Chemistry
Education Research
and Practice

Organic Chemistry Students' Use of Stability in Mental Models on Acid and Base Strength

Journal:	*Chemistry Education Research and Practice*
Manuscript ID	RP-ART-02-2023-000049.R1
Article Type:	Paper
Date Submitted by the Author:	05-May-2023
Complete List of Authors:	Demirdogen, Betul; Zonguldak Bulent Ecevit Universitesi, Secondary Science and Mathematics Education Nelsen, Isaiah; University of South Florida Tampa Campus, Chemistry Lewis, Scott; University of South Florida, Chemistry

Organic Chemistry Students' Use of Stability in Mental Models on Acid and Base Strength

Abstract: The Brønsted-Lowry acid–base model is fundamental when discussing acid and base strength in organic chemistry as many of the reactions include a competing proton transfer reaction. This model requires evaluating chemical stability via a consideration of electronic granularity. The purpose of this study is to identify students' mental models on acid and base strength in terms of granularity and stability. Fourteen students enrolled in organic chemistry participated in this case study. Data were collected through semi-structured interviews including total case comparison tasks on stability, acidity, and basicity. Analysis of data revealed that there were four groups of students differentiated by their reasoning: (1) acid and base strength through structure without association to stability, (2) acid and base strength through electronics without association to stability, (3) acid strength associated with electronically centered stability, and (4) acid and base strength associated with electronically centered stability. This characterization can support teaching and research to promote a reasoning that leads to a more consistent mental model across acid and base strength.

Introduction

The chemistry of acids and bases is foundational to understand much of the content in organic chemistry (Boothe, Zotos, & Shultz, 2023) such as methods of activation, organic synthesis, and classes of reactions (American Chemical Society, 2015; Stoyanovich, Gandhi, & Flynn, 2015) and to perform well at related items in exams (Raker, Holme, & Murphy, 2013). In line with this focus on the chemistry of acids and bases in curricular documents regarding organic chemistry, empirical research on students' prediction of reaction products and reasoning on mechanism problems also indicated that a working knowledge of acid–base chemistry is essential (Anderson & Bodner, 2008; Bhattacharyya, 2014; Bhattacharyya & Bodner, 2005; Graulich, 2015; Grove, Cooper, & Cox, 2012).

The centrality of acid-base chemistry in organic chemistry directed researchers to describe essential learning outcomes for acids and bases (Stoyanovich et al., 2015). This study identified twenty-five organic (e.g., SN1 and aldol condensation) and three biochemical reactions (e.g., Krebs cycle) that necessitate a Brønsted-Lowry acid–base reaction step at some point. Three-quarters of the reactions required identifying the most acidic or basic site in a molecule and one-third of the reactions required determining the stronger/weaker acid or base using relative base stabilities and relevant factors (e.g., resonance and inductive effects). That is, understanding acid and base strength is vital in reasoning about reaction mechanisms. However, students may have difficulties in enacting a scientific mental model of acid strength. They tend to relate acid strength with intrinsic (e.g., atom identity), explicit (e.g., number of specific atoms), and implicit (e.g., polarity) properties (Bhattacharyya, 2006; McClary & Bretz, 2012; McClary & Talanquer 2011a; Shah et al., 2018; Tümay, 2016). In addition, when determining the stability of conjugate bases student responses were influenced by one factor as opposed to a series of related factors (Bhattacharyya, 2006; McClary & Bretz 2012; McClary & Talanquer 2011a; Shah et al., 2018, Tümay, 2016). Despite the emphasis researchers have placed on understanding student knowledge on acid strength in organic chemistry, base strength has not been a specific topic of interest and has been researched only in tandem with acid strength (e.g., Cooper, Kouyoumdjian, & Underwood, 2016; Petterson et al., 2020). Considering the importance of acid and base strength in organic chemistry (Bhattacharyya & Bodner, 2005; Stoyanovich et al., 2015), research on how students conceptualize not only acid but also base strength can aid student success in determining reaction processes. Therefore, this study aimed to reveal students' mental models on acid and base strength.

Mental Models on Acid and Base Strength

Mental modeling is a theory on knowledge organization through which researchers can "explain human cognitive processes of understanding reality, translating reality into internal representations" (Park & Gittleman, 1995, p. 303). The human cognitive system is able to construct mental models that are refined in order to interpret lived experiences (Coll & Treagust, 2003; Clement & Rea-Ramirez, 2008). When constructing a mental model for a system (i.e., real or imaginary situation, event or process), individuals generate mental entities, which represent their perception about the entities including established properties and relationships (Johnson-Laird, 1983; Nersessian, 2008). Individuals may exclude critical entities and their associated properties when forming mental models. When learning science, these characteristics of the mental model result in alternative explanations in relation to scientific knowledge, which can generate misconceptions (Coll & Treagust, 2003; Lin & Chiu, 2007). Although mental models can have limiting characteristics, they are functional to students allowing them to explain, predict, and reason when problem solving (Gentner, 2002). When functioning with mental models, students might retrieve the mental model from their long-term memory (i.e., permanent mental model) or generate a new method on the spot to solve the problem (i.e., temporal mental model) (Gentner, 2002; van der Veer, Kok, & Bajo, 1999; Vosniadou, 2002). That is, mental models are dynamic in nature that might change with the accessible information through remembering (McClary & Talanquer, 2011a), stimulation by the features of the task (Osman & Stavy, 2006), and available implicit cognitive resources (e.g., prior knowledge and intuitive heuristics, Greca & Moreira, 2000). Examination and identification of students' mental models, requires elicitation—making this internal representation external. Elicited mental models (or expressed mental models) (Gilbert & Boulter, 1998) are the external representations of the corresponding mental model. Expressed mental models are accessible through action, speech, and writing (Gilbert, Boulter, & Rutherford, 2000). In this study, students' mental models were identified through their speech and drawing for specific tasks, which was used to infer their reasoning on stability, acidity, and basicity (Gilbert et al., 2000). In doing so, we aimed to reveal students' mental models on acid and base strength. Considering the existence of three scientific acid-base models (i.e., Arrhenius, Brønsted-Lowry, and Lewis), analysis of mental models unavoidably requires defining the context of the tasks (Tümay, 2016). The tasks in this study required students to compare relative acidity and basicity of organic compounds in water, stimulating them to consider the stability of bases and conjugate bases, two emergent properties in the Bronsted Lowry model.

Review of the literature on students' conceptualizations, mental models or alternative conceptions/misconceptions/difficulties on acid strength identified six categories of students considering their expressed mental models. Students in the first category retained an empirical definition of acid that relies on sour taste, red litmus paper, and pH, and they carried over their definition when predicting relative acid strength (Tümay, 2016). In the second category, acidity is viewed as an intrinsic property (Bretz, & McClary, 2015; McClary & Bretz 2012; McClary &

Talanquer 2011a, b; Shah et al., 2018) where explicit features (i.e., structural) such as atom type (e.g., O) or functional groups (e.g., -COOH) are associated with acid strength. For students in the third category, acids are seen as hydrogen ion (H^+) donors (Arrhenius model) when dissolved in water; hence acid strength is related to the degree of ionization influenced by bond strength and polarity (Bhattacharyya, 2006; Tümay, 2016). In the fourth category, students model substances that lose hydrogens or protons relying on intrinsic (e.g., atom identity), explicit (e.g., number of specific atoms), and implicit (e.g., polarity) properties (McClary & Talanquer, 2011a, b). Students in the fifth category identify proton loss based on the stability of the conjugate base influenced by implicit properties (i.e., atom size, atom electronegativity, resonance/delocalization, inductive effect, and hybridization) (Brønsted-Lowry model) (Bhattacharyya, 2006; Bretz, & McClary, 2015; McClary & Bretz, 2012; McClary & Talanquer, 2011a, b; Shah et al., 2018; Tümay, 2016). In the sixth category, students focus on electron acceptance capacity, leading students to take into consideration the number of lone electron pairs or empty orbitals (Lewis model) (McClary & Talanquer, 2011a, b). Mental models, however, are not always consistent and the features present in a task or the nature of the task can result in the existence of multiple mental models across tasks (McClary & Talanquer, 2011a). Our understanding on students' mental models on acid strength has reached a certain level through the empirical evidence available in literature, which helps us to improve the instruction and to advance research on acid strength. However, our understanding on students' mental models on base strength is very limited. Therefore, we intended to identify students' mental models on acid and base strength in terms of granularity and stability.

As of late, granularity has been a relatively prominent term among chemistry education researchers to describe levels in activities and entities in chemical phenomena (Bodé et al., 2019; Deng & Flynn, 2021; Talanquer, 2022). Phenomenological, structural, electronic, and energetics are the fundamental granularity levels (Bodé et al., 2019; Deng & Flynn, 2021). However, different granularity exists depending on context and need (Bodé et al., 2019; Deng & Flynn, 2021, Machamer, Darden, & Craver, 2000). The structural level includes descriptions of structural features of molecules and atoms (Deng & Flynn, 2021). For instance, when comparing the plausibility of alternative mechanisms for given reactants, steric hindrance and number of alpha-carbon substituents would be relative structural granularities in students' explanations. In acid-base chemistry, atom size was proposed as structural granularity that students would enact in their reasoning (Deng & Flynn, 2021). The electronic level captures descriptions of electronic features of molecules and atoms (Deng & Flynn, 2021). For instance, electronegativity and formal charge could be utilized when explaining plausibility of alternative reaction mechanisms (Deng & Flynn, 2021) while delocalization and inductive effects are fundamental in acid-base chemistry. The energetic level includes descriptions of the energetics such as thermodynamic and kinetic considerations. For instance, the stabilities of conjugate acids/bases to reason about the direction of an acid-base equilibrium or activation energy to justify the plausibility of alternative reaction mechanisms are relevant energetic features. The phenomenological level captures descriptions of chemical phenomena, an emergent property, which is the result of entities including their properties and activities (Machamer et al., 2000) using structural, electronic, and energetic features. Within the given context, structural (i.e., size) and electronic (i.e., spreading of charge) features could be used to explain the phenomenon "stability", which then utilized to predict other phenomena (i.e., acid and base strength).

Invoking Stability in Reasoning about Acid and Base Strength

The Brønsted-Lowry model for acid and basis led to both the emergence of conjugate acid-base pair concept and consideration of acid-base reactions as competing proton transfer reactions, which in turn influence acid strength (McClary & Talanquer 2011a; Tümay, 2016). During an acid-base reaction in a solvent, the acid donates a proton in a forward reaction resulting in the formation of a conjugate base. The conjugate base accepts the proton in a backward reaction. In this competing proton transfer reaction; the relative stability of all species determines the direction and extent of this dynamic process, which form the basis of acid and base strength phenomenon. A strong acid readily donates its proton to base in the forward reaction if the resulting negatively charged conjugate base is stable. The stability of the conjugate base is supported by low charge density, which is influenced by multiple factors. Electronegativity of the atom influences the degree to which a charge is localized. Atom size, resonance (delocalization), and electron withdrawal-donation (induction) affect spreading of charge. Hybridization (orbital) of the atom determines the to what degree electrons are held closer to the nucleus. All factors should be considered concurrently when determining how those contribute to the stability of the conjugate base. The more stable a conjugate base is, the weaker base it is and the stronger the originating acid.

