L. M. McClary & Bretz, 2012). The difference in awareness could be attributed to the organization of the questions or to the timeline of the survey's distribution. *Figure 3.2.* summarizes students' reported confidence by their performance in explaining the trends in acidity. The explanations were coded as correct, partially correct, or incorrect as outlined in the **Methods** section.

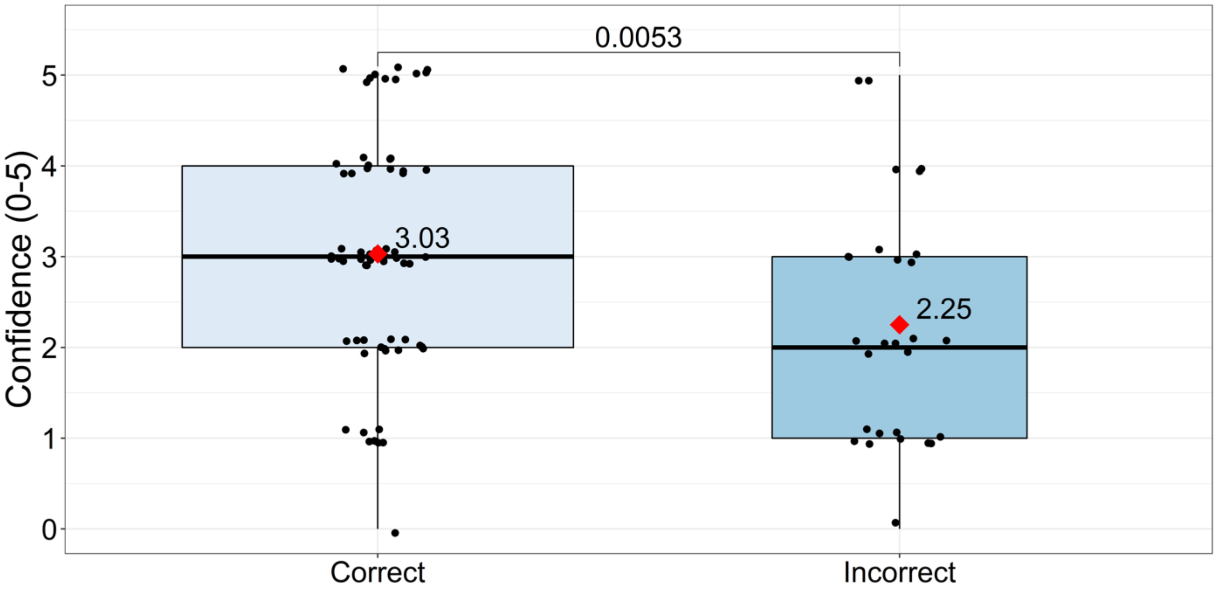


Figure 3.2. A comparison of students' (N = 95) reported confidence based on whether they correctly or incorrectly ranked the acidity of the hybridization structures. Red diamond denotes the mean.

Statistical differences were not observed for students' reported confidence based on the correctness of their explanations. Of the 66 students who correctly ranked the acidity, only 6/66 ≈ 9% provided a correct explanation and 7/66 ≈ 11% provided a partially correct explanation. Given the sizable drop in performance between the two tasks, the responses were analyzed and coded to acquire a greater perspective on students' rationale and to identify alternative conceptions. The qualitative codes and the frequency to which they were observed are outlined in *Table 3.3.*

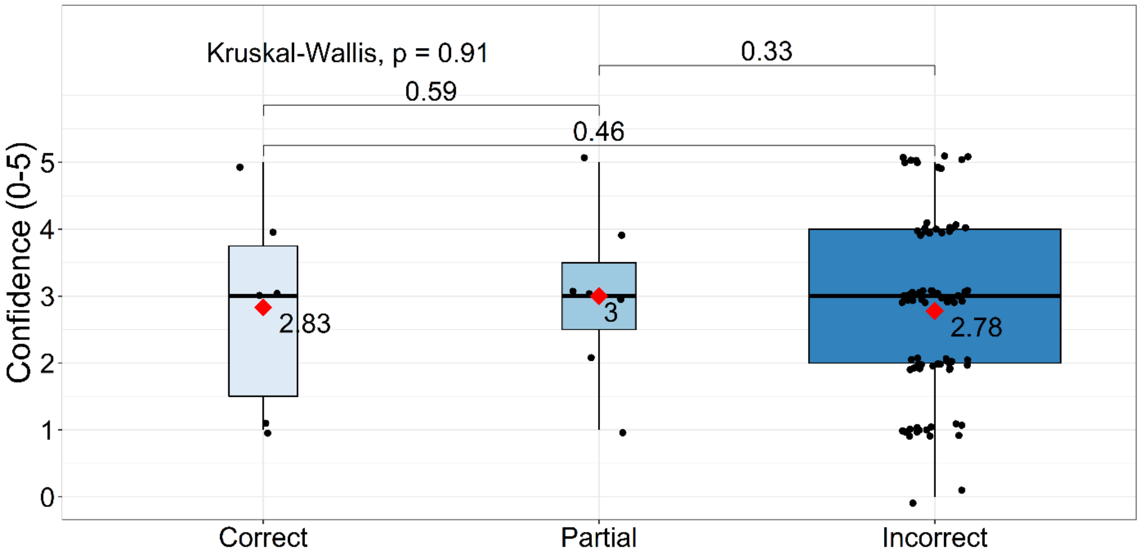


Figure 3.3. A comparison of students' (N = 95) reported confidence and the correctness of their explanations regarding the acidity of the hybridization structures. Red diamond denotes the mean. The Kruskal-Wallis test (p = 0.91) indicates that no statistical difference was observed when comparing all three groups of students. Further analysis using the Mann-Whitney test suggests no statistical differences were observed between any pairs the three groups.

Table 3.3. Deductive and Inductive Codes for Student Explanations to Q1 – Hybridization Acidity

Code Descriptions	Percentage of students (N = 95)
Deductive Codes	
Mentioning conjugate base stability	35
Equating functional groups with acidity	20
Inductive Codes	
Stabilizing the conjugate base makes molecules more acidic	29
Alkynes have more s-character, which makes them more acidic	28
Carbon-centered proton will be deprotonated	22
Alkynes are more acidic than alkenes, which are more acidic than alkanes; no justification provided	15
Increased s-character in the carbon chain means they are more electronegative / inductively electron-withdrawing, which makes alkynes more acidic than alkenes, which are more acidic than alkanes	14
Oxygen-centered proton will be deprotonated	13
Alkynes contribute more to resonance than alkenes and alkanes	12
Alkenes contribute more to resonance than alkynes and alkanes	10
Alkynes and triple bonds are electronegative/ have an inductive electron-withdrawing effect; does not explicitly discuss s-character	7
Alkynes do not contribute as well to resonance compared to alkenes due to the allene/cumulene structure	7
Alkenes have more conjugation, which makes them more acidic than alkynes and alkanes	6
Alkynes have more conjugation, which makes them more acidic than alkenes and alkanes	5
Resonance within the carboxylate makes all three molecules more acidic	4
Alkynes have shorter / stronger bonds than alkenes than alkanes, which makes them more acidic	4
More resonance between the C=C and C=O of alkenes and alkynes makes molecules B and C more acidic	2

The qualitative codes in *Table 3.3.* imply students were successful in ranking the acidities of the hybridization structures despite using flawed logic. The correct reasoning should have considered the inductive effect from the neighboring alkyl, alkenyl, and alkynyl groups, with the alkynyl group being more electronegative because of the increased s-character. More s-character implies a stronger nuclear charge because of the proximity of the s-orbital to the nucleus relative to the p-orbital. An increase in the electronegativity of a neighboring substituent increases acidity through inductive effects, in which neighboring groups withdraw, or pull away electron density through σ bonds. Therefore, the alkynyl substituent "pulls away" more electron density from the carboxylate group in the conjugate base, reducing the electron density on the base. As electron density on the site decreases, conjugate base strength decreases and stability increases, which results in an increase in acid strength. Only 14% of the 95 students surveyed correctly considered both the inductive effects and s-character (hybridization). The inductive effect is normally introduced in lectures using halogen-substituted compounds to illustrate the pull of electron density by the electronegative halogen substituents. *Figure 3.4.* summarizes structures commonly outlined in the textbook and on typical assessments. These structures become the benchmarks students use to rationalize inductive effects.

