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Investigating Students' Reasoning about Acid–Base Reactions

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Supporting Information

ABSTRACT: Acid–base chemistry is central to a wide range of reactions. If students are able to understand how and why acid–base reactions occur, it should provide a basis for reasoning about a host of other reactions. Here, we report the development of a method to characterize student reasoning about acid–base reactions based on their description of *what* happens during the reaction, *how* it happens, and *why* it happens. We show that we can reliably place student responses into categories that reflect the model of acid–base reactivity used and whether the students invoke an electrostatic causal argument. However, the quality of student responses is highly dependent on the structure of the task prompt, which must be structured to provide students with enough information for them to understand what is needed. In general, students who construct responses that invoke a causal mechanistic Lewis model are more likely to draw appropriate curved arrow reaction mechanisms.

KEYWORDS: *Undergraduate/College Chemistry, Acid–Base Reactions, Mechanistic Explanations, Chemistry Education Research, Testing/Assessment*

FEATURE: Chemical Education Research

INTRODUCTION

Acid–base reactions are a major component of chemistry. If students understand acid–base chemistry in all its guises, it becomes possible to predict and explain the outcomes of a wide range of apparently unrelated reactions. For example, students would be able to connect and integrate seemingly diverse phenomena such as proton transfer, transition metal coordination complexes, and organic reactions involving nucleophilic and electrophilic attack. However, as discussed below, there are a wide range of well-recognized problems that students face as they learn acid–base concepts: from misconceptions, to the use of surface level features to identify acids and bases, to difficulties with understanding how to use and move flexibly between models of acid–base chemistry. While there is a great deal of research on student misconceptions about the nature of acids and bases, and the difficulties that students have in recognizing and using the idea of acid–base chemistry, there are fewer reports on student understanding of acid–base reactions themselves. To help us understand how students think about acid–base reactions, we have developed assessment tasks that prompt students to construct explanations about how and why these reactions occur. In this paper, we describe how we use these student responses to develop an approach that allows us to characterize how students reason about acid–base reactions. We also investigate how the model that students use to reason about these reactions might be associated with their mechanistic reasoning. Since mechanistic reasoning is normally operationalized (at least in organic chemistry courses) by drawing mechanistic arrows, we also investigate how students verbal mechanistic reasoning compares to the ways they drew mechanistic arrows.

The goals of this study are guided by three research questions (RQs):

RQ 1: In what ways do students reason about acid–base reactions?

RQ 2: In what ways does the structure of the item prompt affect student responses?

RQ 3: In what ways does student reasoning about acid–base reactions relate to how they draw mechanistic arrows?

STUDENT UNDERSTANDING OF ACIDS AND BASES

There have been a number of approaches to characterize how students understand acids and bases and their chemistry. Much of this research has focused on documenting the misconceptions or non-normative ideas that hinder understanding of acid–base chemistry in high school level,[1−10] undergraduate general chemistry,[11−14] undergraduate organic chemistry,[15−19] and graduate chemistry.[20] Some reports focus on difficulties with mathematical ideas involving acid–base chemistry including difficulty with and the meaning of pH calculations, equilibrium calculations, and buffers.[5,7,13,21,22] Others indicate that difficulty with prior knowledge often hinders understanding. For example, Nakhleh and Krajcik[13] studied student understanding of acids and bases and reported underlying problems such as the inability to distinguish between a molecule, atom, and ion, and how acids and bases are represented. Other researchers[23] have reported on how students recognize acids and bases, for example, by looking

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for the presence of a H or an OH (that is, a surface level feature) to identify acids and bases or by identifying the types of heuristics that more advanced students use as shortcuts when ranking acid strength.[16] It has been shown that students tend to rely on isolated features and heuristics rather than scientifically acceptable arguments. Concept inventories[24] that address a range of misconceptions about acid–base strength in the context of organic molecules have also been developed.

However, there are relatively few studies that investigate how students reason about acid–base reactions—that is, the way acids and bases interact, instead of focusing on acids or bases separately. In this study, we are concerned with the ways that students explain *what* happens during an acid–base reaction and *how* and *why* acid–base reactions occur. After all, acids and bases are inextricably interwoven; acids (or bases) do not exist in isolation—they are part of an acid–base system.

■ STUDENT UNDERSTANDING OF ACID–BASE MODELS

By the time students complete a general chemistry course, it is generally assumed that they have been introduced to the three common models that describe acid–base chemistry: Arrhenius, Brønsted–Lowry, and Lewis. These models can be seen as building on each other; the Arrhenius model is subsumed by the Brønsted–Lowry model, which in turn is subsumed by the Lewis model. While students are typically introduced to the Arrhenius model in high school, the Brønsted–Lowry model is usually the first approach that can be applied to a range of systems. Indeed, many experts use the Brønsted–Lowry model for situations that involve only proton transfer. However, if students can also use the Lewis acid–base model, that is, understand proton transfer as an interaction between an electron pair and a proton, it becomes easier to expand an understanding of acid–base reactions to a wider class of reactions that involve interactions between an electron pair and an electron-deficient center. As has been noted,[18,25] if students learn to use the Lewis model appropriately, it opens up a wide range of reaction types, particularly in organic chemistry, that can be assimilated into a coherent framework to explain *how* and *why* these reactions occur.