Considering the mechanism in an acid-base reaction in Bronsted-Lowry model, stability is an important phenomenon that should be considered when determining not only acid strength but also base strength. From this perspective, both stability and acid-base strength are conceived as emergent in nature since they stem from entities of the substance, activities in the substance, and weighing all these entities and activities in the given task (McClary & Talanquer, 2011a; Tümay, 2016). In this study, we aimed to reveal to what degree students invoke stability in their expressed mental models when predicting acid and base strength. To increase the accessibility of the results, we will present how an idealized response should look like for one of the tasks (Acidity 1). This idealized response was also reviewed by two organic chemistry instructors at the setting. Please see Supporting Information for idealized responses for all the tasks. In Acidity 1, students were asked to compare the relative acidity of acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH) in water. An idealized student response should include the following reasoning:

- The conjugate bases of these acids are acetate ion (CH_3COO^-) and ethoxide ion ($CH_3CH_2O^-$).
- Size and electronegativity of atom: Atoms with negative charges are oxygen in both conjugate bases. Since atoms are the same therefore size and electronegativity are not relevant.
- Resonance/delocalization: Spreading charge lowers free energy and increases stability for acetate ion, which in turn increases the acidity of acetic acid.
- Inductive effect: Electron withdrawing of carbonyl group (-C=O) stabilizes the acetate ion through polarization of sigma bonds of molecule. Therefore, induction increases stability for acetate ion, which in turn increases the acidity of acetic acid.
- Hybridization/Orbital – The negatively charged oxygen on acetic acid is sp^2 whereas the oxygen on ethanol is sp^3. The larger s-character on the oxygen on acetate ion stabilizes the negative charge on the oxygen of acetate relative to the oxygen of ethoxide. Therefore, induction increases stability for acetate ion, which in turn increases the acidity of acetic acid.

Methodology

Research Question

To explore students' reasoning on acid and base strength, this study was guided by the following research question: What are students' mental models on acid and base strength in terms of granularity and inclusiveness of stability?

Research Design

Given the tacit nature of mental models, this research is qualitative-interpretive (Marshall & Rossman, 2011). Among the qualitative strategies, case study guided the design, data collection, and data analysis of this study. Yin (2009) valued this type of research method when "a how or why question is being asked about a contemporary set of events, over which the investigator has little or no control" (p. 13). Since the researchers had no control on students' use of mental model other than asking questions to reveal them, students' reasoning process as a case provided in-depth information about characterization of students' mental models on acid and base strength. Moreover, this case study was designed to expand the theories of mental model and granularity, which are the aims of case study (Yin, 2009). There are several types of case studies depending on the intent of the case analysis (Creswell, 2007; Yin, 2009). This case study is descriptive—the focus was to describe students' reasoning on acid and base strength considering the granularity and inclusiveness of stability.

Participants

Fourteen students participated in the study at a large and research-incentive university in the southeastern U.S. in Fall 2022 after obtaining approval from the university's institutional review board. Seven students from each Organic Chemistry class (I and II) were recruited by announcement. We informed students orally and through the reading of consent form about the purpose of research, their rights, and how the data is processed. The students then submitted their written consent forms. Pseudonyms were used to ensure confidentiality. Student quotes were edited to remove verbal utterances (e.g., um) and repeated phrases to improve clarity. Students' participation was compensated with a 20 dollar gift card. Content coverage in the courses were determined via conversations with the course instructors and a review of course materials. Acids and bases are covered in Organic Chemistry I; more specifically how the stability of a conjugate base relates to acid strength and factors that influence stability (e.g., type of atom, delocalization, induction, orbital). These ideas are also reviewed at the beginning of Organic Chemistry II. Organic Chemistry II emphasizes basicity of amines and requires utilization of acid strength in the context of reaction mechanism (ACS, 2015; Stoyanovich et al., 2015). Assessments include items that measured students' abilities to compare acid strength, compare base strength, and use strength in predicting the position of acid-base equilibrium reactions. Students were interviewed right after their completion of learning and assessment of acid and base strength in both courses. Since students taking either of the two sequential Organic Chemistry classes had experience in learning concepts of stability, acidity, and basicity, they were the subjects of interest.

Data Collection

This study collected data using semi-structured interviews in the form of case comparison tasks. Case comparison tasks have been previously used to identify all relevant variables to the task (Alfieri, Nokes-Malach, & Schunn, 2013) in chemistry education literature (e.g., Kranz, Schween, & Graulich, 2023). While preparing and organizing semi-structured interviews, we considered not only students' learning experiences during organic chemistry classes but also fundamental concepts required to understand stability, acidity, and basicity. Each student was given six case comparison tasks presented in two tasks for each of the three concepts interested in study (i.e., stability, acidity, and basicity, Table 1). Each student was asked to compare the cases in terms of the given concept and provide an explanation for their answers. The cases were selected from the organic chemistry textbook used in the setting (Klein, 2017) and another available textbook (Solomon & Fryhle, 2012). The original study design was to investigate the students' conceptions of resonance, so cases were selected where resonance was present. In addition, there was an attempt to select cases with that were considered to be relatively familiar to students (e.g., acetamide vs. ethyl amine) and less familiar (e.g., propoxide vs. propene-1-olate) to gain more insight on students' reasoning. An additional goal of this investigation was to examine the impact of representations on students' explanations. Two different interview protocols (i.e., Protocol A and Protocol B) were used that had the same content and ordering of questions but differed in how resonance was represented. Students were randomly assigned to Protocol A or B. The impact of resonance representations will be the subject of a future investigation and not discussed further herein. Complete interview protocols can be found in the supporting information.

Table 1. Descriptions of the interview protocols used in the study

		Representations at protocols		
Tasks	**Chemistry Content**	**A**	**B**	**Task description used in this study**
Stability 1	Phenolate vs. Cyclohexanolate	Single Lewis	Single Lewis	Negatively charged ions
Acidity 1	Acetic acid vs. Ethanol	Resonance structures of conjugate base	Resonance hybrid structure of conjugate base	Conjugate base with resonance
Basicity 1	Acetamide vs. Ethyl amine	Resonance hybrid structure of base	Resonance hybrid structures of base	Base with resonance
Stability 2	Allylic carbocation vs. Non-allylic carbocation	Single Lewis structures	Single Lewis structures	Positively charged ions
Acidity 2	Allylic hydrogen vs. Non-allylic hydrogen on a substance	Single Lewis structure	Single Lewis structure	Acid with single Lewis structure
Basicity 2	Propoxide vs. Propene-1-olate	Single Lewis structures	Single Lewis structures	Base with single Lewis structures

Data Analysis

Interview questions included “How do you define stability and how do you use your definition to explain which one is more stable?,” “How do you determine which substance is more acidic?,” and “How does your answer relate to your definition of acid strength?” We focused on these parts of the interview transcriptions where students provide their reasoning at each case comparison task on stability, acidity, and basicity since mental models are meant to support understanding, reasoning, and prediction when solving problems (Gentner, 2002).

We identified how students communicated their mental models that guided their reasoning on each task through their speech and drawing peculiar to the task. This helped us code their expressed mental models. Considering the nature of mental models, researchers coded students’ mental models on stability, acid strength, and base strength in an inductive manner. For instance, if students defined stability in relation to the degree to which electrons are delocalized and focused on this when reasoning which substance is more stable, we coded this mental model on stability as “delocalization”. Examples for coding the mental model at each task are presented in Table 2 and a detailed analysis is included in supporting information. Once the coding scheme was complete two researchers independently coded each student’s mental model at every case comparison task. All discrepancies in coding were discussed to reach a consensus code assignment.

Table 2. Coding examples for students' mental models on stability, acidity, and basicity

Task	Excerpt	Mental Model
Stability	Resonance is basically how much room the electron could take up and the different positions that it could exist in to be stabilized (S10)	Delocalization
	I think it's vynillic. But I guess my point is,…The carbon is it's next to a double bond….So and I think that that increases stability….I don't know why….I just remember the fact. (S2)	Identity
	…the most stable one doesn't need more ions or it doesn't need more bonds or anything like that, we can find the way it is. (S4)	Octet
Acidity	…the least stable base those are the most acidic structure. (S3)	Stability of conjugate base
	…there are two oxygens on the ace acetate ion and then on the ethoxide ion, there's only one oxygen….Oxygen is very electro negative, more electronegative than carbon, and there are more carbons in ethoxide than acetate. (S9)	Electronegative atom
	Acetic acid would be more acidic than the ethanol. This is because there's more oxygens and this is going back to like if you look at a periodic table and like how it is layed out versus like polarity and everything. Since there's more oxygens and then this one has more Hs, this one's going to be more acidic because it's just like, it's just like the difference in the polarity. That it's [referring to acetic acid], like, higher, I would think, because that, like, shows, it's, like, willing to take, like, stuff in order to fill, like those octet to make those charges. (S12)	Polarity and octet
Basicity	If this [O in acetamide] takes an H somewhere, it's going to become an always making it more acidic, but we need more basic. I'm assuming this [ethyl amine] is basic (S14)	Atom identity
	…the acetamide I think would be a weaker base because it's resonance stabilized rather than the ethyl amine, which is not resonance stabilized, making it a stronger base (S2)	Stability of base
	From more basic I would say the propoxide because if you do resonance with the propane-1-olate, you can make it where that double bond will go to that oxygen and then to fulfill like it's charge. So there would be no there'd be no charge, whereas with the propoxide, there's nowhere to do resonance. So it will always have that negative charge. (S12)	Neutralization/Removing charge

Another focus of this study is to reveal the granularity observed in students' mental model on acid and base strength. Granularity levels were characterized as structural or electronic descriptions (Bodé et al., 2019; Deng & Flynn, 2021) as they are the most relevant levels in the phenomena under investigation and different granularity exists depending on context and need (Bodé et al., 2019; Deng & Flynn, 2021, Machamer et al., 2000). Electronic and structural granularity were defined inductively within the context of this study. Structural granularity refers to students' descriptions of features of molecules, atoms, and ions (Deng & Flynn, 2021). In the context of acid and base strength, structural granularity differs from what is proposed in the literature since teaching of acid and base strength in organic chemistry heavily relies on stability (Stoyanovich et al., 2015). Moreover, reasoning about stability requires utilization of structural (e.g., lone pairs, charges, and connectivity of those) and electronic (e.g., delocalization and polarization) granularity levels. For instance, explicit structural features are utilized by students when asked to compare the stability of two ions of which one has the structure (i.e., allylic lone pair) that enables the delocalization of electrons using structural representations (i.e., Lewis). Based on inductive coding, structural granularity was defined as atom identity, atom count, functional group identity, bond type, bond count, electron count, charge, resonance specific representational features, and connectivity of atoms, ions, and molecules.

Electronic level granularity was also conceptualized with the context of this study in mind. We defined electronic granularity as electronic activities and the emergent properties relevant to the phenomenon (e.g., acid and base strength). When assessing electronic granularity, we focused on the instances where students refer to electronic activities in the ion or molecule and the resulting effect. Delocalization of electrons, spreading charge, electron withdrawal, electron donation, bearing charge, and polarization were the codes that emerged during coding for electronic granularity. Detailed information describing each code is presented in the supporting information. Granularity level was coded to consensus using the same procedures as described in mental models.

Following the completion of mental models and granularity analyses, an inductive, constant comparative analysis was conducted. A summary table for students' mental models on each case comparison task (Table 3) and a table for levels of granularity in their explanations (Table 4) were prepared. The tables were examined for similarities, and differences in participants' mental models across all tasks to gain an insight about their reasoning. This examination identified the existence of groups that are dissimilar from other groups both in the way they described stability (i.e., structural vs. electronic) and in the degree they associate stability to predict acid and base strength. Four groups were identified represented by the differing colors in Tables 3 and 4. These four groups of students are the main findings of this study and are characterized in Figure 1 and detailed in the results section.