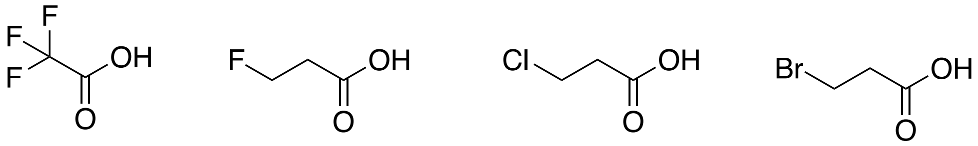


Figure 3.4. A summary of molecules generally used to illustrate the inductive effect. Similar structures were used to illustrate the inductive effect in the standard text (Jones & Fleming, 2010).

A substantial number of students, 46%, applied a resonance or conjugation argument. Resonance is an argument used to account for the differences in the acidity of acetic acid versus methanol, and students have seen this argument in their textbooks, in lectures, and on assessments. Additionally, there are resonance structures that can be proposed with the alkenyl and alkynyl substituents (*Figure 3.5.*), but the argument would not fully account for the differences in acidity. Neither resonance structure B3 nor C3 would be considered a pertinent resonance structure; they would both be exceptionally minor resonance contributors, as they unnecessarily incorporate an incomplete octet on carbon and multiple formal charges. Furthermore, a carbocation is less stable on an sp- compared to an sp^2-hybridized carbon because of the increased electronegativity of the former, which further minimizes the contribution of resonance structure C3, even relative to B3. Finally, resonance structures B3 and C3 also do not illustrate a reduction in electron density at the carboxylate; in fact, the electron density at the carboxylate is greater with both oxygens having a negative formal charge, which would support an increase in basicity and a decrease in acidity. As noted above, the argument that the alkynyl substituent could support additional resonance representations relative to the alkenyl substituent is incorrect, which was stated in 12% of responses. Students are likely using bond order to support this rationale; however, although the alkyne has a triple bond, only one of the two π bonds would contribute to resonance. For resonance and conjugation purposes, the π-systems must be within the same plane. Yet with the alkynyl substituent, only one π bond would be coplanar, while the other would not contribute to the conjugation.

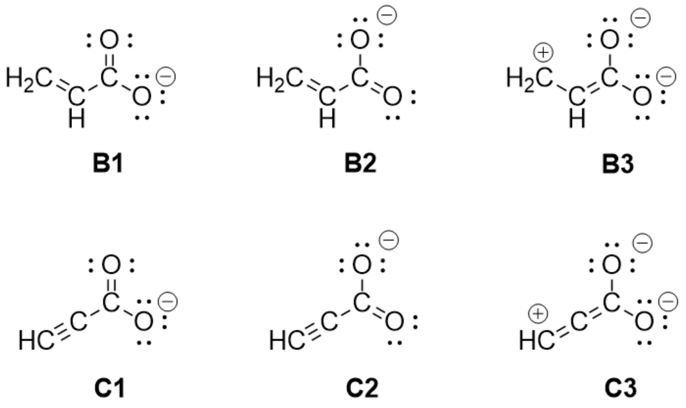


Figure 3.5. Possible resonance structures for the alkenyl- and alkynyl-substituted carboxylic acids.

From the resonance arguments, OC2 students articulated two alternative conceptions as parts of their rationales. The first alternative conception is that resonance can always be used to justify acidity when double or triple bonds are present. Indeed, resonance does play a role as noted, but the resonance forms should be drawn and carefully analyzed to rationalize changes in electron density. Resonance structures constitute key representational models in organic chemistry, but other models and arguments remain pertinent. The second alternative conception is that double and triple bonds yield different numbers of resonance structures. Orbital overlap occurs within a plane (along one axis), and in the triple bond, the two π bonds are orthogonal. Regarding student understanding of resonance, Xue and Stains (Xue & Stains, 2020) found that students focused more on the Lewis structure representations and faced challenges when explaining the concepts of resonance and resonance hybrids. In our study, students identified the importance of resonance, but as with the Xue and Stains' study, students did not accurately explain the connections between resonance structural representations and the property they were rationalizing. Similar ideas were reported (Brandfonbrener, Watts, & Shultz, 2021; Duis, 2011) in which students focused more on drawing resonance structures without understanding the embedded concepts.

In lectures, the acidity of the C-H bond of alkanes, alkenes, and alkynes is compared using s-character, with the alkyne C-H bond being more acidic because of the increased s-character and subsequent increase in electronegativity. The acidity of the alkyne C-H bond was noted in 43% of responses, but there was no additional elaboration for why this is significant for this system. Additionally, 22% argued the C-H bond would be deprotonated instead of the more acidic O-H bond of the carboxylic acid. Therefore, a potential alternative conception can be proposed based on these arguments in which students are considering a less acidic proton. This could stem from either only using facts from lectures or not fully analyzing all potential acidic protons in the structure. Using the acidity of the C-H bonds, students could correctly rank the structure in terms of increasing acidity, but as with resonance, this works only by coincidence and does not demonstrate a complete understanding to rationalize the acid-base properties.

The following responses, ordered correct, partially correct, and incorrect, provide representative explanations from the survey. These responses reiterate the points noted above regarding the incorrect use of resonance or the incomplete use of s-character to justify their ranking.

Survey Response 1 [Correct]

"sp hybridized carbons are more electronegative than sp2, which is more electronegative than sp3. Carboxylic acids lose the proton bound to the oxygen when in the presence of a base, creating a carboxylate anion. Due to the polar effect, the more electronegative sp hybridized carbon can stabilize the negative charge on the oxygen of the anion better than the sp2 carbon, which can stabilize the anion better than the sp3 carbon."

Assessment: The student correctly identifies the loss of the oxygen-centered proton to form the carboxylate, understands the relationship between hybridization and inductive effects, and correctly predicts relative acidity.

Survey Response 2 [Partial]

"sp-hybridized carbon atoms (50% s character) are more electronegative than sp2-hybridized carbon atoms (33% s character), which are more electronegative than sp3-hybridized carbon atoms (25% s character). Because of this, the negative charge of the conjugative base is best stabilized by the alkyne group, then the alkene group, then the alkane group."

Assessment: The student uses a hybridization argument and accurately connects hybridization to electronegativity. However, they do not make the final connection to inductive effects. It is also unclear if they are referring to the carbon- or oxygen-centered proton.

Survey Response 3 [Incorrect]
"Alkynes are the most acidic as it forms the weakest and most stable conjugate base as it does not want to receive any hydrogens. Alkynes also have more S character, making protons more easily released."

Assessment: The student focuses on the deprotonation of the alkyne based on the s-character. The student correctly recalls the role of the s-character but does not consider the acidity of the carboxylic acid.

Survey Response 4 [Incorrect]
"Alkynes have a lower pK_a value than alkenes, which have a lower pK_a value than alkanes."

Assessment: The student recalls a set of facts but does not apply concepts beyond a recall level.

Survey Response 5 [Incorrect]
"The conjugate bases of B and C are more stable due to there being more resonance. Of these two, the alkyne has even more resonance."

Assessment: The student rationalizes that a higher bond order results in more resonance.

The Sankey diagram in *Figure 3.6.* illustrates students' trajectories in successfully ranking and explaining the acidity of the hybridization structures. The diagram supports conclusions drawn above in which students were able to accurately rank the acidity using incorrect logic. Notable is the sizable drop in the accuracy of the ranking task compared to the explanation.