The ability to move flexibly between appropriate models is one of the hallmarks of a sophisticated understanding of the scientific enterprise,[26] and it has been shown that students often have trouble understanding the nature of models, particularly in chemistry.[27,28] Typically, younger students tend to understand models as concrete representations of reality rather than tools with which to predict and explain.[29,30]

Ideally, as students enter college and move to more advanced chemistry ideas, they would move toward a more sophisticated use of models as predictive tools. Moving flexibly among models, understanding the limitations of models, and choosing appropriate models that can predict and explain outcomes requires that students understand the nature of scientific models as ways of thinking that are not direct representations of reality but rather that they are ways to abstract the important components of a system.[26] However, it has been shown that even organic chemistry students have difficulty in moving between the accepted models of acid–base chemistry.[18] As Paik[31] has noted, as students move from Arrhenius to Brønsted, they are moving from a view of acids and bases as a type of matter to a process by which a proton is transferred. That is, they must move from isolated ideas about what an acid or a base is to an acid–base reaction system. This change in distinct ontological categories, that is, from "matter" to "process" is what Chi considers to be difficult.[32]

While both Brønsted and Lewis models describe acid–base reactions as a process, in fact, the Brønsted model only requires a description of *what* is happening; that is, a proton is transferred from the acid to the base. The switch from Brønsted to Lewis requires that students become comfortable thinking about the system in a flexible and more expert-like way. The transfer of a proton is indeed a process, but *how* that proton is transferred falls under the Lewis model. Cartrette and Mayo[18] investigated whether students think about acids and bases using Brønsted or Lewis ideas, both, or neither and found that while all students could define Brønsted acids and bases, less than half could do the same for Lewis acids and bases, and that most participants relied heavily on the Brønsted definition—even when it was not warranted. Indeed, a number of authors have speculated that if students use the Lewis model to think about acid–base reactions, they should develop a more robust framework on which to build their understanding of a broader range of chemical reactions;[18,25] however, there is currently little empirical evidence to support this hypothesis.

One further reason to support earlier emphasis on the Lewis acid–base model is that it provides an entrée into reasoning about chemical reactions from a mechanistic view by helping students think about how reactions occur. If students think about acid–base reactions as proton transfers, without considering how the transfer happens, they will be less likely to make the connection between acid–base reactions and (for example) nucleophilic substitutions. The move to Lewis acid–base theory means that students will be introduced to mechanistic reasoning. In fact, some organic texts[33,34] discuss Lewis acid–base models as an introduction to the formal drawing of mechanistic arrows.

■ MECHANISTIC AND CAUSAL REASONING

As has been discussed by Krist et al.,[35] mechanistic reasoning occurs at a scale or grain size below that of the phenomenon being explained. While the Brønsted model describes a proton transfer, using the Lewis model requires that students understand the process as an interaction between the lone pair of the Lewis base and an empty orbital (or incipient empty orbital) on the Lewis acid. That is, students must reason mechanistically about *how* the reaction occurs. In organic chemistry, mechanistic reasoning is usually operationalized by "arrow pushing". Most instructors of organic chemistry emphasize the need for students to learn how to construct mechanisms for the reactions they are learning. That is, students learn to draw arrows from electron source to sink and by doing this are able to predict the outcome of many organic reactions. This is a powerful tool that can take organic chemistry from the realm of memorization to a coherent framework which can tie together many seemingly unrelated systems of reactions. Studies on how students actually go about drawing mechanisms have shown that many (most) students do not use mechanistic arrows in the ways they are intended. For example, in our prior studies,[36] we found that, even when explicitly asked to write mechanisms for reactions, about half of the students did not draw arrows but instead wrote the (memorized) product directly. In fact, about 20% of the students who drew arrows actually did so after they had produced the product, thus doubling the amount of material they had to memorize. Further, the number of students drawing any type of mechanisms did not increase over the course of the

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two-semester sequence; this despite the fact that mechanism users were significantly more likely to produce the correct product for an unfamiliar reaction. Other qualitative studies support these findings,[37,38] for example, studies on how and why graduate students construct mechanisms indicate that even at this level many students are not aware of the power of mechanistic arrows or what they actually mean.[39] That is, many students do not seem to be aware that (except for some electrocyclic reactions) the arrows are indicative of an interaction between sites of differing polarities. Arrow pushing is a formalized shorthand to show how interactions begin and how electron density shifts over the course of a reaction, but if students fail to recognize this, it is unlikely that they will be able to use arrows with any degree of success. For example, many students use arrows to indicate the movement of the hydrogen atom itself (in acid–base reactions) rather than the attraction of electron-rich sites to electron-poor sites via movement of electrons.[36]