Table 3. Students' mental models on stability, acidity, basicity across all case comparison tasks

	Tasks					
Student	**Stability 1**	**Acidity 1**	**Basicity 1**	**Stability 2**	**Acidity 2**	**Basicity 2**
4[b]	Octet	Identity, bond strength and octet	Identity, bond strength, and octet	Octet	Bond strength	Identity, bond strength, and octet
5[b]	Bond strength	Bond strength and donating proton	Donating electron	Bond strength	Bond strength and donating proton	Bond strength and accepting electron
9[a]	Identity	Electronegative atom	Stability of molecule	Identity	Electronegative atom	Stability of molecule
1[b]	Spreading charge	Stability of conjugate base	Accepting proton	Identity	Donating proton and accepting electrons	Accepting proton and donating electron
6[b]	Delocalization and octet	Polarity	Accepting proton and donating electron	Delocalization and octet	Delocalization of electrons	Accepting proton and donating electron
11[a]	Delocalization	Neutralization/ Donating electrons	Accepting electron	Identity	Comparison to basicity using delocalization	No specific conception
12[a]	Bond strength	Polarity and octet	Removing charge/ Neutralization	Removing charge/ Neutralization	Delocalization of electrons	Removing charge/ Neutralization
7[b]	Spreading charge and delocalization	Stability of conjugate base	Accepting proton	Spreading charge	Stability of conjugate base	Accepting proton
14[a]	Delocalization	Stability of conjugate base	Atom identity	Spreading charge	Stability of conjugate base	No specific conception
2[b]	Spreading charge	Stability of conjugate base	Stability of conjugate acid (accepting proton)	Identity	Stability of conjugate base	Stability of base
3[b]	Delocalization	Stability of conjugate base	Stability of base	Delocalization	Stability of conjugate base	Stability of base
8[a]	Spreading charge and delocalization	Stability of conjugate base	Stability of base	Spreading charge and delocalization	Stability of conjugate base	Stability of base
10[a]	Delocalization	Stability of conjugate base	Stability of base and donating electrons	Spreading of charge	Stability of conjugate base	Stability of base
13[a]	Spreading charge	Stability of conjugate base	Stability of base	Spreading charge	Delocalization of electrons	Stability of base

[a] indicates students in Organic Chemistry I
[b] indicates students in Organic Chemistry II

Table 4. Granularity in students' explanations when predicting stability, acidity, basicity across all case comparison tasks

	Tasks					
Student	**Stability 1**	**Acidity 1**	**Basicity 1**	**Stability 2**	**Acidity 2**	**Basicity 2**
4[b]	S	S	S	S	S	S
5[b]	S	S - E	S	S	S - E*	S
9[a]	S	S	S - E	S	S	S
1[b]	S - E	S - E	S	S	S - E*	S - E
6[b]	S - E	S – E*	S	S - E	S - E	S - E
11[a]	S - E	S - E	S - E	S	S - E	S - E
12[a]	S	S	S - E	S - E	S - E	S-E
7[b]	S - E	S - E	S	S - E	S - E	S - E
14[a]	S - E	S - E	S	S - E	S - E	S
2[b]	S - E	S - E	S	S	S - E	S - E
3[b]	S - E	S - E	S - E	S - E	S - E	S - E
8[a]	S - E	S - E	S - E	S - E	S - E	S - E
10[a]	S - E	S - E	S - E	S - E	S - E	S
13[a]	S - E	S - E	S - E	S - E	S - E	S - E

S indicates use of structural granularity
S - E indicates use of structural and electronic granularity
*indicates use of electron withdrawal as electronic granularity without mentioning delocalization and/or spreading charge
[a] indicates students in Organic Chemistry I
[b] indicates students in Organic Chemistry II

Results

Analysis of data revealed that there were four groups of students indicating various reasoning when they predicted acid and base strength. These groups are distinguished in Figure 1 on two dimensions where one dimension indicates granularity in students' explanations and the other corresponds to inclusiveness of stability when predicting acid and base strength. The following descriptions represent the four groups: (1) acid and base strength through structure without association to stability, (2) acid and base strength through electronics without association to stability, (3) acid strength associated to electronically centered stability, and (4) acid and base strength associated to electronically centered stability.

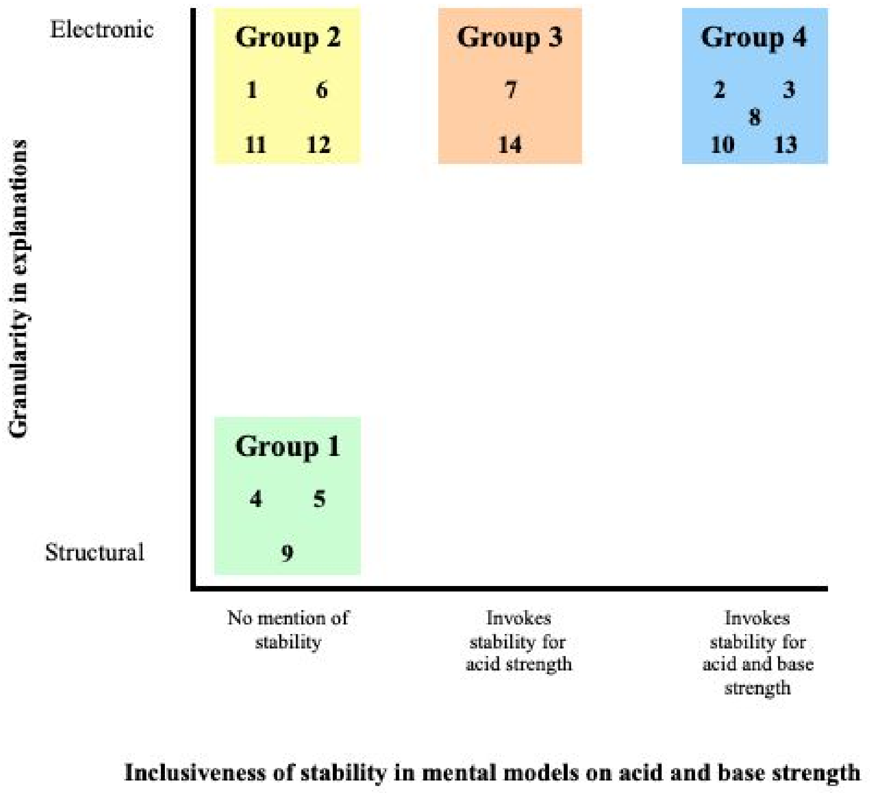


Figure 1: Groups of students with different reasoning when predicting acid and base strength

Group 1: Acid and base strength through structure without association to stability

One group of students focused on structural level granularity (S4, S5, S9), highlighting features like atom count and bond type. The origin of their structurally focused mental model rested in two approaches: either electronic features were mentioned in passing with a far heavier focus on structural features, or the mental models remained strictly structural (Table 4).

When defining stability, S5 chose a situational definition, explaining, “stability is like the ability to hold the bond together so that the atoms will not go away.” This definition was apparent as the student relied on bond strength with a focus on atom identity and bond type when determining the stability of each molecule. S4 showed a similar affinity for this mental model, utilizing the octet rule and more specifically examining the bond type in each molecule to determine stability. When asked to determine the more stable molecule the student reasoned, “I'd say phenolate. It's more stable because of the double bonds.” Akin to S5 and S9, this student’s mental model is contingent on bonds from a structural perspective; this definition of stability can be described as a rule in which more bonds equal greater stability.

As these students (S4, S5, and S9) progressed to the topic of acidity, these students did not connect stability to acid strength. Upon being asked to determine the more acidic molecule in Acidity 1, S9 responded “Honestly, I just think I remember the CH_3COO being more negatively charged than the ethoxide ion, but I am not a hundred percent sure." S9 then emphasized the number of oxygens, highlighting the element's electronegative nature as her mental model. S4 and S5 were able to remain relatively consistent in their mental models without invoking stability. Initially, both students cited the differences in bond strength as the causal factor for determining acid strength. Interestingly, S5 also used resonance, a concept grounded in electronic granularity; however, this student inappropriately applied this principle. From S5's perspective, the existence of resonance within a system induces a weaker bond and results in a better hydrogen donor. Although resonance was mentioned, the mental model used was based on a structural framework (i.e., bond strength). S5's reliance on structural features was even more apparent in Acidity 2, where no resonance features were provided. The student again emphasized bond strength, but this time focused on each bond's proximity to oxygen. S4 established a connection between bond strength and acidity, but her reasoning was inconsistent as she first utilized atom identity and then upon further questioning settled on the explanation "because of its full of octet."

Basicity appeared to generate many of the same problems that each student experienced when differentiating acidity. S4 again utilized structural features in her mental model to argue bond strength's role in determining base strength. In Basicity 1, she reasoned "Acetamide also has double bonds in its structure and double bonds are also stronger... as well, like the charges as well, like, this one was a plus charge, and then it only can have three bonds to it. So, like in terms of like stability, those are more stable…" Despite the mention of stability, it is important to note that the student displayed no conception of how this stability influences the basicity of a molecule even after being prompted by the interviewer. A similar phenomenon was witnessed in Basicity 2, when S9 introduced the idea of stability, yet showed little to no understanding of its implications. S9 clarified "the pi bonds just means it's super stable. But I don't know if the pi bonds has anything to do with basicity." S9 experienced a similar issue with Basicity 1, recognizing the presence of resonance but unable to explain the connection between resonance and basicity. S5, however, formulated a new mental model for base strength involving electron donation/acceptance. In Basicity 1, she relied on electron count, a concept grounded in structural granularity since lone pairs and bonding electrons are explicitly represented on the structures given. Attempting to stay consistent, S5 approached Basicity 2 with a similar electron donation/acceptance mental model. Nonetheless, the student realized the shortcomings of this model and reverted back to his bond strength mental model seen in acidity, confessing "So the weaker the bond I mean, if it is weaker, the oxygen is less likely to receive the electron, but I am not too sure. I still don't know."

Group 2: Acid and base strength through electronics without association to stability

Four of the students (S1, S6, S11, S12) within this study utilized a mental model contingent on electronics when determining acidity and basicity whereas explanations of students in group 1 included more structurally focused granularity. However, within their model, the association between electronics and stability was not established when analyzing acid and base strength.

In establishing the means by which stability is determined within Stability 1 and 2, each student provided congruent reasoning using primarily electronic granularity as the central focus (Table 3 and 4). The two mental models employed by these students were the delocalization of electrons and the spreading of the charge. Structural granularity such as bond type, atom count, and connectivity occasionally operated as substitutions for their electronic counterparts. With Stability 1, S1 and S6 expressed that an increased ability for electron delocalization results in greater stability. From here, they both recognized the charge present on the oxygen and recalled that the existence of a charge generates instability. Attempting to connect this idea with their mental model of delocalization, both students attempted to illustrate the delocalization being described, but after multiple drafts, both students were unable to move the charge as shown by S6 in Figure 2. S1 acknowledged, “I know that there is a way to move this down. I just don't know what it is.” S11 was also unfamiliar with the utility of delocalization in resonance, describing her knowledge on the subject more as a memorized concept explaining, “I just know that. Okay, I just have that in my head that like the more resonance, the more stable.” When all three of these students were asked to carry out a similar task in Stability 2, two out of the three students (S1 and S11) were unable to use electronics and isolated connectivity as their main argument. S6 likewise began with noticing that the positive charge retained an allylic nature (connectivity) however expounded on this observation with electronic granularity explaining that “it can do resonance and the resonance will make it more stable.” S12 followed a more structural mental model when assigning stability, using bond type as the determining factor. In Stability 1, S12 cited the presence of a double bond was the greatest indication of stability, however in Stability 2 she cited delocalization.

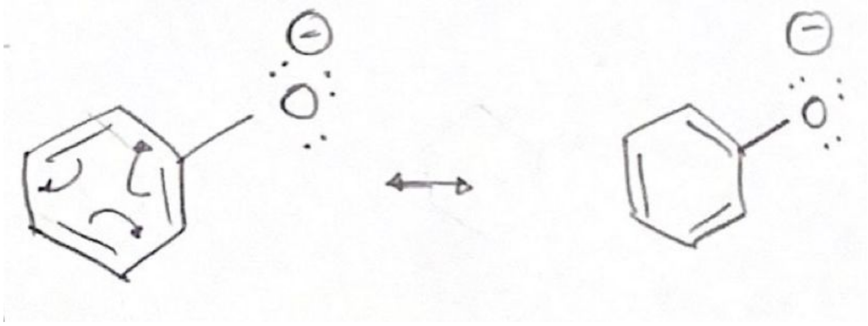


Figure 2: S6’s Illustration of electron delocalization without the spreading of the charge

Each student in this group did not carry over their electronically centered mental models of stability in determining acid strength. Although stability was not employed when determining acidity, each student was still able to exhibit a mental model loosely grounded in electronic granularity (Table 4). Three students (S1, S6, and S12) incorporated some mode of electronegativity into their mental model of acid strength referencing the idea of polarity several times. S6 highlighted her mental model of polarity stating “So when an atom is electronegative, they become, their electron cloud they're not even anymore... when the cloud is bigger on one side than the atom is gonna have more charge. And then that charge will make the molecule more acidic or basic.” Likewise, in Acidity 2 S1 denotes hydrogen’s proximity to an electronegative atom as the determining factor in acid strength. S12 referred to a polarity mental model as well yet provided an explanation by connecting the concept with resonance. This student hypothesized “if there's like a cloud around that whole like structure, for example, then say it's like then the clouds are going to be bigger towards the oxygen showing that there's more like resonance over there.” The only outlier within this session of the interview was S1’s decision to use the stability of the conjugate base as a mental model for Acidity 1 as expressed by her “the more stable one would be the more acidic”. She was able to utilize both structural (bond type) and electronic granularity (delocalization) to describe how a more stable conjugate base results in a more acidic molecule, however this was not used in Acidity 2.