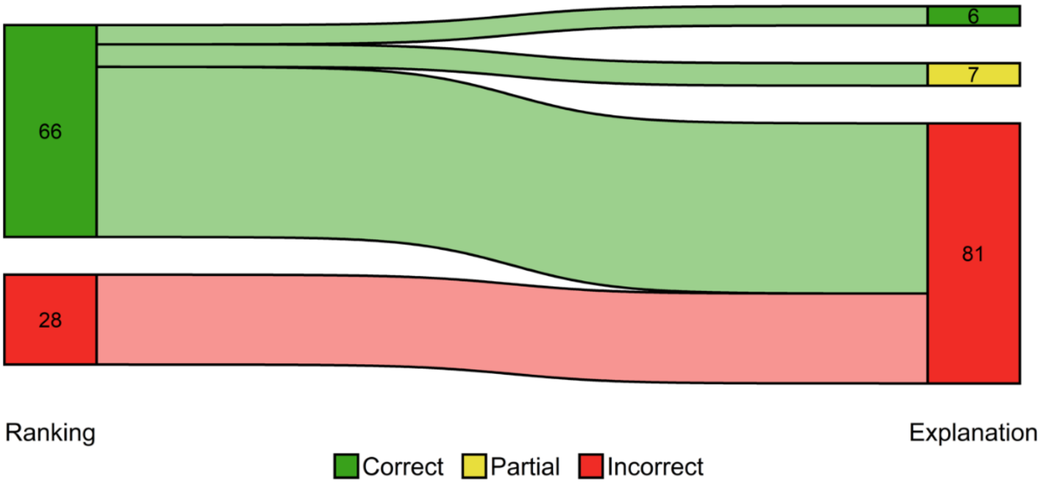


Figure 3.6. A Sankey diagram comparing students' ranking and explanations on the hybridization question in the survey (N = 94, one removed due to incomplete response). Note the sizable number of students who were able to successfully rank the acidity of the structures but were unsuccessful in correctly explaining the rationale.

Additional statistical analysis of reported confidence based on the ranking and explanation correctness was completed as shown in *Figure 3.7*. Note the statistical difference between students who incorrectly ranked the acidity versus those who correctly ranked the acidity but incorrectly explained their rationale. There was no statistical difference between students who correctly ranked and explained versus those who correctly ranked but incorrectly explained their rationale. Students who incorrectly ranked the molecules were statistically less confident in their responses than the other groups. It appears that students who knew the trends for alkane, alkene, and alkyne acidity, and knew resonance was a key factor, had a high degree of confidence in their answers, even if their rationale may have been flawed. This illustrates considerations when designing assessments: Can students correctly answer assessment questions without actually understanding the content? What are we truly assessing, and are the questions achieving that purpose? Ranking items are quite common tasks on organic chemistry assessments, particularly in the United States. This illustrates that while common, these types of assessment items have their limitations.

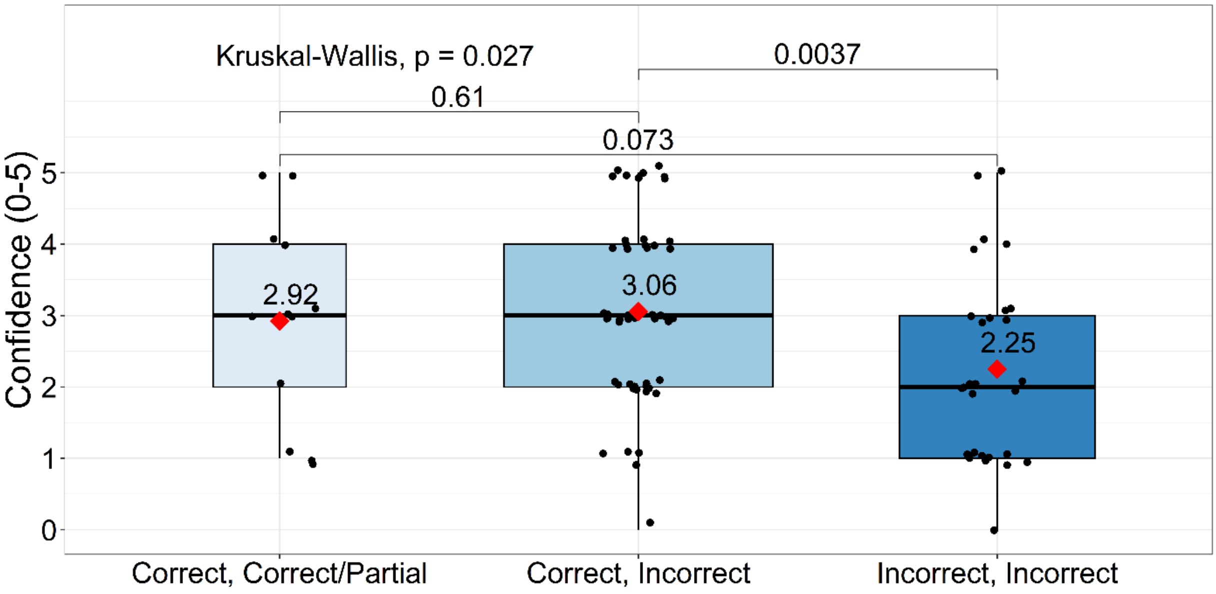


Figure 3.7. A comparison of confidence for students (N = 94) based on their ranking and explanation, correctness formatted as [Ranking, Explanation]. Red diamond denotes the mean. The [Correct, Correct] and [Correct, Partial] groups were aggregated following the results of *Figure 3.3.* and *Figure 3.6.*; there was no statistically significant difference in the students' confidence, and all students who explained correctly or partially correctly also ranked correctly. The Kruskal-Wallis test (p = 0.027) indicates that a statistical difference was observed when comparing all three groups. Further analysis compared each cohort using the Mann-Whitney test. Between the specific cohorts, a statistical difference was observed between the [Correct, Incorrect] and [Incorrect, Incorrect] groups.

To validate the survey findings, 10 interviews were conducted. Students' interview responses are summarized in the Sankey diagram in *Figure 3.8.* Of the 10 students interviewed, 5 correctly ranked the acidity, but none of the students were able to successfully explain the ranking. Similar explanations were provided as outlined above in which resonance, the acidity of the C-H bond, conjugation, and s-character were all noted, but these concepts were applied incorrectly or only partially correctly to account for the observed trend. Example explanations from the interviews are provided below:

Interview 1 [Incorrect (B > C > A), Incorrect]

Student: "Okay, so I think I'm going to put C as the most acidic, so C as 1, B as 2, and then A. So, I guess I can start talking. The reason I'm a little hesitant — I think B is definitely above A because you get more resonance there, which can kind of help, and it's also conjugated, and conjugation is happiness, from what I've learned. But with C, I'm a little scared, because if I'm thinking about, like, the hydrogen on the oxygen goes away, and you get a resonating carboxylate -- with that alkyne, if it chooses to participate in, and kind of help out — it's going to have like, I forgot the molecule, like, allene — I don't remember if there's any stability things we need to remember about allenes, but a little hesitant about that. So, I might honestly, you know, not super confident on this one, but let's put B above C, because C is a little bit weird. The reason I wanted to put C in the start is obviously, like, alkynes are the most acidic out of our little branchy things, because you have, like, the most s-character. Also, for acidity, I remember I talked with Professor X, my old professor for OC1, and he mentioned like, when you look at really niche pK_a stuff, you should always think of it like, the other hydrogens. So I'm looking at C, and like, there's one other hydrogen on the other side, which would be the most acidic carbon-hydrogen, hydrogen attached to a carbon. Let's just keep B > C > A, why not."

Assessment: The student rationalizes the acidity trends using both resonance and s-character. They rationalize that the alkynyl-substituted acid will be more acidic based on the alkyne acidity. The student does expand on why they are assessing the acidity of the alkyne by assessing the acidity of all protons. This is a valid point—we always assess the acidity of all protons. The limiting factor with the response is the failure to connect the ideas and utilize the inductive effect to explain the trend.