As we have noted earlier,[40] there is a great deal of evidence to support the idea that asking students to explain why a phenomenon occurs leads to deeper learning. That is, having students approach mechanistic reasoning in organic chemistry systems by helping students articulate *why* reactions occur may help them construct a framework with which to reason. However, there is considerable evidence that most students do not consider the underlying reasoning for *why* mechanistic arrows are drawn this way. That is, students do not seem to associate arrow drawing with the *causal mechanism* by which the reaction occurs. Constructing a causal mechanistic explanation about an acid–base reaction would require that students do more than describe the course of the reaction (whether it be by proton transfer or movement of electrons), rather it would require that students discuss the cause of the reaction as beginning with an interaction between the lone pair on an electronegative atom (e.g., oxygen) and the electropositive proton. That is, students should understand that acid–base reactions start with an electrostatic interaction between moieties of opposite (partial) charge. Understanding the mechanism (how the reaction occurs) is not the same as understanding the causal mechanism (why the reaction occurs). Similarly, it is possible to provide causal reasoning without providing a mechanism (as discussed below).

■ ASSESSMENT OF STUDENT REASONING

Our goals are to characterize the ways in which students reason about acid–base reactions and to develop an assessment protocol for acid–base mechanistic reasoning. To capture such reasoning requires the design of tasks that can elicit evidence of student understanding.[41] In our work on such tasks, we are using a modified evidence centered design (ECD) framework.[42] ECD is an approach to assessment development that relies on the idea of assessment as an evidentiary argument. That is, assessments must elicit evidence which can be used to make an argument about student understanding. Using this approach typically involves several steps:

(1) *Define the construct that is to be assessed or characterized.* In this study, the construct is how students reason about acid–base reactions. Note that the construct is more than knowledge; we are interested not only in student knowledge about acid–base reactions but also the ways in which students reason about why such reactions occur.

(2) *Decide what evidence is acceptable to support the argument that students understand the construct.* Evidence of student reasoning about acid–base reactions can be elicited by asking students to provide causal mechanistic explanations for why these reactions occur: by which we mean that students should be able to identify an acid–base reaction, describe the scientific principles or evidence that supports their identification, and provide reasoning about why this reaction is occurring. There is a great deal of evidence to support the use of tasks that involve having students provide causal mechanistic explanations for phenomena.[40]

(3) *Design assessment tasks that would elicit the types of evidence specified in step 2.* We have designed open-ended tasks because we believe they will provide stronger evidence about student reasoning than forced choice items. As discussed in the Methods section, the structure of the prompt to which students respond is crucial.[43] It must provide enough information to signal to students what is expected but should not "over-prompt" the students so that they are guided to an answer that they would not otherwise have given. In a similar vein, it has been reported that multiple choice tests tend to overestimate the level of student understanding when compared to open-ended responses.[44]

(4) *Decide how to analyze the evidence elicited in the assessment tasks.* Evidence from student-constructed responses can be analyzed in a number of ways. For example, much of the prior work on student understanding has focused on the identification of types of misconceptions or the model of acid–base behavior used. However, we are eventually interested in comparing student responses across courses and over time, and for this, we have developed an approach based on the type of reasoning of the student response (see discussion below). That is, rather than "right" or "wrong" responses, we would like to identify how the student reasons about acid–base chemistry, and ideally, we would like to gain some measure of the level of sophistication of the response.

■ METHODS

Student Participants

The development of assessment tasks to elicit student acid–base reasoning included several groups of students enrolled in college level general chemistry and organic chemistry at two different universities (Table S1 in the Supporting Information). All administrations of the assessment tasks were conducted at the end of the semester indicated except where noted. In addition, all students involved in this research agreed to participate in this study and signed informed consent forms. In this paper, however, we highlight two groups of second-semester general chemistry (GC2) students to discuss the development of the assessment task: (1) students enrolled at a medium-sized public southeastern research university (University 1) in the spring 2012 (referred to as SP12) semester ($N = 121$) and (2) students enrolled at a large public midwestern university (University 2) during the spring 2015 (referred to as SP15) semester ($N = 107$).

These two groups of students were selected to illustrate how, by changing the task prompt, we were able to elicit stronger evidence about the ways in which students reason about acid–base reactions. Both of these groups of students were enrolled in transformed second-semester general chemistry courses at these two institutions. At University 1 ($N = 121$), the assessment was administered in the accompanying laboratory course for credit to the whole class, and at University 2, it was administered as an extra credit assignment out of class to a

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representative sample ($N = 107$) of the whole class population ($N = 812$). We found no significant difference in the students' course grades between the students who completed the assessment and those who did not complete the assessment using a Mann–Whitney test (U = 35503, $p = 0.33$, median = 3.0).