This set of students also attempted to use electronic granularity to the base strength questions. For instance, in Basicity 1, two students (S1 and S6) defined bases through an accepting proton mental model, electing to determine base strength through electron count. As S1 described “It has a... lone pair which means it has more of a potential to accept an extra hydrogen into it's because it has the NH_2 plus the lone pair which means okay, there's more space to accept the hydrogen.” S11 followed a similar mental model for Basicity 1 by recognizing a positive charge and arguing that this impacts electron acceptance, which is an indication of a mental model on base congruent with Lewis definition. A considerably different narrative arises for S1 and S11 in Basicity 2 where both students showed frustration and settled on the explanation that the additional double bond was the deciding factor in base strength. Nevertheless, two students were still able to find ways to incorporate their mental model of electronics. For S6 in Basicity 2, the explanation was that propoxide’s ability to “do resonance” resulted in increased ability to accept protons. S12 provided a consistent line of reasoning for both Basicity 1 and 2, utilizing resonance and charge neutralization to explain differences in base strength. Students in this group provided no description of how electronics corresponds to stability and the impact of stability on basicity or acidity.

Group 3: Acid strength associated to electronically centered stability

Two students utilized their mental models of electronically centered stability when predicting acid strength but not base strength (S7 and S14), which contrasts with the previous groups. In group 3, students compared acid strength using the stability of the conjugate base while holding electronic granularity as the determining factor in their mental models on stability (Tables 3 and 4). Nevertheless, they were not able to use the stability of the base when differentiating base strength between two molecules.

Students in this group denoted stability as the degree to which charge is spread through the delocalization of electrons. In their explanations, charge as structural granularity and electronic granularity including spreading charge and delocalization of electrons were evident. For instance, when comparing the stability of two negatively charged ions (Stability 1), S7 expressed that although charge destabilizes an atom “resonance contributes to stability” explaining: "I think it's because the charge can be more evenly distributed across the atoms and that's why it's more stable”. The student depicted this phenomenon in Figure 3 and verbally, “but the electrons on the oxygen, they could resonate down to form like, a double bond.” Similarly, S14 elucidated how delocalization aids in the spreading of charge on the allylic cation presented in Stability 2. The student reasoned “…because the carbon is lacking the electrons…it will want to move there to make it more stable. the carbon…by the resonance again…but then the plus sign will move to here”

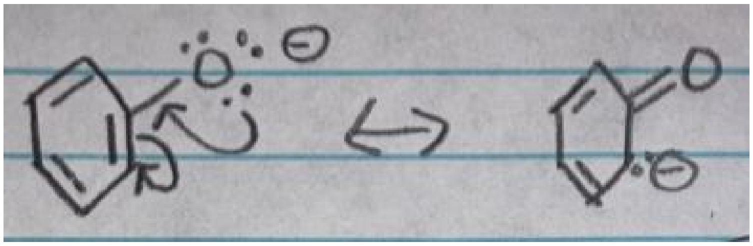


Figure 3: S7's drawing of how delocalization occurs in phenolate

The students stayed consistent in their framework and implement their electronic mental models of stability when predicting acid strength in two cases (Table 4). They used delocalization of electrons as electronic granularity in both cases whereas different structural granularity existed in each case comparison. For instance, in Acidity 1 where students were given conjugate bases with resonance to compare acidity of acetic acid and ethanol, S14 explained "…I think there's maybe conjugate base tells me why it's more acidic…it's even shown [referring resonance structures of acetate ion], like, showing me how the electrons are moving…But then it's just a resonance again, making it more stable". Even in Acidity 2 where conjugate base structures were not provided, each student was still able to use the same mental model when predicting acid strength of two hydrogens in a molecule. S7 expressed why the hydrogen closest to the carbonyl group was more acidic reasoning "I'm thinking like if…that hydrogen leaves that nitrogen will be left with…a negative charge. And that can be like resonance stabilized onto the oxygen". The student further elaborated on why delocalization does not occur for another hydrogen through structural granularity, more specifically connectivity.

These two students differed in terms of their mental models on basicity and neither cited stability (Table 3). S7's mental model on basicity relied on the Bronsted-Lowry definition. The student was also able to recognize the resonance present within the structures yet was not able to associate how this impacted stability and proton acceptance. In Basicity 1 where only structural granularity was observed, she explained "I will define a base as being a proton acceptor, and I determined that it was acetamide over ethyl amine because when I looked at the resonance structures, I saw that the second and third structures both have a negative oxygen". Defining a base and predicting base strength seemed to be more challenging for S14 due to the inconsistency in her mental model. She elected identity as the approach when comparing the base strengths' of acetamide and ethylamine. During the interview she explained "It's usually I think there was like a structure. As I said here NH_2, oxygen [referring to OH], there was like and a halide. And it usually goes this way. And this is more acidic going to more acidic side [referring to order beginning from NH_2 and ending with halide]". For this student, acid is an intrinsic property, which can be inferred from atom identity. Relying on this, she reasoned that acetamide is more acidic because of oxygen, which makes it less basic. When the student was asked why propoxide was more basic than propene-1-olate (Basicity 2), she explained, "the difference is just the pi bond there. But I'm not sure how it helps with that. But I'm not sure if I have learned this before, if I should have. I don't know".

Group 4: Acid and base strength associated to electronically centered stability

Five students employed electronically centered stability as a framework for predicting both acid strength and base strength (S2, S3, S8, S10 and S13), differing from Group 3 in their extension of the stability model to the basicity prompts. Each of these student's mental model of acid strength was related to the stability of the conjugate base while base strength was determined by the stability of base as well.

These students related stability to the degree to which the charges on negatively and positively charged ions were dispersed and/or how the electrons delocalized. (Stability 1 and Stability 2 in Table 3). For instance, S10 defined stability as "how much room the electron could take up and the different positions that it could exist in to be stabilized" indicating a focus on delocalization. S13 elected an alternative approach, claiming stability was related to the spreading of the charge, stating, "I can…disperse…Just the negative." One student's mental model (S8) included not only delocalization but also the spreading of charge, equating stability to the movement of the pi bond and dispersal of charges as depicted in Figure 4. Students utilized functional group identity (aromatic ring, S2 and S8) or connectivity (allylic, S3 and S13) or both (S10) as structural granularity to enact how delocalization and/or spreading of charge stabilizes ions in the tasks. There was only one student (S2) who defined stability in relation to identity when comparing the stability of two positively charged ions (Stability 2). This student reasoned, "The carbon is it's next to a double bond and I think that that increases stability." S2 could not provide an explanation when questioned further, as evidenced in his statement "I don't know why…I just remember the fact."

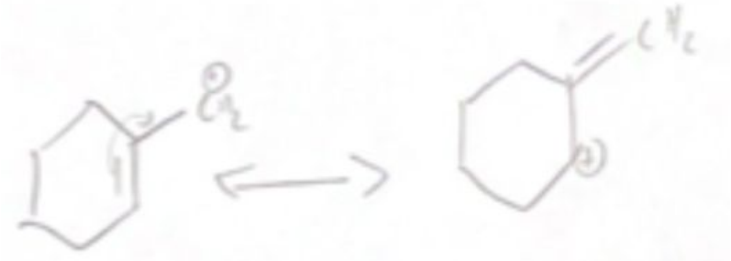


Figure 4: S8's drawing of how delocalization and spreading charge occur in an allylic carbocation

All students, apart from S13, were consistent in their mental models of acid strength, implementing their knowledge on the stability of the conjugate base in both acidity tasks (Table 3). S8 explained his mental model by emphasizing the most stable negative charge upon deprotonation. This student depicted his model in Figure 5. S13 was distinct from the others in his approach to Acidity 2 in which delocalization was emphasized, reasoning "I would say that..it's like the blue hydrogen just because…It has the ability to do resonance with the oxygen or not with oxygen, but rather with the source of electrons that are right here". S2 followed a similar mental model in Acidity 1. Regardless of their mental models, resonance specific representational features in Acidity 1 and connectivity in Acidity 2 were the common structural granularities in all students' reasoning. Nevertheless, in terms of electronic granularity, students selected a wider variety of features. Delocalization was the shared electronic granularity for all students in both tasks; however, only some students were able to activate spreading charge in both acidity tasks (S2 and S8) while others utilized it specifically for Acidity 1 (S3 and S13) where resonance specific representations were provided. Moreover, one of the students in this group (S3) also included electron withdrawal in her explanations for both cases. She expressed "induction would be greater than this one [referring to ethoxide] because this [referring to acetate] has two Os to the carbon and this [referring to ethoxide] only has one oxygen."

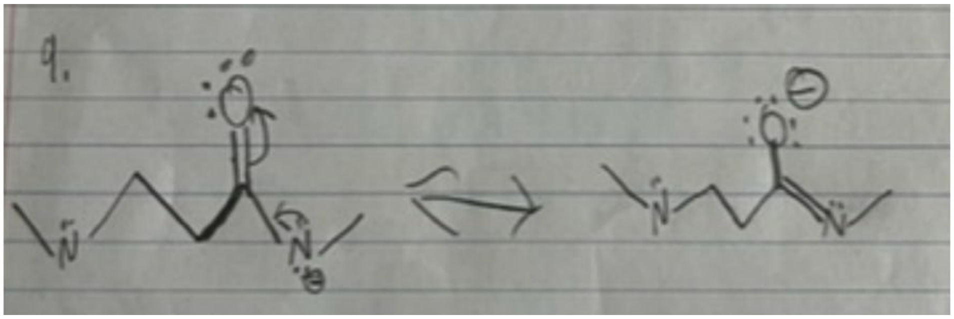


Figure 5: S8's drawing of how delocalization and spreading charge occur after deprotonation

With the exception of S2, all students utilized their electronic centered stability mental models when reasoning for base strength in two cases (Table 3). For instance, S3 focused on stability to explain why acetamide was less basic, reasoning "…the acetamide I think would be a weaker base because it's resonance stabilized". Moreover, S10 expounded, "it is more basic. If it's less stable" when comparing bases with single Lewis structures (Basicity 2). S2 applied the stability mental model in an alternative manner, determining the stability of the conjugate acid rather than that of the base. Relying on Bronsted-Lowry definition of a base, he elaborated "…I put a…theoretical hydrogen…on the oxygen [referring to the one in acetamide] and then one on the nitrogen of the ethyl amine and…I determined which one of those two would be more stable." While S2 was able to determine base strength through stability, the granularity remained strictly structural in his reasoning. (i.e., atom identity, electron count, and charge). In the context of electronic granularity, students' explanations showed partiality toward electron delocalization (excluding S10 in Basicity 2). For instance, S13 explained "the pi bonds move, that source of electrons moves around the structure, not around, but rather from the one oxygen, the top oxygen to the right nitrogen". Spreading of charge was also enacted by one student in Basicity 2 (S2) while it was observed in two students' reasoning (S8 and S10) in Basicity 1. Although used less frequently, other types of electronic granularity (i.e., polarization, electron withdrawal, and bearing charge) existed in students' explanations for Basicity 1 when resonance specific representations were provided. For instance, S3 focused on atom identity and its effect on polarization reasoning "…this has a nitrogen [referring to acetamide] as well, but oxygen has a higher electronegativity…which decides the polarity".