Interview 2 [Incorrect (A > B > C), Incorrect]

S: "Yeah, so B and C — electrophilicity, I believe is tied to acidity. So, if you have a more electrophilic compound, it would be more acidic. And if you look at B and C, there's resonance, and if a carbocation were to form on the carbonyl, there would be resonance with the carbon-carbon double bond, and with the alkyne in C. That would just reduce electrophilicity, that partial positive charge on the carbonyl right there, and that's how it reduces the acidity. That would just make it a lot harder for that acidic hydrogen on the right (-OH) to be pulled off, if you have resonance right there. And then if you look at A, there's no resonance there, so that's just a typical carboxylic acid."

Interviewer: "Okay, are you saying C has more resonance than B because it has two double bonds, or two π bonds?"

S: "See, I was debating that but I'm not sure. Yeah, I don't know. I mean, yeah, I don't know if we've ever — we might've, or maybe I just forgot it, but like, doing resonance with alkynes. Yeah, I'm not entirely sure, but yeah I'll just stick with my answer."

Assessment: The student uses a resonance argument to justify the answers. However, the student's rationale is jumbled. The student acknowledges an increase in acidity due to resonance but does not adequately explain why. Several statements are unclear, such as, "if a carbocation were to form on the carbonyl." The student realizes there are no resonance structures with the alkane moiety in molecule A, but they do not fully illustrate a grasp on either resonance or how resonance arguments can be used to justify acidity. Furthermore, when probed to consider similar resonance structures in C as in B, they fall back onto recall patterns; if it was not discussed in class, it probably does not play a role.

Interview 3 [Correct (C > B > A), Incorrect]
S: I know the oxygen on the carboxylic acid is what's going to leave, and off the top of my head, I feel like alkynes are more acidic because there's more s-character, so then I would rank C as the most acidic, and then B as the second one, and then A is the third.

I: Okay, and so you said this oxygen from the carboxylate is going to be the one leaving, is that what you said?
S: Well yeah, the H.
I: So, the proton attached to this oxygen.
S: Yeah, it's going to form a carboxylate.
I: Okay, and then you also said alkynes are more acidic than alkenes, which are more acidic than alkanes, because these carbons have more s-character, right?
S: Yes.
I: So, I have a question then. Your first statement is referring to this proton (-OH) being the most acidic. Your second statement is referring to this carbon-centered proton being the acidic one.
S: Yes.
I: Which one do you want to focus on?
S: I'm guessing only one proton is going to leave?
I: Uh-huh.
S: I think my ranking is still going to stay the same. But for C, I think the proton on the alkyne is more likely to leave than the proton that leaves to form the carboxylate.
I: Okay. So, you're saying for C, at least, this alkyne proton is going to be the one that leaves, whereas for B and A, it's going to be the carboxylate proton?
S: Yes.
I: Okay, we can go with that.
S: Okay, yeah, I'll go with that.
I: Alright, and then, how would you justify this ranking then, based on the protons that leave?
S: Okay, so the first one, for C, I would justify that because of the s-character I mentioned before — the higher s-character makes it more acidic. And I think that (alkyne) one is more likely to leave than the carboxylate, just because, in my head it seems like a stronger acid.
I: Okay, and so, why does more s-character make something more acidic?
S: I think it's due to the positioning of the orbitals, so with that carbon (alkyne), it is sp-hybridized. And since this is a triple bond, there are two orbitals that are going to be perpendicular — two orbitals are used to form the additional bonds — and then, I feel like the one orbital that's attached to the hydrogen is like, pointing away, which makes it easier to be deprotonated.

Assessment: The student accurately recalls the relationship between s-character and acidity; the student also understands the orientation of the π bonds in the alkyne. However, they argue the deprotonation will occur at carbon in the alkynyl-substituted molecule, versus the oxygen in the other two, reflecting a tendency to latch onto the idea of "alkynes being more acidic."

Interview 4 [Incorrect (B > C > A), Incorrect]
S: I think it's A > B > C. Oh, hold up, but then again, resonance probably has a role in this. So, I'd say B is the least acidic.

I: B is the least, okay. So, like this, A > C > B?
S: Yeah.
I: Okay, and what makes you say this ranking?
S: So, this is my reasoning. So, B is resonance-stabilized, which makes it more stable, which means it doesn't want to — it's going to be a weaker acid — oh wait, never mind — B is the most acidic, I change my mind. Because the conjugate base can be resonance-stabilized, making it more stable.
I: Okay. Where is the resonance in the molecule?
S: Because there's a double bond attached to the oxygen, and the double bond (C=O) can be moved around across the three double bonds. There's going to be a lone pair on the oxygen attached to the H, which can contribute to the resonance as well.
I: Okay, so you're saying, after we lose this proton (-OH), we'll have an extra lone pair on the oxygen, and then that oxygen, plus these two double bonds (C=O and C=C) will all be in resonance.
S: In resonance, yes.
I: Okay.
S: And then, so I think that's the most acidic. And then, I think the alkyne will be the least acidic because the triple bond is going to withdraw the electron charge — never mind, so that's more acidic than A — so it goes B > C > A, last answer.
I: Okay.
S: So, I think the alkyne is more acidic because the triple bond withdraws electron density from the H, making it more acidic.
I: Okay, and then A has none of those things that you just talked about, right? So, it will be the least acidic.
S: Yeah. I guess all can form resonance with the double-bond O, B just forms it with the other double bond too.
I: Okay, so you're saying all of them have resonance at this right side of the molecule (carboxylate moiety), but B also has resonance with the left part of the molecule (carbon chain).
S: Yeah.
I: I have a question for you then. Does C have that same kind of resonance as B?
S: Because it's a triple bond, I don't remember ever — I'm not sure — I don't remember ever learning about triple bonds contributing to resonance. I don't think so, but I could be wrong.

Assessment: The student is applying a resonance argument but demonstrates uncertainty between the alkenyl- and alkynyl- substituted carboxylic acid. Again, like in Interview 2, when probed further about similar resonance within molecule C as in B, the student falls back onto memory recall strategies. However, this represents a gap in the thought process; just because a concept is discussed in class does not mean it is applicable in every scenario. In this hybridization-focused question, the tendency of some students to latch onto resonance between double bonds reflects a lack of critical thinking during the problem-solving process, where they immediately grasp at models they have seen before without considering their limitations.

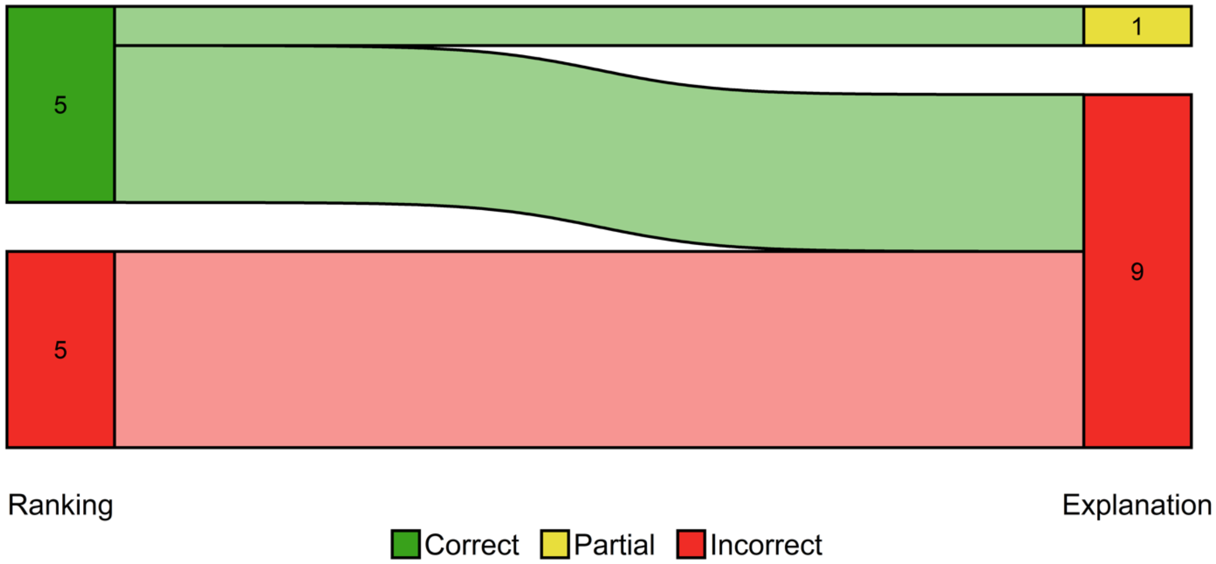


Figure 3.8. A Sankey diagram comparing students' (N = 10) ranking and explanations on Q1 in the interview. Only half of the interviewees were successful in ranking the items, and of these only one provided partially correct reasoning.