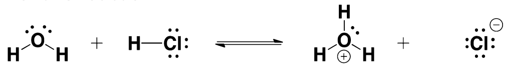
Even though these students attended different universities, both of the groups of students used the same two-semester general chemistry curriculum *Chemistry, Life, the Universe and Everything* (CLUE).[45] In the CLUE curriculum, three models (Arrhenius, Brønsted–Lowry, and Lewis) of acid–base reactions are introduced and developed in such a way that each subsequent model is shown to build on and supersedes the last. That is, students are reminded that they may have encountered the Arrhenius model in their earlier education and then introduced to the Brønsted model. Care is taken to show how all Arrhenius acid–base reactions can be described using the Brønsted model, while the reverse is not true. Finally, the Lewis acid–base model is introduced in the same way, and students see that it can be used to describe all Arrhenius and Brønsted reactions, but again, the reverse is not true. At the same time as the Lewis model, students are also taught to draw simple reaction mechanisms (i.e., mechanistic arrows) for acid–base reactions and for simple nucleophilic substitutions. In addition, acid–base chemistry is threaded throughout the second semester as the focus of sections on equilibrium reactions and networked biological reactions.

The SP12 and SP15 students were compared to determine if the two groups were similar according to the available demographic information and assessment measurements. The students' final course grades in the CLUE curriculum and their incoming ACT composite scores were compared using a Mann–Whitney analysis (Table S2 in Supporting Information). Although there were no significant differences between the students' final course grades, their ACT scores were different (SP12 average ACT 28, SP15 average ACT 26) with a medium effect size. The ratio of males and females within each group were compared using a χ^2 analysis (Table S3 in Supporting Information), and we found no significant differences. Although the SP12 students had slightly higher average ACT scores, we believe that the two groups are similar enough for our comparison purposes here (particularly since the SP15 students constructed more sophisticated explanations for the assessment item as discussed below). It should also be noted that, in our earlier work, students from University 2 (SP15) performed at the same level as those from University 1 (SP12) on a different assessment task involving understanding intermolecular forces.[46] The results from the statistical analyses are shown in Tables S2 and S3 in the Supporting Information.

Development of the Assessment Tasks

The assessment tasks were designed to elicit molecular level mechanistic reasoning about acid–base reactions. The initial iteration of the assessment (Figure 1) was developed as part of a series of studies on student understanding of structure–property relationships.[46−51] Based on this previous work, we designed the tasks around simple reaction systems in which the full Lewis structures and the products were provided. In the preliminary iterations of the assessment tasks, we explored how presenting students with representations of condensed structures (without any structural cues) compared to providing Lewis structures (Table S1 in Supporting Information, early spring 2012). We found that students were less likely to mention lone pairs during their discussion of the molecular level explanations when presented with the condensed structural representations. Since our goal in this study was to elicit reasoning about the acid–base reaction, and because in our previous work we found that it was helpful to focus students' attention on the goal, we decided to provide students with the structural cues (i.e., Lewis structures) rather than have students get side-tracked by worrying about how to draw the structure or grappling with an unfamiliar structurally complex system. Therefore, in the study, a common acid–base reaction was presented to students (reaction of hydrochloric acid (HCl) with water (H_2O)).

For this reaction:



a. How would you classify the above reaction? Please explain your reasoning.
b. Please explain your reasoning for what you think is happening at the molecular level for this reaction.

Figure 1. Initial iteration of the assessment tasks (SP12).

The first iteration of the assessment tasks was administered at the end of the second semester of general chemistry during the spring semester of 2012 at University 1, referred to as SP12 ($N = 121$). Since this iteration required only written responses from students, it was administered using *SurveyMonkey*, an online survey program, and was composed of questions about the reaction of hydrochloric acid (HCl) with water (H_2O) (Figure 1).

As we analyzed the student responses, it became clear that the prompt "explain your reasoning for what you think is happening at the molecular level" did not elicit responses that would provide us with evidence about student understanding. Rather, the majority of students provided a descriptive response, telling us *what* was happening in the reaction, rather than reasoning about *how* or *why* it was happening, as shown in Laura's response "The equation is turning from an acid–base to its conjugate acid/base pair. The HCl acid donates its H^+ to create a base, while the H_2O gains an H^+ to become an acid". That is, many students merely stated what atoms were rearranging instead of explaining *why* these atoms rearrange.