Discussion

Teaching on acid and base strength in organic chemistry heavily relies on a consideration of stability (Stoyanovich et al., 2015). Building on this statement, the results from this study lead to three assertions. First, students in this study can be demarcated by the whether or not they associated acid and base strength with chemical stability. Second, students that employ electronic-based stability displayed a more consistent mental model across acid and base strength (group 4) than students that focused on structural features (group 1) or did not associate stability to electronic features (group 2). Third, evaluating base strength is more challenging than acid strength even among students who enacted electronic-based stability for acids (group 3).

First, students are different from each other when reasoning on acid and base strength in relation to the degree to which they consider stability. Students in groups 1 and 2 did not associate the stability of bases and conjugate bases when comparing relative basicity and acidity. Among those, students in group 2 gravitated towards electronics (e.g., bond polarity, electronegativity, and donating electrons) in their processes. This could be explained by students' enactment of various mental models consistent with different scientific models on acids and bases. Arrhenius (i.e., gives hydrogen when dissolved in water) and Lewis models (i.e., electron transfer) could stimulate students' reliance on electronics when predicting acid and base strength (Bhattacharyya, 2006; McClary & Talanquer 2011a; Tümay, 2016). Although students have spent a considerable amount of time in Organic Chemistry I on the factors affecting acid and base strength, lack of explicit focus on the factors in relation to Bronsted-Lowry model (de Vos & Pilot, 2001; Furio´-Ma´s et al., 2005) might lead students to enact different models of acids and bases. Group 1 students did not associate stability with acid and base strength; instead, they gave prominence to structural features (e.g., atom identity, electron count, and bond type) that are accessed easily (Heckler, 2011; Shah & Oppenheimer, 2008) when predicting acid and base strength. The tendency to use surface similarity (e.g., functional group identity) and overgeneralization (e.g., bond strength or electronegativity or octet) could explain this group of students' reasoning (Talanquer, 2014). This tendency may hinder students' understanding of scientific concepts, which can result in missing relevant scientific concepts and in generating conflicting responses (Tümay, 2016). Either electronics or structural centered, most of the time, students' uses of models were triggered by the features of the task (McClary & Talanquer, 2011a; Osman & Stavy, 2006), which is accompanied by the use of relational heuristics (e.g., McClary & Talanquer, 2011a, 2011b; Tümay, 2016). For instance, S4 enacted a hybrid mental model on acid strength including identity, citing the COOH functional group, bond strength, comparing C to O versus CH_2 and CH_3, and octet, citing a full valence, when explaining why acetic acid is more acidic (Acidity 1, Table 3). However, she expressed a single mental model where bond strength is central for Acidity 2 (Table 3). She explained that "And basically when you see a lot of CH bonds you know it's basic because their structure they are weak bonds, whereas the C double bonds O, wouldn't be a shorter bond and I assume acid…the stronger."

Second, students that enact electronic-based stability displayed a more consistent mental model across acid (group 3 and 4) and base strength (group 4) than students who utilized alternative methods (groups 1 and 2). That is, the stability of conjugate base was their major focus for acid strength while the stability of base was considered for base strength across all tasks. Consistent use of stability in relative acidity and basicity is more aligned with the scientific assumptions on acid and base strength in Bronsted-Lowry model (McClary & Talanquer, 2011a; Tümay, 2016). Electronic-based stability could trigger the retrieval of a mental model of acid and base strength from long-term memory that is based on foundational principles (Gentner, 2002; McClary & Talanquer, 2011a; Vosniadou, 2002) and support students' reasoning on relative acid and base strength (Gentner, 2002). Another factor that explains why students with electronic-centered stability are more consistent in their mental models across relative acidity and basicity could be related to the type of reasoning. Invoking stability could help students to apply analytical reasoning (i.e., Type 2) instead of heuristic reasoning (i.e., Type 1) (McClary &

Talanquer, 2011a; Talanquer, 2014). Considering stability for acid and base strength is the relevant knowledge in Bronsted-Lowry model (McClary & Talanquer, 2011a; Tümay, 2016) and strong relevant knowledge in a topic could support analytical reasoning (Evans, 2008). Analytical reasoning may result in more consistent and scientific mental models (group 3 and 4) whereas heuristic reasoning (group 1 and 2) could lead to conflicting responses (Tümay, 2016). Students with electronic-centered stability searched for the following cues that help to determine how these influence relative acidity and basicity; factors effecting polarizability and bearing charge (i.e., size and electronegativity of atom), and delocalization. However, students stopped searching for inductive effects and hybridization, which were evidenced as more difficult for students (McClary & Talanquer, 2011a). Students' stopping the search for all relevant factors might be related to their difficulty in conceptualizing acid strength as an emergent property (Tümay, 2016).

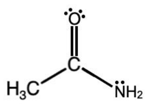
Third, base strength is more challenging than acid strength even for students who expressed electronic-centered stability. That is, the stability of conjugate base was considered by half of the students when predicting acid strength whereas fewer students utilized stability of the base when comparing relative basicity. One explanation may be the lack of emphasis on base strength relative to acid strength in the curriculum. The organic chemistry textbook used at the setting of this study (Klein, 2017) describes acid strength in relation to several factors influencing the stability of conjugate base extensively through explanations and worked examples, whereas base strength is not as thoroughly explored. Base strength is also mentioned in relation to nucleophilicity and addressed in amines instead of a phenomenon by itself. Another reason for why base strength is more challenging than acid strength could be the switch in framing of stability in the judgment making process. In judging acid strength, one must identify the most stable conjugate base, while in judging base strength one must identify the least stable base. Switching this frame of reference may be difficult for some students and may require explicit modeling.

Implications

To help students understand chemical stability and the role of stability in acidity, and basicity, chemistry instruction could benefit from scaffolding the emergent nature of stability (Wilensky & Resnick, 1999) and how stability relates to acid and base strength (Kranz et al., 2013). To emphasize the emergent nature, instructors should use the terms "emergence" and "system" explicitly since chemical systems are emergent in nature including entities and their properties and activities, in increasing complexity that results in novel properties (Machamer et al., 2000). It is also important that students should be informed about the acid-base model that is used when comparing relative acidity and basicity. Since Bronsted-Lowry model is the fundamental model in organic chemistry (Stoyanovich et al., 2015), chemistry instructors could emphasize this model at first introducing examples as "an acid–base reaction system" instead of "an acid–base reaction". Then, students can be prompted "How do acidic and basic properties emerge in an acid-base reaction system?" and finally focus on relative acid and base strength. Student discussions can be directed toward the relative stability of all species determines the direction and extent of this dynamic process, which form the basis of acid and base strength. Moreover, "delocalization" should be used as an alternative to "resonance" when discussing chemical stability. Although the term resonance has been used since its introduction in 1950s, electron delocalization describes the physical reality more than the term resonance (Kerber, 2006). In summary, instruction may benefit by focusing on three sequential learning outcomes: (1) explicit teaching of stability, (2) explicit mapping of basicity onto the construct of stability, and (3) mapping of acidity onto the construct of stability of the conjugate base.

As explicit teaching of stability requires comprehension of the emergent nature of stability, we proposed an example scaffold based on Deng and Flynn's model (2021). The scaffold, shown in Figure 6, uses three prompts: evaluating the relevance of each factor contributing emergence of stability for two molecule systems (correct responses are shown in red), comparing the relative effect of relevant factors (i.e., entities and activities) for two systems, and reasoning about stability emerged from the interaction of all entities and activities in the molecule system. Chemistry instructors could model how to reason on emergence of stability in different molecule systems.

A



B

$CH_3—CH_2—\ddot{N}H_2$

1. Identify the relevancy of each factor contributing the emergence of the stability of molecule systems if at all.

Charge	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Atom size	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Electronegativity	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Delocalization	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Hybridization	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Electron withdrawal	Stabilizes A more than B	Stabilizes B more than A	Not relevant
Electron donation	Stabilizes A more than B	Stabilizes B more than A	Not relevant

2. Which factor(s) has (have) the greater effect on the relative stability in this case?

Atom (N) is the same. Therefore, size and electronegativity of the atom are not relevant. Delocalization lowers free energy and hence increases stability of acetamide. Electron withdrawing of carbonyl group (-C=O) stabilizes the acetamide through polarization of sigma bonds of molecule. The nitrogen on acetamide is sp^2 whereas the nitrogen on ethylamine is sp^3. The lone pair on the amide is in a p-orbital, whereas the lone pair on the amine is sp^3. The larger s-character of the lone pair on nitrogen on ethylamine (sp^3) is more stabilizing than on nitrogen on acetamide. That is, this is opposite of delocalization and inductive effect.

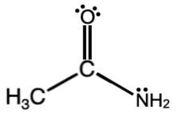
3. Based on your reasoning in 1 and 2, which of the molecule system emerge as more stable and why?

Delocalization is more important factor than hybridization for making the acetamide more stable. With the consideration of inductive effect acetamide is more stable than ethylamine.

Figure 6: Example scaffold to model the emergent nature of stability

Following a scaffold on chemical stability, a similar scaffold can be used regarding relative basicity (Figure 7) also based on the Deng and Flynn's model (2021). Before utilizing the scaffolding prompts, chemistry instructor could emphasize how relative stability determines relative base strength within a competing proton transfer system. Student responses to prompts 2 and 3 in Figure 7 can elucidate the extent the students' employ stability considerations in making basicity predictions. Various worked examples on emergence of basic property that requires consideration of different type and number of factors might help students to build a more conceptual understanding.

A



B

$CH_3—CH_2—\ddot{N}H_2$

1. Identify the relevancy of each factor contributing the emergence of the basicity of each molecule system, if at all.

Charge	Increases basicity of A more than B	Increases basicity of B more than A	[✓ Not relevant]
Atom size	Increases basicity of A more than B	Increases basicity of B more than A	[✓ Not relevant]
Electronegativity	Increases basicity of A more than B	Increases basicity of B more than A	[✓ Not relevant]
Delocalization	Increases basicity of A more than B	[✓ Increases basicity of B more than A]	Not relevant
Hybridization	[✓ Increases basicity of A more than B]	Increases basicity of B more than A	Not relevant
Electron withdrawal	Increases basicity of A more than B	[✓ Increases basicity of B more than A]	Not relevant
Electron donation	Increases basicity of A more than B	Increases basicity of B more than A	[✓ Not relevant]

2. Which factor(s) has (have) the greater effect on the relative basic property in this case?

Atom is the same (N). Therefore, size and electronegativity of the atom are not relevant. Delocalizing the lone pair on nitrogen and giving the nitrogen atom a partial positive charge and makes it less available for bonding a proton for acetamide. Electron withdrawing of carbonyl group (-C=O) (inductive effect) increases stability for acetamide, which in turn decreases the basicity of acetamide. The nitrogen on acetamide is sp^2 whereas the nitrogen on ethylamine is sp^3. The lone pair on the amide is in a p-orbital, whereas the lone pair on the amine is sp^3. The larger s-character of the lone pair on nitrogen on ethylamine (sp^3) is more stabilizing than on nitrogen on acetamide (p orbital). Therefore, orbital decreases the stability of acetamide, which in turn increases the basicity. That is, this is opposite of delocalization and inductive effect.

3. Based on your reasoning in 1 and 2, which of the molecule system emerge as more basic and why?

Delocalization is more important factor than hybridization for making the acetamide more stable and less basic. With the consideration of inductive effect acetamide is less basic than ethylamine.

Figure 7: Example scaffold to model the relative base strength

Finally, chemistry instructors could map acidity onto the construct of stability of the conjugate base. Before mapping, chemistry instructor could emphasize why stability is the determining factor for the emergence of acidic property in Bronsted-Lowry model. A similar scaffold can be developed for relative acid strength with students rating the conjugate base for two molecule systems. Responses to prompts 2 and 3 can then explore how students invoke chemical stability of the conjugate bases and how this rating relates to relative acid strength. The explicit teaching of emergent nature of stability, acidity, and basicity and the use of scaffolds may prevent students' reliance on heuristics driven by their mental models that can be triggered by the tasks and hence help students to form a better comprehension of these phenomena.