To reiterate the research questions, because of the double and triple C-C bonds on the substituents, 46% used a resonance argument to explain the trends in acidity. The s-character or hybridization was explained in 43% of responses but some students (22%) argued that the C-H bond would be the more acidic site instead of the O-H bond of the carboxylic acid. Therefore, regarding *the first research question: How do OC2 students apply the concepts of hybridization, inductive effects, resonance, and conjugation to rationalize acid strength?* It is clear that students remember key facts from lectures or textbooks, but often they did not extend and apply these concepts to new structures. Similar findings have been reported about students' application of resonance (Brandfonbrener et al., 2021) and with explaining acid-base trends (Bretz & McClary, 2014), but this study provides an extension by asking students to identify the most appropriate model to explain the trend. *The second research question focused on the alternative conceptions students demonstrate.* Three alternative conceptions were identified: the first two focus on resonance, with one being that resonance is always the "answer" regarding structures that have double or triple bonds. The second alternative conception is the idea that as bond order increases (from a double to a triple bond), the number of resonance structures also increases. Resonance is introduced in introductory chemistry and reiterated throughout organic chemistry, which may explain its prevalence as an alternative conception that influences student rationale. The third alternative conception focuses on the more acidic site. Some students used structural cues and rote memory to identify the more acidic sites rather than carefully analyzing the acidity of each proton, which is consistent with similar studies in organic chemistry (Bhattacharyya, 2006; Bretz & McClary, 2014). *Finally, regarding the third subpart in every question probing confidence*, students who incorrectly ranked the acidity did report statistically lower confidence in their answers, but students who correctly ranked the items using flawed logic reported the highest confidence in their answers of the three groups. This was expected given the design of the problem—in which students were expected to use incorrect models in their justifications.

Q2: Aromatic Acidity

To provide a comparison with our findings concerning the hybridization structures, the second survey question focused on the acidity of substituted aromatics compounds. This is a standard question in organic chemistry, and students have certainly encountered similar problems in the textbook, during lectures, and on assessments. Because of this familiarity, we hypothesized that students would be more confident and would perform better on both the ranking and explanation questions for the aromatic structures relative to the hybridization structures. *Figure 3.9.* summarizes the confidence of students who correctly and incorrectly ranked the acidity of the aromatic structures. As hypothesized, students who successfully ranked the aromatic molecules did report higher confidence compared to the hybridization problem, likely because they had seen similar questions earlier in the semester. A statistically significant difference was observed between the reported confidence for students who correctly versus incorrectly ranked the acidity.

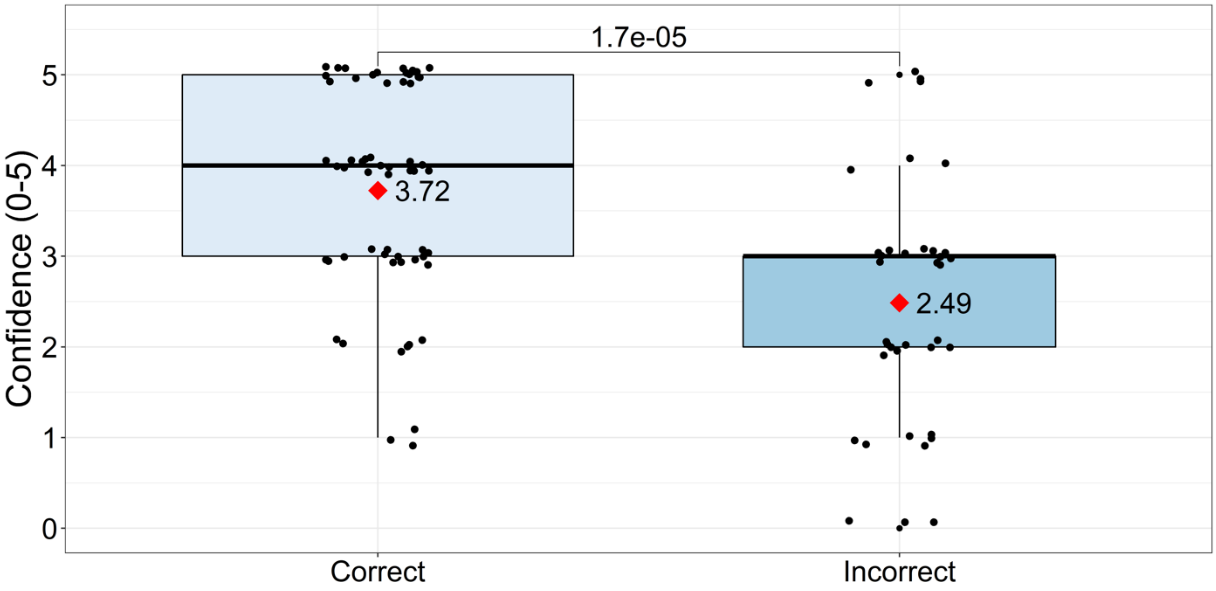


Figure 3.9. A comparison of students' (N = 95) reported confidence based on whether they correctly or incorrectly ranked the acidity of the aromatic structures. Red diamond denotes the mean.

Figure 3.10. summarizes the reported confidence for students based on the correctness of their explanations to justify the ranking of the acidity of the aromatic structures. Again, the responses were coded as correct, partially correct, or incorrect as outlined in the Methods. There was a statistical difference in the confidence reported for students providing correct and partially correct explanations versus incorrect explanations. There were no statistical differences in confidence reported for students who provided correct or partially correct explanations. The responses were qualitatively coded and tabulated as shown in *Table 3.4.*

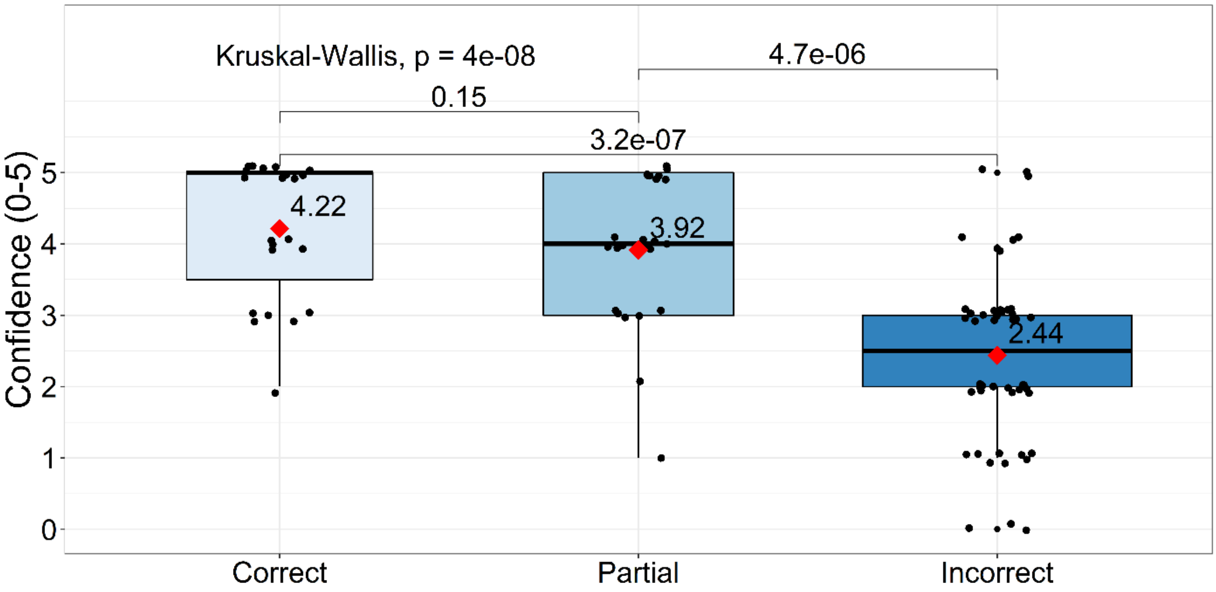


Figure 3.10. A comparison of students' (N = 95) reported confidence and the correctness of their explanations regarding the acidity of the aromatic structures. Red diamond denotes the mean. The Kruskal-Wallis test ($p << 0.05$) indicates that a statistical difference was observed when comparing all three groups of students. Further analysis using the Mann-Whitney test to make pairwise comparisons revealed a statistical difference between the correct versus incorrect, and partially correct versus incorrect groups.