As Jin and Anderson[43] noted, the structure of the prompt is crucial in designing assessments that are intended to provide evidence of student reasoning. It must be accessible so that all levels of students can understand what is intended, and it should also provide enough structure so that students understand what is required to answer the question. We want students to provide as much relevant information as they can, but they must understand what is needed. Many students are "bilingual" in that they are capable of answering a question on many levels, and it is important to provide enough structure to indicate the type of response required. On the other hand, overstructuring the prompt may provide students with enough information to answer the question in ways that they may not have thought of otherwise. By providing too much information in the prompt, we may encounter the problem found with multiple choice questions that have been shown to over-estimate student understanding,[44] or it may even send students off in an unproductive direction.

Over the next administrations, the structure of the task prompt was modified in an attempt to elicit rich student

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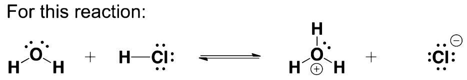
responses, without "over-prompting" students. For example, one iteration asked students to consider "electronegativity" in their responses, and while students did include this word in their responses, some of their answers were no more meaningful.

The iteration of the assessment discussed here (Figure 2) was administered at the end of the spring semester 2015 to second-semester general chemistry students at University 2, referred to as SP15 ($N = 107$). This iteration of the survey was administered using *beSocratic*, an online system where students can construct written and drawn free-response answers.[52,53] In this iteration (SP15), we separated the explanation into separate prompts: describe *what* is happening at the molecular level and finally *why* it is happening. In addition, another question that asked students to draw mechanistic arrows for the reaction was added. Since this iteration of the assessment was administered in the *beSocratic* system, we could replay each student's response to determine whether the student has drawn mechanistic arrows and the sequence in which they were drawn.

For this reaction:



a. How would you classify this reaction? Please explain why you chose that classification.
b. Describe in full detail **what** you think is happening on the molecular level for this reaction. Specifically, discuss the role of each reactant.
c. Using a molecular level explanation, please explain **why** this reaction occurs. Specifically, why the reactants form the products shown.
d. Please draw arrows to indicate how this reaction occurs.

Figure 2. Final iteration of the assessment tasks (SP15).

To make sure that students understood what was meant by the task, we interviewed five students toward the end of the spring 2015 general chemistry course before the final iteration (SP15) was administered. The interviews were geared toward gauging students' interpretation of the questions and the alignment of their responses. We found that students were consistently able to provide explanations that were aligned with the provided prompts, and therefore no further interviews were necessary.

DATA ANALYSIS

The student responses for both *what* was happening on the molecular level (Figure 2b) and *why* the reaction occurs (Figure 2c) were combined for analysis purposes since some students responded to the *why* prompt in the *what* response space (and vice versa). Since we were interested in identifying the type of reasoning in the student response (rather than right or wrong, misconception, or model used), we placed these responses into categories that were aligned with student reasoning, as shown in Table 1.

That is, students who provided simple descriptions were simply categorized as General Descriptive, if the student provided a more extensive descriptive response that used the Brønsted–Lowry model, it was designated Brønsted Descriptive. For students who use the Brønsted model but also added some causal reasoning (indicated by discussion of polarity or ideas about attractive forces), the response was designated Brønsted Causal. Students who used the Lewis model to discuss how the reaction occurred were Lewis Mechanistic, and if they added causal reasoning, they were designated as Lewis Causal. These characterizations are further discussed in the Results and Discussion section.

The three authors coded a random sample of 20% of student-generated explanations from each SP12 and SP15 assessment to establish inter-rater reliability, resulting in pairwise Cohen's Kappa ranging from 0.73 to 0.79. The three authors further discussed the coding scheme, which resulted in a Kappa value of 0.90.

The arrow pushing mechanisms that students constructed for this reaction were also inspected and coded for (1) whether the first arrow was shown in the correct direction, from the lone pair on the oxygen in water to the hydrogen in HCl and (2) whether the complete mechanism was correct, as shown in Figure 3.

RESULTS AND DISCUSSION

A majority of students from both implementations of the assessment task were able to identify that the reaction provided was an acid–base reaction (SP12, 81% and SP15, 94%). Other responses included redox, displacement, hydrolysis, and substitution reactions. That is, most students recognized without prompting that the given reaction was an acid–base reaction.

RQ 1: In what ways do students reason about acid–base reactions?

Examples of each type of student reasoning are shown in Table 1. In both SP12 and SP15 administrations, relatively few students provided Non-normative answers. For example, Donald wrote, "The electrons are being excited and therefore causing the hydrogen bonding to occur", and Bob indicated that "The chlorine is losing electrons and the oxygen is gaining electrons."

Responses assigned to the General Descriptive category invoked an acid–base reaction and typically included a generic description of *what* is happening to the reactants and products without any indication of *how* or *why* the reaction happens, such as Aiden's response, "Because there is a conjugate base formed and the acid is gone." General Arrhenius explanations were also included in this category. For example, Kate provided the following explanation: "HCl is being dissociated completely by the water."