This study has been one of the first attempts investigating students' understanding of base strength to the best of the researchers' knowledge. In this study, students had difficulties in explaining how the relative stability of bases relates to the relative base strength. Additional research can adopt the prompts presented in Figures 6 and 7 to utilize in a larger scale study where the focus is on students understanding of various factors that influence the stability of bases and their strength. The results from a study of this form can offer additional insight into the challenges students may face with base strength.

Limitations

There were several limitations inherent to this study. First, the conclusions are limited to the students at the research institution where the study was conducted. However, we attempted to expand the theories of mental model (Park & Gittleman, 1995) and granularity (Luisi, 2002; Talanquer, 2022), which is one of the aims of the case study (Yin, 2009). This study provided evidence for the applicability of those models to stability and basicity since available literature utilized those when investigating acid strength (e.g., Tümay, 2016) and acid-base reactions (e.g., Deng & Flynn, 2021). Researchers can benefit from using theories of mental model and granularity to reveal whether conclusions reached in this study is valid in their institutions. Also, the conclusions can be a foundation to devise questions for a larger scale study where students' reasoning on acid and base strength are investigated. Second, limitations rest in the exploratory nature of this study. We did not prepare interviews to identify whether students invoke stability in their mental models on acid and base strength. However, through follow-up questions, we were able to capture to what degree students relate stability with relative acidity and basicity. Further research could benefit from questions that intentionally reveal students' consideration of stability. Finally, it is unknown the extent that assessments in the course promoted students' use of electronic granularity or stability in making predictions of relative acid or base strength. Future research that investigates the extent to which students use these features during their assessments would inform instruction and assessment design.

Conclusion

Four groups of students emerged, differentiated by their reasoning on acid and base strength: (1) acid and base strength through structure, (2) acid and base strength through electronics, (3) acid strength associated with electronically centered stability, and (4) acid and base strength associated with electronically centered stability. Among those groups, a more consistent mental model across acid and base strength was observed in students that enact electronic-based stability. In addition, students employing electronic-based stability for acids experienced difficulty in relating their mental model of stability to base strength.

Conflicts of Interest: The authors report no conflicts of interest for this work.

Acknowledgements: This material is based upon work supported by the National Science Foundation under Grant No 2142324. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation. Author BD would like to thank The Scientific and Technological Research Council of Turkey for their support (TÜBITAK 2219) and Zonguldak Bülent Ecevit University. The authors wish to acknowledge Ayesha Farheen, Dianna Kim, Jessica D. Young, and Pallavi Nayyar for feedback on project development. The authors also acknowledge the students who participated in the interviews and instructors for feedback on the instructional setting.

References

Alfieri, L., Nokes-Malach, T. J., & Schunn, C. D. (2013). Learning through case comparisons: A Meta-analytic review, *Educational Psychology, 48*, 87-113.

American Chemical Society (2015). *Committee on professional training. Organic chemistry supplement*. https://www.acs. org/content/dam/acsorg/about/governance/committees/ training/acsapproved/degreeprogram/organic-chemistry- supplement.pdf (accessed January 2023).

Anderson, T. L., & Bodner, G. M. (2008). What can we do about 'Parker'? A case study of a good student who didn't 'get'organic chemistry. *Chemistry Education Research and Practice, 9*(2), 93-101.

Bhattacharyya, G. (2006). Practitioner development in organic chemistry: How graduate students conceptualize organic acids. *Chemistry Education Research and Practice, 7*(4), 240–247.

Bhattacharyya, G. (2014). Trials and tribulations: Student approaches and difficulties with proposing mechanisms using the electron-pushing formalism. *Chemistry Education Research and Practice, 15*(4), 594-609.

Bhattacharyya, G., & Bodner, G. M. (2005). "It gets me to the product": How students propose organic mechanisms. *Journal of Chemical Education*, *82*(9), 1402-1407.

Bodé, N. E., Deng, J. M., & Flynn, A. B. (2019). Getting past the rules and to the WHY: Causal mechanistic arguments when judging the plausibility of organic reaction mechanisms. *Journal of Chemical Education*, *96*(6), 1068-1082.

Boothe, J. R., Zotos, E. K., & Shultz, G. V. (2023). Analysis of post-secondary instructors' pedagogical content knowledge of organic acid–base chemistry using content representations. *Chemistry Education Research and Practice*, *24*(2), 577-598.

Bretz, S. L., & McClary, L. (2015). Students 'understandings of acid strength: How meaningful is reliability when measuring alternative conceptions? *Journal of Chemical Education*, *92*(2), 212-219.

Clement, J. J. & Rea-Ramirez, M. A. (2008). *Model based learning and instruction in science*, New York: Springer.

Coll, R. K., & Treagust, D. F. (2003). Investigation of secondary school, undergraduate, and graduate learners' mental models of ionic bonding. *Journal of Research in Science Teaching*, *40*(5), 464-486.

Cooper, M. M., Kouyoumdjian, H., & Underwood, S. M. (2016). Investigating students ' reasoning about acid–base reactions. *Journal of Chemical Education*, *93*(10), 1703-1712.

Creswell J. W. (2007). *Qualitative inquiry and research design: Choosing among five traditions*, London, UK: Sage.

De Vos, W., & Pilot, A. (2001). Acids and bases in layers: The stratal structure of an ancient topic. *Journal of Chemical Education, 78*(4), 494–499.

Deng, J. M., & Flynn, A. B. (2021). Reasoning, granularity, and comparisons in students ' arguments on two organic chemistry items. *Chemistry Education Research and Practice*, *22*(3), 749-771.

Evans, J. S. B. (2008). Dual-processing accounts of reasoning, judgment, and social cognition. *Annual Review of Psychology, 59*, 255-278.

Furio´-Ma´s, C., Calatayud, M. L., Guisasola, J., & Furio´-Go´mez, C. (2005). How are the concepts and theories of acid–base reactions presented? Chemistry in textbooks and as presented by teachers. *International Journal of Science Education, 27*(11), 1337–1358.

Gentner, D. (2002), Mental models, psychology of. In Smelser N. J. and Bates P. B. (Eds.). *International encyclopedia of the social and behavioral sciences* (pp. 9683–9687.), Amsterdam, Netherlands: Elsevier Science.

Gilbert, J. K. & Boulter, C. J. (1998). Learning science through models and modeling, in Fraser B. J. and Tobin K. G. (Eds.), *International handbook of science education* (pp. 53–66.*)*, Amsterdam: Kluwer Academic Publishers

Gilbert, J. K., Boulter, C. J., & Rutherford, M. (2000). Explanations with models in science education, in J. K. Gilbert and C. J. Boulter (Eds.). *Developing models in science education* (pp. 193-208). Dordrecht: Springer

Graulich, N. (2015). The tip of the iceberg in organic chemistry classes: how do students deal with the invisible? *Chemistry Education Research and Practice, 16*(1), 9-21.

Greca, I. M., & Moreira, M. A. (2000). Mental models, conceptual models, and modelling. *International Journal of Science Education*, *22*(1), 1-11.

Grove, N. P., Cooper, M. M., & Cox, E. L. (2012). Does mechanistic thinking improve student success in organic chemistry? *Journal of Chemical Education, 89*(7), 850-853.

Heckler, A. F. (2011). The role of automatic, bottom-up processes: In the ubiquitous patterns of incorrect answers to science questions, in Mestre, J. P. and Ross, B. H. (Eds.). *Psychology of learning and motivation* (Vol. 55, pp. 227-267). San Diego, CA: Academic Press.

Johnson-Laird, P. N. (1983). *Mental models: Towards a cognitive science of language, inference, and consciousness* (No. 6). Harvard University Press.

Kerber, R. C. (2006). If it's resonance, what is resonating? *Journal of Chemical Education, 83*(2), 223.

Klein, D. (2017). *Organic chemistry* (4th Ed.), New York, NY: Wiley.

Kranz, D., Schween, M., & Graulich, N. (2023). Patterns of reasoning–exploring the interplay of students' work with a scaffold and their conceptual knowledge in organic chemistry. *Chemistry Education Research and Practice*, *24*(2), 453-477

Lin, J. W., & Chiu, M. H. (2007). Exploring the characteristics and diverse sources of students ' mental models of acids and bases. *International Journal of Science Education*, *29*(6), 771-803.

Luisi, P. L. (2002), Emergence in chemistry: Chemistry as the embodiment of emergence, *Foundations of Chemistry, 4(*3), 183–200.

Machamer, P., Darden, L., & Craver, C. F. (2000). Thinking about mechanisms, *Philosophy of Science, 67*(1), 1–25.

Marshall, G. B. & Rossman, C. (2011). *Designing qualitative research* (5th Ed.), London: Sage.

McClary, L. M., & Bretz, S. L. (2012). Development and assessment of a diagnostic tool to identify organic chemistry students 'alternative conceptions related to acid strength. *International Journal of Science Education, 34*(15), 2317–2341.

McClary, L., & Talanquer, V. (2011a). College chemistry students 'mental models of acids and acid strength. *Journal of Research in Science Teaching, 48*(4), 396–413.

McClary, L., & Talanquer, V. (2011b). Heuristic reasoning in chemistry: Making decisions about acid strength. *International Journal of Science Education, 33*(10), 1433–1454.

Nersessian, N. J. (2008). *Creating scientific concepts*, Cambridge: MIT Press.

Osman, M., & Stavy, R. (2006). Development of intuitive rules: Evaluating the application of the dual-system framework to understanding children's intuitive reasoning. *Psychonomic Bulletin & Review*, *13*(6), 935-953.

Park, O. C., & Gittelman, S. S. (1995). Dynamic characteristics of mental models and dynamic visual displays. *Instructional Science*, *23*(5), 303-320.

Petterson, M. N., Watts, F. M., Snyder-White, E. P., Archer, S. R., Shultz, G. V., & Finkenstaedt-Quinn, S. A. (2020). Eliciting student thinking about acid–base reactions via app and paper–pencil based problem solving. *Chemistry Education Research and Practice*, *21*(3), 878-892.

Raker, J., Holme, T., & Murphy, K. (2013). The ACS exams institute undergraduate chemistry anchoring concepts content map II: Organic chemistry. *Journal of Chemical Education*, *90*(11), 1443-1445.

Shah, A. K., & Oppenheimer, D. M. (2008). Heuristics made easy: An effort-reduction framework. *Psychological Bulletin, 134*(2), 207-222.

Shah, L., Rodriguez, C. A., Bartoli, M., & Rushton, G. T. (2018). Analysing the impact of a discussion-oriented curriculum on first-year general chemistry students' conceptions of relative acidity. *Chemistry Education Research and Practice*, *19*(2), 543-557.

Solomons, T. G., & Fryhle, C. B. (2012). *Organic chemistry* (7th Ed.). New York, NY: Wiley.

Stoyanovich, C., Gandhi, A., & Flynn, A. B. (2015). Acid–base learning outcomes for students in an introductory organic chemistry course. *Journal of Chemical Education*, *92*(2), 220-229.

Talanquer, V. (2014). Chemistry education: Ten heuristics to tame. *Journal of Chemical Education,* 91(8), 1091-1097.

Talanquer, V. (2022). The complexity of reasoning about and with chemical representations. *JACS Au, 2*(12), 2658–2669.

Tümay, H. (2016). Emergence, learning difficulties, and misconceptions in chemistry undergraduate students ’conceptualizations of acid strength. *Science and Education*, *25*, 21-46.

van der Veer, G. C., Kok, E., & Bajo, T. (1999). Conceptualizing mental representations of mechanics: A method to investigate representational change, in D. Kayser and S. Vosniadou (Eds.) *Modeling changes in understanding: Case studies in physical reasoning* (pp 44–60). Oxford: Elsevier

Vosniadou, S. (2002). Mental models in conceptual development. In: L. Magnani and N. J. Nersessian (Eds.), *Model-based reasoning* (pp 353–68). Boston, MA: Springer.