Table 3.4. Deductive and Inductive Codes for Student Explanations to Q2 – Aromatic Acidity

Code Descriptions	Percentage of students (N = 95)
Deductive Codes	
Mentioning conjugate base stability	32
Equating functional groups with acidity	31
Inductive Codes	
Para-EWGs are more acidic than *meta*-EWGs because they participate in resonance	35
EWGs increase acidity; no further discussion	29
Para-EWGs are more acidic than *meta*-EWGs / *meta*-EWGs are less stabilizing than *para*-EWGs	20
NO_2 is an EWG, CH_3 is an EDG; identification of unique substituents	19
Meta-EWGs are less acidic than *para*-EWGs because they only exert inductive effects	13
EDGs decrease acidity; no further discussion	10
EDGs increase electron density at the oxygen in the conjugate base, which makes the molecules less acidic	8
EWGs decrease electron density at the oxygen in the conjugate base, which makes the molecules more acidic	8

Table 3.4. continued

EWGs stabilize the conjugate base through inductive effects	7
Para-substituted phenols are always more acidic than *meta*-substituted because *para*- has more resonance structures	7
Activation/activation of the aryl ring determines acidity; more activated rings are less acidic, more deactivated rings are more acidic	7
Meta-EWGs are more acidic than *para*-EWGs because they are closer to the hydroxy group, so they exert a stronger inductive effect	4
Para-EWGs are less acidic than *meta*-EWGs / *meta*-EWGs are more stabilizing than *para*-EWGs	4

In comparison to the hybridization question, a larger proportion of student explanations were correct and applicable, but often insufficient detail was provided to fully explain the acidity ranking. For example, from *Table 3.4.*, the following statements are correct and applicable, but more information is needed to fully explain the trend:

1. NO_2 is an EWG, CH_3 is an EDG; identification of unique substituents
2. *Meta*-EWGs are less acidic than *para*-EWGs because they only exert inductive effects
3. EWGs increase acidity; no further discussion
4. EDGs decrease acidity; no further discussion

The four statements are applicable for this problem, but students needed to draw connections that were largely missing in explanations. Namely, students needed to relate both the substituent effect (i.e., electron-donating or electron-withdrawing) and its position (i.e., *ortho*, *meta*, or *para*) relative to the acidic proton. Student explanations were limited and focused on only one of the two items. Both resonance and inductive effects should have been emphasized to fully explain the trend. The following responses (ordered correct, partially correct, and incorrect) provide representative explanations from the survey:

Survey Response 1 [Correct]

"The negative charge of the phenoxide can be delocalized through resonance to the nitro in the para position, but not to the nitro group in the meta position. However, the compound with the nitro group in the meta position can still stabilize the negative charge through an inductive effect. Compound A is the least acidic because the methyl is an electron donating group that destabilizes the negative charge of the phenoxide."

Assessment: The student accurately classifies the substituents as electron-donating and electron-withdrawing and accurately describes trends using both resonance and inductive effects.

Survey Response 2 [Partial]

"After deprotonation, the strongly electron withdrawing NO2 group will stabilize the electron density in the conjugate base. This effect is most prominent in the para-positioning. The meta-positioning still stabilizes the electron density to an extent, and the electron-donating nature of the methyl group provides less stability to the conjugate base."

Assessment: The student accurately rationalizes that EWGs stabilize the conjugate base, and EDGs destabilize the conjugate base. However, they do not explicitly distinguish between *para*-nitro and *meta*-nitro; "to an extent" does not mean only inductive effects versus inductive + resonance effects.

Survey Response 3 [Partial]
"B is the most acidic because the electron withdrawing group being in the para position allows resonance/electron delocalization to occur for c, the EWG in the meta position does not allow resonance for a, the methyl at the para position is an electron donating group that activates the ring."

Assessment: The student correctly rationalizes the role of electron-withdrawing groups versus electron-donating groups for increasing or decreasing the acidity. The student also correctly identifies the substituents as electron-withdrawing or electron-donating. The presence of resonance stabilization in the *para*-substituted molecule is correctly identified. Collectively, the student has all pieces except for the rationalization of the inductive effects from the *meta*-substituted group in C.

Survey Response 4 [Incorrect]
"Molecule B would be most acidic because the loss of the hydrogen could allow for resonance stabilization with the really good Electron withdrawing group in the para position to take on the charge in resonance structures well, then A next because the methyl group does a helpful inductive effect, not as much as electron withdrawing but still helpful in para position, and then the NO_2 in the meta position last because the NO_2 is a good EWG but isn't really that helpful when in the meta position."

Assessment: Although the student correctly notes that a *para*-nitro group allows for resonance stabilization of the conjugate base, the other statements are incorrect. The methyl group does not exert a "helpful inductive effect"; it destabilizes the conjugate base instead. Furthermore, the student states that the *meta*-position prevents substituents from exerting inductive effects.

Survey Response 5 [Incorrect]
"B has the most ability to delocalize charge with resonance when the OH is deprotonated negative charge can be pushed all the way around the ring onto the NO_2 oxygens. C has a nitro group in the meta position, making it ineffective at stabilizing the ion that forms."

Assessment: The student accurately explains the delocalization (presumably through resonance) for the *para*-nitrophenol. The role of the methyl group is not discussed, and the student notes that the nitro group in C has no impact (presumably through resonance). The inductive effects of the *meta* group in structure C are not considered.

Survey Response 6 [Incorrect]
"EDG of Me will allow for the molecule to be more stable. NO_2 is an EWG so when it is meta to the OH group it prevents electron stability. Stability will increase acidity since the negative charge of losing the hydrogen can be better distributed."

Assessment: The student does not understand the impact of an electron-donating versus electron-withdrawing group on increasing or decreasing acidity. The *meta*-substitution is said to "prevent electron stability" supporting that only resonance effects are being considered.

From the sample responses, the responses have correct ideas but fail to fully incorporate each of the key points required to explain the trend. The difference in electron-donating versus electron-withdrawing groups is emphasized to explain the reactivity of aromatic compounds. Given the focus on substituents to explain both acidity and reactivity, most students likely memorize the substituents that act as electron-donating versus electron-withdrawing groups. Therefore, while students readily draw on memorized knowledge and recognize when certain arguments are pertinent, they fall short of fully synthesizing each idea to explain trends cohesively. The primary alternative conception that emerged from this question is the idea that substituents in the *meta* position do not modulate acidity. Resonance models work when relating acidity for certain substituents with an *ortho* or *para* substitution, but they cannot be used to gauge the impact of substituents in the *meta* position. Resonance structures are drawn extensively when discussing aromatic molecules, which explains why students gravitate toward these models. Additionally, resonance structures provide tangible representations that students can draw and visualize in place of models such as inductive effects that are not as easily drawn on paper. However, inductive effects are pertinent for considering the role of electron-withdrawing or electron-donating groups in the *meta* position. *Figure 3.11.* illustrates the Sankey diagram for the aromatic acidity ranking and explanations. Additional statistical analysis of reported confidence based on the ranking and explanation correctness was completed as shown in *Figure 3.12.*

As with the hybridization structures, students were more successful at ranking the acidity of the aromatic structures than explaining the trend, but the difference in success rates was less substantial. This question was designed to serve as a control question, and distractors were not incorporated. Students either knew how to approach the problem or did not. Students whose explanations were marked as partially correct were likely not thorough or explicit enough with their explanations to earn a correct score but still had a decent understanding of the rationale. With the hybridization structures, distractors were incorporated, such as conjugation and the C-H bonds on the alkyl, alkenyl, and alkynyl substituents to promote the wider array of models implemented to gauge alternative conceptions. For the aromatic structures, students who readily apply the models they had previously encountered were more likely to successfully rank the acidity and explain their rationale. Therefore, the reported confidence more closely aligns with their success in ranking and explaining the acidity of the aromatic structures.