In the Brønsted Descriptive category, students now identify which reagent is the acid and base in the reaction and generally provide some description of *what* happens during the reaction and using a Brønsted model of acid–base for the explanation. For example, Hannah's response, "HCl is acid and H_2O is base. HCl is proton donor, H_2O is proton acceptor, this means the H in HCl transfer to H_2O and form the H_3O^+ which is an conjugate acid. And Cl^- becomes conjugate base." While this is a quite complete description of *what* is happening during the reaction, it does not include any description of *how* or *why* the reaction happens. On the other hand, responses that invoked a causal mechanism, for example, by including terms such as *attraction*, *pulling off*, and *interacting partial charges* were all considered as a demonstration of causal accounts. Freddy's response, "This occurs because the hydrogen is attracted to the most electronegative atom, which is the oxygen, thus creating the hydronium molecule. The chlorine is then left alone with a full octet", was assigned to the Brønsted Causal category.

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Table 1. Characterization Scheme for Student Reasoning about Acid−Base Reactions

Characterizations	Examples
No Response	Viktor: *"I do not really have a reasoning"*
No answer or their explanations were unreadable or incomprehensible	
Non-normative	Raymond: *"The hydrogen on the HCl is donating its electron to the oxygen on the water"*
Students provide non-normative or unrelated explanations. In addition, students do not recognize it is an acid−base reaction and instead attribute the mechanism to other types of reactions or other macroscopic observations	
General Descriptive (what)	Catherine: *"The acid is reacting with the base and the acid is a proton donor while the base is a proton acceptor"*
Students provide scientifically simplistic description and may discuss bond breaking or forming	
Brønsted Descriptive (what)	Heather: *"The HCl is the acid meaning it is a proton donor and the water is the base meaning it is a proton acceptor. At the molecular level the hydrogen from the HCl is breaking off and the water is gaining it forming H_3O^+"*
Students provide Brønsted acid−base explanation including identification of acid and/or base and discussion of proton transfer	
Brønsted Causal (what and why)	Remy: *"The oxygen is extremely electronegative and attracts the proton of the hydrogen. The hydrogen donates its electron to the chlorine so that its proton can go to the oxygen"*
Students provide Brønsted acid−base causal reasoning that includes discussion of polarity of one or both of the reactants	Claire: *"The oxygen atom in water bonds to the hydrogen atom in hydrochloric acid as the hydrogen and chlorine atom break apart. The partial negative oxygen in water is attracted to the partial positive hydrogen in hydrochloric acid. When the oxygen and hydrogen form a bond the hydrogen and chlorine break their bond creating the products H_3O^+ and Cl^-"*
Lewis Mechanistic (what and how)	Jackie: *"The O in the H_2O gives its electrons to the H in the HCl bond, and simultaneously the HCl bond breaks, placing those electrons onto the Cl. This reaction happens because it is more favorable"*
Students provide Lewis acid−base explanation, including role of lone pair (may also encompass the Brønsted explanation)	
Lewis Causal (what, how and why)	Doug: *"HCl acts as a proton donor and donates a proton to water which is the proton acceptor. H_2O and HCl are attracted to each other because of their partial charges. When the H on HCl interacts with the lone pair on O, the HCl bond breaks and the Cl is left with the bonding electrons"*
Students provide Lewis acid−base causal reasoning that includes discussion of polarity of one or both of the reactants (may also encompass the Brønsted explanation).	Francis: *"The lone pair on the water molecule attracts the Hydrogen from the HCl. The H−Cl bond is broken and forms a new bond with oxygen. The reaction occurs because the partial negative charge on the oxygen attracts the partial positive charge on the hydrogen. The bond between the Hydrogen and Cl is less strong than the bond that forms between hydrogen and oxygen"*

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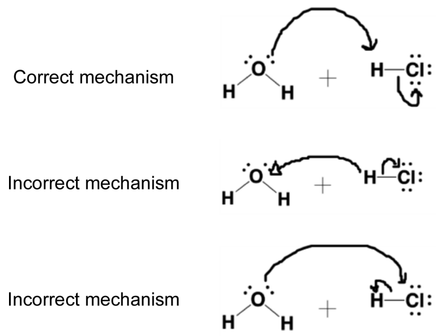

Figure 3. Examples of correct and incorrect mechanistic arrow drawings by students from SP15.

Responses that described the involvement of the lone pair on the base were assigned to the Lewis category. For example, LeAnn's explanation of "Oxygen's electrons reach out and grab the Hydrogen (proton). So the bond breaks and the electrons go back to the Cl from the HCl bond" invoked the Lewis model and was assigned to the Lewis Mechanistic category. In contrast Guadalupe invokes both cause and mechanism for the reaction, and her response is categorized as Lewis Causal: "The H_2O is the base. It is a proton acceptor. It will accept the proton from the HCl. The HCl will donate its proton to the H_2O. The polarity of the H_2O is what first attracts the partially negative oxygen to the partially positive H in the HCl. Since O is highly electronegative, it will pull off the H from the HCl and make a bond with one of its lone pair of electrons. The electrons from the bond of the HCl will stay on the Cl since it is more electronegative than H." It should be noted that, like Guadalupe, some students used both models, for example, by talking about proton transfer but invoking an electron pair description of the mechanism. In these cases, responses were designated as Lewis because while they discussed *what* is happening using the Brønsted model, they discussed *how* and *why* it is happening using the Lewis model.