Wilensky, U., & Resnick, M. (1999). Thinking in levels: A dynamic systems approach to making sense of the world. *Journal of Science Education and Technology, 8*(1), 3–19.

Yin, R. K. (2009). *Case study research: Design and methods* (4th Ed.). Thousand Oaks, CA: Sage.

Organic Chemistry Students' Use of Stability in Mental Models on Acid and Base Strength

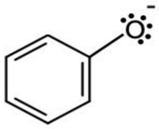
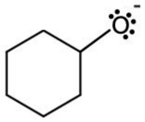
Supporting Information

Interview Protocols

Protocol A

<u>Section 1:</u>

Prompt 1: Structures of phenolate ($C_6H_5O^-$) and cyclohexanolate ($C_6H_{11}O^-$) ions are given below.

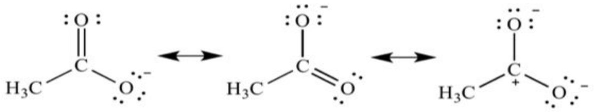
Phenolate ($C_6H_5O^-$)	Cyclohexanolate ($C_6H_{11}O^-$)
	

Considering the structures, compare the stability of phenolate ($C_6H_5O^-$) and cyclohexanolate ($C_6H_{11}O^-$) ions.

1.1. **<u>Which ion</u>** (phenolate ($C_6H_5O^-$) and cyclohexanolate ($C_6H_{11}O^-$)) is more stable?

1.2. Using molecular structures, explain **<u>why</u>** you made such a stability order for phenolate ($C_6H_5O^-$) and cyclohexanolate ($C_6H_{11}O^-$).

Prompt 2: Structures of acetate ion (CH_3COO^-) and structure of ethoxide ion ($CH_3CH_2O^-$) are given below.

Acetate ion (CH_3COO^-)	Ethoxide ion ($CH_3CH_2O^-$)
	

Considering the structures, compare the acidity of acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH) in water.

$$CH_3COOH(aq) + H_2O(l) \rightleftharpoons CH_3COO^-(aq) + H_3O^+(aq)$$

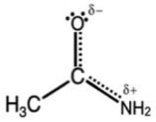
$$CH_3CH_2OH(aq) + H_2O(l) \rightleftharpoons CH_3CH_2O^-(aq) + H_3O^+(aq)$$

2.1 **<u>Which one</u>** (acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH)) is more acidic?

2.2. Using molecular structures, explain **<u>why</u>** you made such an acidity order for acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH)?

Prompt 3: Structure of acetamide (CH_3CONH_2) and structure of ethylamine ($CH_3CH_2NH_2$) molecules are given below.

Acetamide (CH_3CONH_2)	Ethylamine ($CH_3CH_2NH_2$)

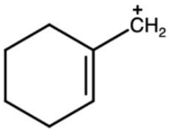
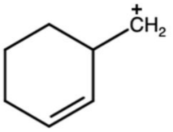
	$CH_3-CH_2-\ddot{N}H_2$

Considering the structures, compare the basicity of acetamide (CH_3CONH_2) and ethylamine ($CH_3CH_2NH_2$) in water.

3.1. **Which one** (acetamide (CH_3CONH_2) and ethylamine ($CH_3CH_2NH_2$)) is more basic?
3.2. Using molecular structures, explain **why** you made such a basicity order for acetamide (CH_3CONH_2) and ethylamine ($CH_3CH_2NH_2$)?

Section 2:

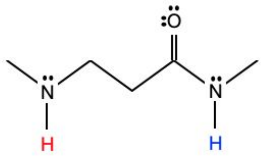
Prompt 1. Structures of Ion A and Ion B are given below. Compare the stability of following ions.

Ion A	Ion B
	

Considering the structures, compare the stability of ion A and ion B.

1.1 **Which ion** (Ion A and Ion B) is more stable?
1.2. Using molecular structures, explain **why** you made such a stability order for ion A and ion B.

Prompt 2: Structure of an acid is given below. Compare the acidity of hydrogen atoms.



Considering the structure, compare the acidity of hydrogens?

2.1. **Which hydrogen** (red and blue) is more acidic?
2.2. Using molecular structure, explain **why** you made such an acidity order for hydrogens (red and blue).

Prompt 3: Structures of propene-1-olate and propoxide are given below. Compare the basicity of following ions.

Propene-1-olate	Propoxide
	

Considering the structures, compare the basicity of propene-1-olate and propoxide in water.

3.2. **Which one** (propene-1-olate and propoxide) is more basic?

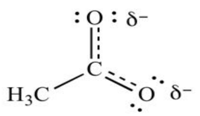
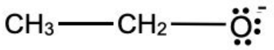
3.2. Using molecular structures, explain **why** you made such a basicity order for propene-1-olate and propoxide.

Protocol B

Section 1:

Prompt 1: Prompt is the same with the prompt 1 in section 1 in protocol A.

Prompt 2: Structure of acetate ion (CH_3COO^-) and structure of ethoxide ion ($CH_3CH_2O^-$) are given below.

Acetate ion (CH_3COO^-)	Ethoxide ion ($CH_3CH_2O^-$)
	

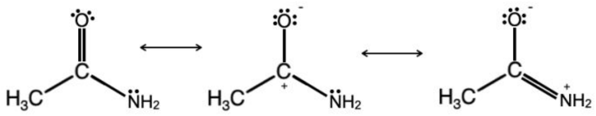
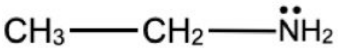
Considering the structures, compare the acidity of acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH) in water.

$$CH_3COOH(aq) + H_2O(l) \rightleftharpoons CH_3COO^-(aq) + H_3O^+(aq)$$

$$CH_3CH_2OH(aq) + H_2O(l) \rightleftharpoons CH_3CH_2O^-(aq) + H_3O^+(aq)$$

2.1. **Which one** (acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH)) is more acidic?
2.2. Using molecular structures, explain **why** you made such an acidity order for acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH)?

Prompt 3: Structures of acetamide (CH_3CONH_2) and structure of ethylamine ($CH_3CH_2NH_2$) molecules are given below.

Acetamide (CH_3CONH_2)	Ethylamine ($CH_3CH_2NH_2$)
	

Considering the structures, compare the basicity of acetamide (CH_3CONH_2) and ethylamine ($CH_3CH_2NH_2$) in water.

3.1. **Which one** (acetamide (CH_3CONH_2) and ethyl amine ($CH_3CH_2NH_2$)) is more basic?
3.2. Using molecular structures, explain **why** you made such a basicity order for acetamide (CH_3CONH_2) and ethylamine ($CH_3CH_2NH_2$)?

Section 2:

Prompts in this section in protocol B is the same with the prompts in section 2 in protocol A.

Correct Responses for the Case Comparison Tasks in Interviews

Stability 1

Phenolate is more stable than cyclohexanolate. When comparing the stability of phenolate vs cyclohexanolate, the relevant factors are;

- Atom is the same therefore size and electronegativity not relevant
- Resonance/delocalization - spreading charge lowers free energy of phenolate
- Inductive effect - Through induction sp^2 carbon groups are electron withdrawing through sigma bonds whereas sp^3 carbon groups are electron donating through sigma bonds. Phenyl group is electron withdrawing which further stabilizes the phenolate ion (by spreading the charge of the anion across a larger area). Cyclo group is electron donating which destabilizes the cyclohexanolate ion (by concentrating negative charge on the oxygen).
- Orbital - The oxygen on phenolate is sp^2 whereas the oxygen on cyclohexanolate is sp^3. The larger s-character on the oxygen on phenolate stabilizes the negative charge on that oxygen relative to the oxygen on the cyclohexanolate.

Stability 2

Ion A is more stable than ion B. When comparing the stability of ion A and ion B, the relevant factors are;

- Atom is the same therefore size and electronegativity are not relevant
- Resonance/delocalization - spreading the charge lowers free energy of Ion A
- Inductive effect - Through induction sp^2 carbon groups are electron withdrawing through sigma bonds whereas sp^3 carbon groups are electron donating through sigma bonds. On the left structure the next-door sp^2 carbon is electron withdrawing which destabilizes the carbocation through induction (by concentrating more positive charge at the carbocation). On the right structure the next-door sp^3 carbon is electron donating which stabilizes that carbocation (by spreading the charge of the carbocation across a larger area). Therefore, induction decreases the stability of ion A. That is, this is opposite from the overall stability of these two ions because resonance has a larger effect than induction.
- Orbital is not relevant.

Acidity 1

Acetic acid is more acidic than ethanol. When comparing the acidity of acetic acid (CH_3COOH) and ethanol (CH_3CH_2OH) in water, relevant factors are;

- Atom is the same therefore size and electronegativity not relevant.
- Resonance/delocalization - spreading charge lowers free energy and increases stability for conjugate base of acidic acid, which in turn increases the acidity of acetic acid.
- Inductive effect - electron withdrawing of carbonyl group (-C=O) stabilize the acetate ion through polarization of sigma bonds of molecule. Therefore, induction increases stability for conjugate base of acidic acid, which in turn increases the acidity of acetic acid.
- Orbital - The oxygen on acetic acid is sp2 whereas the oxygen on ethanol is sp^3. The larger s-character on the oxygen on acetic acid stabilizes the negative charge on the oxygen of acetate relative to the oxygen of ethoxide. Therefore, induction increases stability for conjugate base of acidic acid, which in turn increases the acidity of acetic acid.

Acidity 2

- Blue (amide) hydrogen is more acidic than red (amine) hydrogen. When comparing the acidity of blue (amide) and red (amine) and hydrogen, relevant factors are;
- Atom is the same therefore size and electronegativity are not relevant.
- Resonance/delocalization - spreading charge lowers free energy and increases stability for conjugate base of blue (amide) hydrogen, which in turn increases the acidity of blue hydrogen.

- Inductive effect - electron withdrawing of carbonyl group (-C=O) stabilize the ion formed after donating blue (amide) hydrogen through polarization of sigma bonds of molecule. Therefore, induction increases stability for conjugate base of blue (amide) hydrogen, which in turn increases the acidity of blue (amide) hydrogen.
- Orbital - The nitrogen bonded to blue hydrogen (amide) is sp^2 whereas the nitrogen bonded to red hydrogen (amine) is sp^3. The larger s-character of nitrogen bonded to blue hydrogen (amide) stabilizes the negative charge on the nitrogen of the conjugate base formed after donation of blue hydrogen (amide) relative to the negative charge on nitrogen of the conjugate base formed after donation of the red hydrogen (amine). Therefore, orbital increases stability of conjugate base formed after donation of blue (amide) hydrogen, which in turn increases the acidity of blue (amide) hydrogen.

<u>Basicity 1</u>

Ethylamine is more basic than acetamide. When comparing the basicity of acetamide (CH_3CONH_2) and ethyl amine ($CH_3CH_2NH_2$) in water, relevant factors are;

- Atom is the same therefore size and electronegativity are not relevant.
- Resonance/delocalization - delocalization lowers free energy and hence increases stability of acetamide. Delocalizing the lone pair on nitrogen and giving the nitrogen atom a partial positive charge and makes it less available for bonding a proton for acetamide.
- Inductive effect - electron withdrawing of carbonyl group (-C=O) stabilize the acetamide through polarization of sigma bonds of molecule. Therefore, induction increases stability for acetamide, which in turn decreases the basicity of acetamide.
- Orbital - The nitrogen on acetamide is sp^2 whereas the nitrogen on ethylamine is sp^3. The lone pair on the amide is in a p-orbital, whereas the lone pair on the amine is sp^3. The larger s-character of the lone pair on nitrogen on ethylamine (sp^3) is more stabilizing than on nitrogen on acetamide (p orbital). Therefore, orbital decreases the stability of acetamide, which in turn increases the basicity. That is, this is opposite of the overall effect since delocalization through resonance is a more important factor making the acetamide more stable and thus less basic.