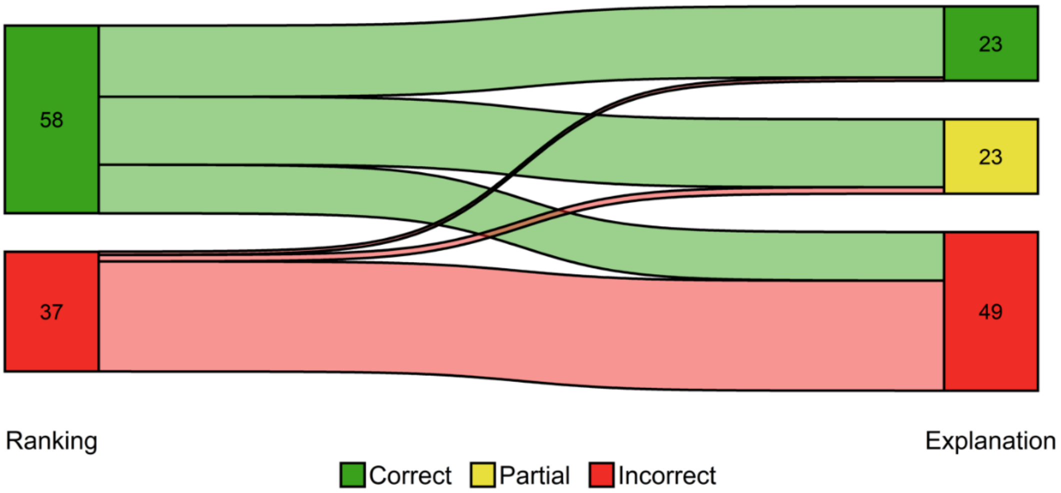


Figure 3.11. A Sankey diagram comparing students' (N = 95) ranking and explanations on the aromatics question on the survey. Note that some students reversed the ranking in the first part but were able to provide a correct or partially correct explanation. The incorrect ranking could have been associated with not carefully reading the problem prompt.

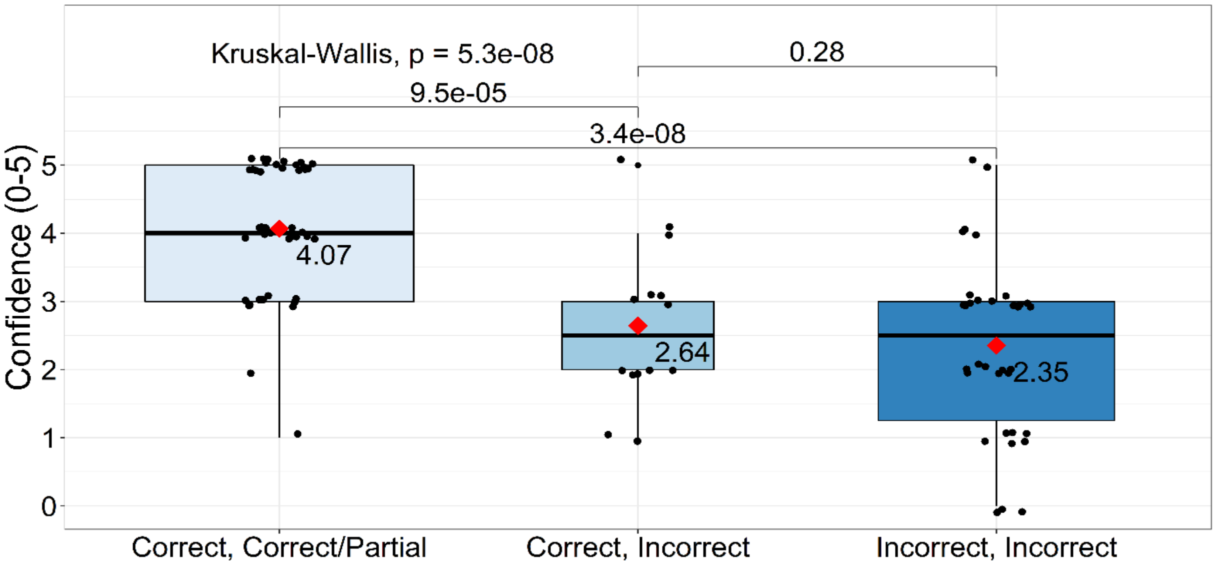


Figure 3.12. A comparison of confidence for students (N = 92) based on their ranking and explanation, correctness formatted as [Ranking, Explanation]. Red diamond denotes the mean. Again, the [Correct, Correct] and [Correct, Partial] groups were aggregated following the results of *Figure 3.10***.** and *Figure 3.11.;* there was no statistically significant difference in the students' confidence, and nearly all students who explained correctly or partially correctly also ranked correctly. The Kruskal-Wallis test ($p << 0.05$) indicates that a statistical difference was observed when comparing all three groups. Further analysis compared each cohort using the Mann-Whitney test and found a statistical difference between the [Correct, Correct/Partial] and the other two groups.

Figure 3.13. summarizes student performance on the hybridization and aromatic ranking items. The Sankey diagram illustrates students performed better with ranking the acidity of the hybridization structures relative to ranking the acidity of the aromatic structures. On the other hand, *Figure 3.14.* illustrates students were less successful in explaining their reasoning on the hybridization item. This was expected given the design, with the hybridization structures providing distractors to provide insight into students' alternative conceptions. The differences between success in ranking versus explaining the items can be attributed to several factors. 1) With the hybridization structures, students could successfully rank the acidity using incorrect models, which was reiterated through the explanations. 2) With the substituted aromatic structures, students were required to incorporate several models to explain the trends based on both the effect and position of substituents, a task that necessitates a more sophisticated use of models. However, distractors were not included in the aromatic structures, which necessitated the recalibration of how models are used to explain the observed trends. Consequently, 3) success in the ranking was attributed less to luck or memory for the aromatic structures. This explains why there was a smaller gap between success in ranking and explaining the trends in acidity for the substituted aromatic molecules.

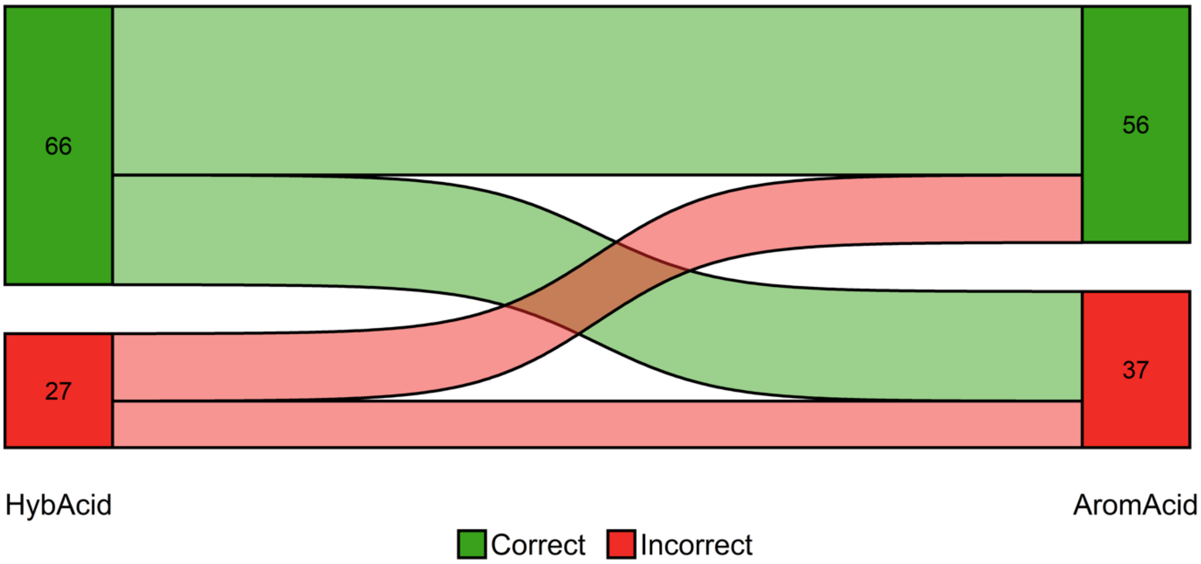


Figure 3.13. A Sankey diagram comparing students' ranking for the hybridization and aromatic structures on the survey (N=93).