RQ 2: In what ways does the structure of the item prompt affect student responses?

To determine how the change in prompt impacts student reasoning, we compared the responses from SP12 and SP15. As shown in Figure 4, it is clear that the SP15 iteration has elicited a larger proportion of Lewis causal mechanistic responses. There is a clear (and significant) difference between the two iterations of the assessment tasks. For instance, the χ^2 analysis of the two groups showed a significant difference between SP12 and SP15, with a medium effect size, $\chi^2 = 48.55$, $p < 0.001$, $\varphi = 0.46$.[54]

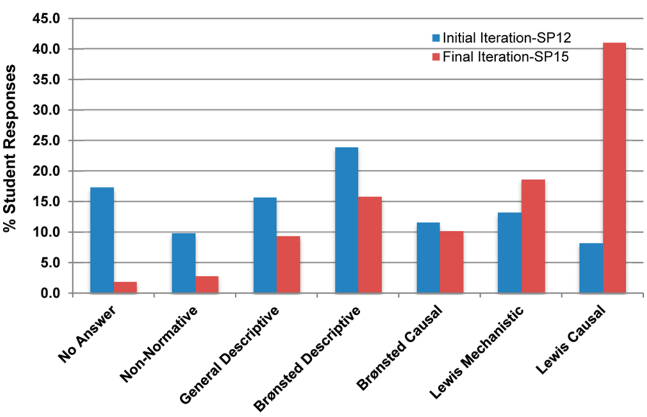

Figure 4. Classification of students' constructed explanations for SP12 and SP15 activities.

Analysis of the SP12 assessment showed that a large number of responses elicited (40%, $N = 48$) were descriptive (General Descriptive and Brønsted Descriptive), while 21% ($N = 26$) of the responses were mechanistic—that is, they invoked a Lewis model (Lewis Mechanistic and Lewis Causal), and 20% ($N = 24$) invoked some cause (Brønsted Causal and Lewis Causal). The largest group of students described, in varying detail, what they saw happening in the reaction scheme provided. In retrospect, this is not surprising. The nature of the prompt did not appear to provide students with enough structure to elicit an explanation for *how* or *why* the reaction is happening. We also note that 17% ($N = 21$) of the students did not have a response or wrote, "I do not know" which may also indicate that students were somewhat unsure of what was being asked of them.

In contrast, the SP15 assessment task required two separate responses from students. Students were asked to describe *what* is happening on the molecular level during the reaction and, then in a separate prompt, asked *why* the reaction occurs (Figure 2). Inherent in the structure of the prompts was the idea that merely describing *what* happens is not sufficient. It should be re-emphasized that we actually coded these responses together as one response since many students answered both tasks in the same response box. In this implementation, we see a significant shift in the pattern of responses. Now 60% ($N = 64$) of the students provide a mechanistic account, and in fact, 41% ($N = 44$) provide a causal mechanistic account. Only 2% ($N = 2$) of students did not answer and 3% ($N = 3$) provided non-normative ideas (as opposed to 10% ($N = 12$) of the SP12 activity).

We believe that the difference between the two iterations is primarily due to the change in prompt. By providing students with more scaffolding, we were able to help them structure their response to provide more evidence of understanding. While the two groups of students were from different universities, there were no major differences in the demographic data that we compared, as discussed in the Methods section (also shown in the Supporting Information Tables S2 and S3), except that students at University 1 (SP12) had a slightly higher incoming average ACT composite score. Both groups of students were enrolled in general chemistry courses that used the same curriculum materials,[45,55] had approximately the same time on task, similar homework assignments and examinations, and the same set of learning objectives. Therefore, though it was not feasible to administer the items in an identical manner to both cohorts, we believe that the difference in responses stemmed from a refinement of the task prompt.

RQ 3: In what ways does student reasoning about acid−base reactions relate to how they draw mechanistic arrows?

In SP15 assessment, students were also asked to draw mechanistic arrows for the acid−base reaction. The responses were coded simply for (1) is the first arrow correct? (i.e., starting on the lone pair of the oxygen and ending on the proton to be transferred), and (2) is the mechanism completely correct? In SP15, 73% of students drew the first arrow correctly and 71% of the students drew the complete mechanism correctly. That is, those students who drew the first arrow

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correctly were almost all able to provide a complete correct mechanism (97%). In contrast, our earlier mechanistic studies[36,56] showed that only about half the students even attempted to draw mechanisms, and only about 20−30% drew an appropriate full mechanism. While the tasks in our earlier studies were more difficult (e.g., electrophilic addition across a double bond), the students in those studies also had almost a full year of organic chemistry. The students in this study are enrolled in a general chemistry course.