<u>Basicity 2</u>

Propene-1-olate is more basic (less stable) than propoxide. Propanal pKa~17 and propanol pKa~16. When comparing the basicity of propene-1-olate and propoxide in water, relevant factors are;

- Atom - Most important factor in determining basicity. On the propene-1-olate, the negative charge is on both the oxygen and the carbon. The resonance structure drawn contributes more to the overall structure but the other structure does place a decent amount of partial negative charge on the carbon. Negative charge on a less electronegative atom (C) is less stable making the propene-1-olate more basic.
- Resonance/delocalization - making propene-1-olate less basic. Spreading charge lowers free energy and hence increases stability of propene-1-olate. Delocalizing the lone pair on oxygen and giving the oxygen atom less of a negative charge and makes it less available for bonding a proton for propene-1-olate
- Inductive effect - Through induction sp^2 carbon groups are electron withdrawing through sigma bonds whereas sp^3 carbon groups are electron donating through sigma bonds. On propene-1-olate, the next-door sp^2 carbon is electron withdrawing which stabilizes the ion (by spreading the charge of the anion across a larger area). On propoxide, structure the next-door sp^3 carbon is electron donating which destabilizes the anion (by concentrating negative charge on the oxygen). Therefore, propene-1-olate is less basic. Orbital - The oxygen on propene-1-olate is sp^2 whereas the oxygen on propoxide is sp^3. The larger s-character on the oxygen on propene-1-olate stabilizes the negative charge on that oxygen relative to the oxygen on propoxide. Therefore, propene-1-olate is less basic.

Codebook for Granularity

Category	Code	Definition and criteria for inclusion	Examples
Structural	Atom identity	Participants refer to a particular atom(s) by stating the name (e.g., oxygen) and/or symbol (e.g., O, N, C, and H) of the atom(s).	“Because oxygen is electronegative atom. And that makes the whole like, molecule become more electronegative, electronegative…” (S6)
	Atom count	Participants refer to number of particular atom(s) by counting or stating total number.	“…there’s two oxygen atoms and one of them has an electronegative charge, there is only one oxygen here” (S1)
	Functional group identity	Participants refer to particular functional group(s) by stating the name (e.g., aromatic ring, amine, amide, carboxyl, carbonyl, hydroxyl, six membered ring with three double bond, carbon ring, benzylic ring, the ring, phenol, phenyl etc.) or formula (e.g., $-NH_2$, $-CONH_2$, $-C=O$) of that functional group(s).	“Um, for me, it was the presence of the carbonyl” (S8)
	Bond type	Participants refer to bond(s) by stating type of bond (e.g., sigma bond/single bond, pi bond/double bond/alkene, single bond has sp^3, double bond has sp^2).	“the only difference is the double bond, so I'd assume the bond would be more strength and then in other one single bond be weaker, which would be more basic.” (S4)
	Bond count	Participants refer to number of particular bond(s) by counting (e.g., sigma and pi bond) or stating total number or making inference about hybridization (e.g., sp3, sp2, and sp) based on number of sigma and double bonds.	“acid ion it has. This is 1, 2, 1, 2, 3 bonds” (S6)
	Connectivity of atoms, ions, and functional groups	Participants refer to how atoms, ions, and functional groups are connected either explicitly (e.g., atom, ions, and functional groups are next to or adjacent to or in close proximity or connected to or attached to or bonded to other atoms, ions, and functional groups, a lone pair adjacent to C+,) or implicitly (e.g., Allylic lone pair, Allylic carbocation, lone pair on the atom because the pi bond is just right there, sp^2 is/being closer to CH_2 plus, sp^2 but it's one extra carbon away).	“I know it makes it less stable. I'm not sure as much as to why it makes it less stable. I mostly focused on allylic, but I do know on that greater than flow chart I was talking about vynyllic was like negative below primary.” (S11)
	Electron count	Participants refer to number of electron either explicitly by counting or implicitly (e.g., atom with complete/incomplete octet based on number of electrons, lone pairs, valance shell).	“And it has the amine and the amine is here with the complete octet, I think, is a very big indicator to me that it's a more it's more basic compared to that of an Acetamide.” (S1)

	Charge	Participants refer to partial or negative charge on the structures explicitly featured.	“Um, for that I looked at I saw in structures two and three, they both had negative charge on the oxygen, but the first one didn’t” (S8)
	Resonance specific representational feature	Participants refer to explicit features (e.g., double headed arrow, dashed/dotted lines, delta) of structures peculiar to resonance.	“the dash, the dash is showing that the bonds can be formed or broken? And it's basically simultaneous” (S9)
Electronic	Electron withdrawal	Participants refer to electron withdrawal by describing this using various verbs and nouns (e.g., atom withdraws electrons, pull of electrons, pull on the atom, electron withdrawing).	“Yeah. the pull on the on the carbon would be greater than that on the one with the one oxygen and the carbon” (S3)
	Bearing charge	Participants refer to the capacity of bearing charge (e.g., charge is strongly attached to more electronegative atom and atom can hold negative charge better than the other atom).	“Carbon is I mean, they can hold negative charges, but they don't hold them as well as oxygen to. So that's why I would go to Blue hydrogen” (S7)
	Spreading charge	Participants refers to spreading of charge either by explicitly stating how charge is spread (e.g., convert negative charge to a neutral charge, balance out negative charge, neutralize negative charge, charge can be evenly distributed, pull negative charge, resonate charges that can jump around, charge can not really move from the atom over, positive charge would leave that atom then positive charge would be on that atom) and/or the use of a drawing indicating charge separation from formal negative charge on one atom to partial negatives on multiple atoms.	“Oh, and no, I was just saying that the resonance allows it to move the negative charge around and be, and stabilize while the ethoxide, it can't perform resonance” (S2)
	Delocalization of electrons	Participants refer to delocalization of electrons by explicitly stating how electrons are delocalized (e.g., electrons to move around, pi/double bond/s can move, pi bonds can move interchangeably, pi bond can move over here/there and that/this one can move over here/there or that/this one can move up/down, move lone pairs down/up/here/there, change where the electrons are, electrons can shift, delocalization/delocalized electrons, free movement of electrons, do resonance, resonate down, resonance can keep going, how much room the electron could take up and the different positions that it could exist in) and/or the use of a drawing indicating delocalization of electrons.	“Like the double bond could go up to the O and that this could make a pi bond which would then make the nitrogen positive and then that wants to accept” (S12).

Granularity Analysis- Stability

Interviewee	Granularity	Coding for Stability 1	Coding for Stability 2
S1	Structural	Atom identity Connectivity	Connectivity
	Electronic	Delocalization of electrons Spreading charge	
S2	Structural	Functional group identity	Connectivity
	Electronic	Delocalization of electrons Spreading charge	
S3	Structural	Atom identity Connectivity Charge	Atom count Bond count Connectivity
	Electronic	Delocalization of electrons	Spreading of charge Delocalization of electron
S4	Structural	Bond type Charge	Atom count Bond count Connectivity
	Electronic		
S5	Structural	Atom identity Bond type	Bond type Bond count
	Electronic		
S6	Structural	Atom identity Atom count Functional group identity Electron count Charge	Connectivity Electron count Charge
	Electronic	Delocalization of electron	Spreading of charge Delocalization of electron
S7	Structural	Connectivity Functional group identity Charge	Connectivity Electron count Charge
	Electronic	Spreading of charge Delocalization of electron Electron withdrawal	Delocalization of electron
S8	Structural	Atom count Functional group identity Charge	Connectivity
	Electronic	Spreading of charge Delocalization of electron	Spreading of charge Delocalization of electron
S9	Structural	Bond type	Connectivity
	Electronic		
S10	Structural	Connectivity Functional group identity Bond count	Connectivity
	Electronic	Delocalization of electron	Spreading of charge Delocalization of electrons
S11	Structural	Bond count Atom count	Connectivity
	Electronic	Spreading of charge Delocalization of electron	
S12	Structural	Bond type Atom identity Atom count	Bond type Connectivity
	Electronic		Delocalization of electrons
S13	Structural	Connectivity	Atom identity Bond count

			Connectivity
	Electronic	Spreading of charge Delocalization of electron	Spreading of charge Delocalization of electron
S14	Structural	Bond type Electron count Charge	Charge
	Electronic	Spreading of charge Delocalization of electron	Spreading of charge Delocalization of electron

Granularity Analysis- Acidity

Interviewee	Granularity	Coding for Acidity 1	Coding for Acidity 2
S1	Structural	Atom identity Atom count Bond type Charge Resonance specific representational feature	Atom identity Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading charge	Electron withdrawal
S2	Structural	Atom identity Charge Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons Spreading charge
S3	Structural	Atom identity Atom count Charge Resonance specific representational feature	Atom identity Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading of charge Electron withdrawal	Delocalization of electrons Electron withdrawal
S4	Structural	Bond type Bond count Charge Electron count Functional group identity	Atom count Bond type Connectivity of atoms, ions, and functional groups
	Electronic		
S5	Structural	Resonance specific representational feature	Atom identity Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons	Electron withdrawal
S6	Structural	Atom identity Atom count Bond count Bond type Connectivity of atoms, ions, and functional groups	Atom identity Connectivity of atoms, ions, and functional groups Electron count
	Electronic	Electron withdrawal Polarization	Delocalization of electrons
S7	Structural	Functional group identity Resonance specific representational feature	Connectivity of atoms, ions, and functional groups Atom identity Functional group identity
	Electronic	Delocalization of electrons	Bearing charge Delocalization of electrons Spreading charge
S8	Structural	Atom identity Charge Resonance specific representational feature	Functional group identity
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons Spreading charge
S9	Structural	Atom identity Atom count Charge	Atom identity Connectivity of atoms, ions, and functional groups
	Electronic		
S10	Structural	Atom identity	Connectivity of atoms, ions, and functional

		Charge Resonance specific representational feature	groups
	Electronic	Delocalization of electrons	Delocalization of electrons
S11	Structural	Charge Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons	Delocalization of electrons
S12	Structural	Atom identity Atom count Charge	Connectivity of atoms, ions, and functional groups
	Electronic		Delocalization of electrons Electron withdrawal
S13	Structural	Charge Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons
S14	Structural	Charge Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons

Granularity Analysis- Basicity

Interviewee	Granularity	Coding for Basicity 1	Coding for Basicity 2
S1	Structural	Charge Electron count Functional group identity	Bond type
	Electronic		Delocalization of electrons
S2	Structural	Atom identity Charge Electron count	Connectivity of atoms, ions, and functional groups
	Electronic		Delocalization of electrons Spreading charge
S3	Structural	Atom identity Charge Electron count Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Polarization	Delocalization of electrons
S4	Structural	Atom identity Bond type Bond count Charge Functional group identity	Atom identity Atom count Bond type Charge
	Electronic		
S5	Structural	Charge Electron count Functional group identity	Bond type
	Electronic		
S6	Structural	Atom identity Atom count Electron count Functional group identity	Atom count Electron count
	Electronic		Delocalization of electrons Spreading charge
S7	Structural	Atom identity Charge Resonance specific representational feature	Bond type Charge Connectivity of atoms, ions, and functional groups
	Electronic		Delocalization of electrons Spreading charge
S8	Structural	Atom identity Charge Electron count Resonance specific representational feature	Bond type
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons
S9	Structural	Atom identity Bond type Charge Electron count Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons	
S10	Structural	Charge Resonance specific representational feature	Bond type

	Electronic	Delocalization of electrons Spreading charge Electron withdrawal	
S11	Structural	Atom identity Charge Electron count	Bond count Charge Electron count
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons
S12	Structural	Bond type Resonance specific representational feature	Connectivity of atoms, ions, and functional groups
	Electronic	Delocalization of electrons Spreading charge	Delocalization of electrons
S13	Structural	Atom identity	Bond type
	Electronic	Bearing charge Delocalization of electrons	Delocalization of electrons
S14	Structural	Charge Functional group identity Electron count	Bond type
	Electronic		