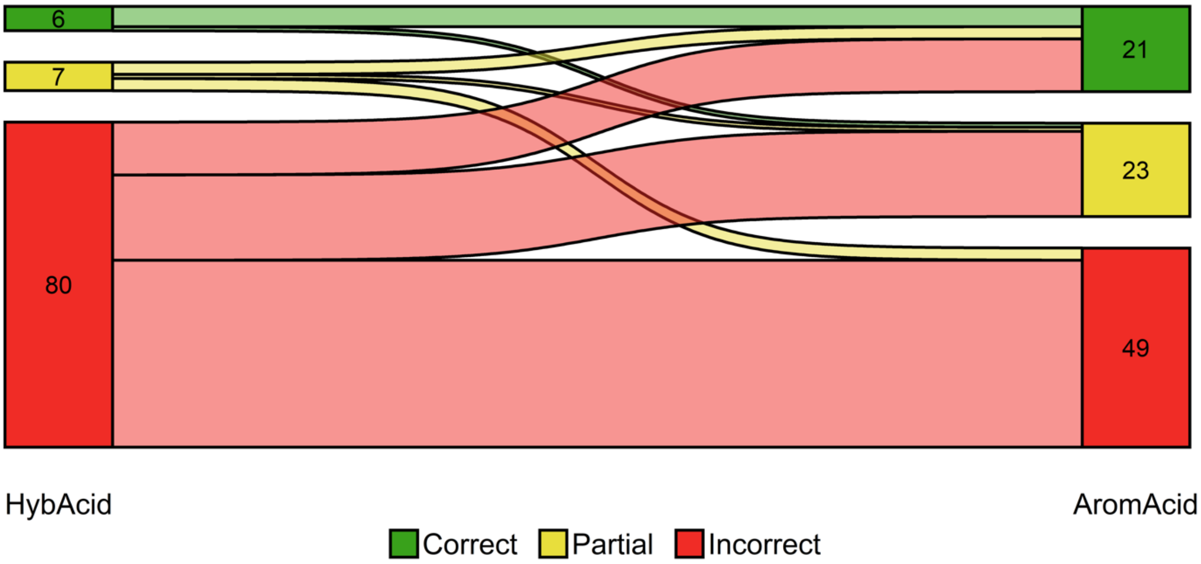


Figure 3.14. A Sankey diagram comparing students' explanations for the hybridization and aromatic structures on the survey (N=93).

To reiterate the research questions for the aromatic structures: students demonstrated a greater tendency to apply and accurately explain the role of resonance in modulating acidity in the presence of a *para*-substituted electron-withdrawing group. To correctly explain the trend in acidity, students needed to consider both resonance and inductive effects as well as their competing electronic effects. As with the hybridization structures, students demonstrated a greater tendency to apply resonance but a weaker ability to identify and apply inductive arguments. The primary alternative conception identified from the survey responses for the aromatics question is the notion that the *meta* substituents do not impact acidity because of the lack of resonance delocalization. This reiterates students' tendency to attempt to use resonance arguments for conjugated systems, despite the existence and applicability of other models. The origin of this alternative conception may be the extensive use of resonance structures to explain aromatic reactivity and regioselectivity. Students demonstrated a greater awareness of their abilities with statistical differences in the reported confidence between correct and incorrect rankings and/or explanations. Given this problem was not designed to act as a distractor, this finding supports that students do gain insight into their abilities as they progress in chemistry. This finding is counter to McClary and Bretz's finding (L. M. McClary & Bretz, 2012), but the timing of the survey and prior course experiences could be used to account for the differences.

Conclusions and future work

The findings from the analysis of the survey and interview data illustrate that students have difficulty rationalizing acid-base trends. The challenges with acid-base chemistry are widely reported in general chemistry, and these challenges persist longitudinally across the chemistry curriculum. A solid understanding of acid-base chemistry is paramount in organic chemistry because many reactions can be rationalized using the frameworks of acid-base chemistry. Students are introduced to models to rationalize these trends, but many experience challenges with identifying and applying these models to novel situations. This research illustrates that with ranking items and explanations, students implement ideas from memory, based on familiar structural features. For the alkyl, alkenyl, and alkynyl-substituted carboxylic acids, students latched onto hybridization, often recalling trends relating to s-character. However, they did not fully develop ideas from this concept. They know that carbon atoms with more s-character are more acidic, but few students made the connection to electronegativity, and even fewer students extended that to inductive stabilization of negative charge. There is a considerable gap between hybridization and inductive effects that most students, near 90%, are not bridging. Using these facts, many students were successful at comparing the acidity of structures differing in hybridization alpha to a carboxylic acid. However, when asked to explain, students did not link and synthesize these facts into a cohesive explanation. Students applied one or more of these potentially memorized facts incorrectly despite correctly ranking the acidity.

Students exhibited a similar strategy with ranking the acidity of the aromatic structures in which they recalled facts, such as classifying substituents as electron-donating or electron-withdrawing, to explain the trends in acidity. Unlike ranking the acidity of the carboxylic acids, successfully ranking the acidity of the substituted aromatic molecules required using multiple pieces of information including substitution pattern and substituent effects; it was not possible to apply a single fact to be successful with the ranking. However, there were no embedded distractors that were designed to limit the efficacy of specific models for explaining the trend. As expected, there was a smaller gap in the performance on the ranking and explanation for the aromatic structures than the carboxylic acids.

Future directions for the research will provide strategies for improving students' identification, understanding, and application of models in organic molecules. The research is expanding into general chemistry and the first semester of organic chemistry, with an overarching goal of developing a longitudinal model for students' progression with acid-base chemistry. Through these studies, we aim to identify alternative conceptions students develop in general chemistry that propagate through the curriculum, with the goal being to develop interventions aimed at promoting cognitive dissonance, such that students become aware of their alternative conceptions. Much like these surveys, which required explanations, the interventions will have students explore the scope and limitations of models. One possible intervention would be to perform our scoring criteria analysis with chemistry students, which would help them gain a better grasp on how to implement models and reiterate the importance of not solving problems using only rote memorization. From our findings, many second-semester organic chemistry students, despite a considerable background in chemistry, still appear to rely on memorized facts and knowledge from previous examples to tackle new problems. The goal of organic chemistry is to develop a toolbox to make predictions regarding novel reactions, which requires successful synthesis of concepts and application of models, in lieu of primarily factual recollection.

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Statement of contributions

SG led the project and contributed to the literature review, design of the research instruments, development of frameworks for analyzing data, and collection of interview data. TCO assisted with developing frameworks for coding survey and interview data and collaborated with SG and JGL to code data. JGL assisted with coding the survey and interview data. AF assisted with the statistical analysis. JLR assisted with the design of the research instruments and aided in collecting data. CM contributed to the design of the research instruments. CTC provided mentorship for the research design, data collection, and data analysis. All authors contributed to the preparation of the manuscript.

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