As seen in Table 2, which shows the student type of reasoning paired with their success in drawing mechanistic arrows for the same reaction, students who invoke mechanistic (Lewis) explanations about acid−base reactions are more likely to construct a correct mechanism than those who provide Brønsted or general descriptions, and the ratio of correct to incorrect mechanisms for all responses. The trend is clear: as students move from general descriptive to Brønsted to Lewis models, they are more likely to draw a correct arrow pushing mechanism. Students who use a Lewis model to reason about acid−base reactions are around 3 times more likely to draw a correct arrow pushing mechanism for the reaction than those who use a Brønsted model or who give a general description. A similar but less pronounced pattern is seen for students who provide causal reasoning. The ratio for Lewis Causal is 4.5 and for Brønsted Causal is 2.7 (Table 2), indicating that while causal reasoning seems to be associated with correct arrow pushing, using a Lewis model is even better.

Table 2. Distribution of Students' Incorrect and Correct Mechanism Drawings and the Ratio of Correct to Incorrect Drawings by Each Type of Student Response[a]

	Student Responses by Type (*N*)							
Answer Category	NA	NN	GD	BD	BC	LM	LC	Total
Incorrect mechanism	2	2	5	7	3	4	8	**31**
Correct mechanism	0	1	5	10	8	16	36	**76**
Ratio correct/incorrect	0	0.5	1.0	1.4	2.7	4.0	4.5	**2.5**

[a]NA = No Answer, NN = Non-normative, GD = General Descriptive, BD = Brønsted Descriptive, BC = Brønsted Causal, LM = Lewis Mechanistic, LC = Lewis Causal.

It is interesting to note that the ratio of incorrect to correct responses increases across Table 2, with students who provide Lewis Causal explanations being most likely to draw correct mechanisms **and** to provide the most scientifically sophisticated explanations. We believe that this provides support for the idea that our classifications actually correspond to levels of sophistication of student reasoning, and that they may be used to monitor trajectories for student understanding over time.

CONCLUSIONS AND IMPLICATIONS

The findings from this study indicate that students use a variety of ways to reason about acid−base reactions that can be characterized using a framework which allows responses to be classified according to the model used and whether the students invoke a causal explanation. In essence, by looking for how students describe *what* is happening, *how* it is happening, and *why* it is happening, we have also shown:

(1) The nature of the prompt can dramatically change the types of responses that students provide, and that explicitly asking both *what is happening on the molecular level during a reaction* and *why the* reaction *occurs* is more likely to trigger responses that provide mechanistic, rather than just descriptive explanations.

(2) Students who provide mechanistic (Lewis model) responses are more likely to construct appropriate mechanisms using curved arrows.

(3) Students who provide causal reasoning tend to have higher success at constructing mechanisms with curved arrows, than students who use the same model (e.g., Brønsted) but do not provide causal reasoning.

As discussed in the Introduction, a number of authors have hypothesized that helping students develop an understanding of Lewis acids and bases may support their ability to construct mechanisms as ways to predict and explain the course of many organic reactions, rather than memorizing reaction paths or "decorating" them with arrows. Here, we have provided evidence that students who use Lewis models are indeed more likely to construct appropriate mechanisms. However, as noted earlier, students in this study were enrolled in a transformed general chemistry course designed to emphasize causal mechanistic reasoning. As students progress through the course they are asked to articulate *what*, *how*, and *why* chemical phenomena occur and are expected to provide both written and drawn responses.[45] Since many instructors may not desire, or may not be in a position, to adopt transformed curricula, there are several suggestions resulting from our findings that instructors might incorporate into their teaching.

(1) Lewis acid−base models should be introduced and emphasized in general chemistry (especially for those students who are going on to organic chemistry). If this is not possible, organic chemistry instructors should take time to carefully introduce Lewis acid−base models at the beginning of organic chemistry and help students move flexibly between Brønsted and Lewis models. In our experience, this process takes time and repetition; that is, a one-shot "fly by" of the concept is unlikely to provide enough support for students to use Lewis models. This approach we recommend is important, not only to help students in learning about mechanisms but also to reinforce the idea that the use of appropriate models is part of the scientific enterprise, and the choice of model can influence subsequent learning.

(2) When the Lewis model is taught, it should be accompanied by an expectation that students provide written explanations for *why* the reaction is happening, while at the same time learning to draw mechanistic arrows. That is, students should be asked to articulate both what the arrows mean and *why* they are drawn from electron source to sink. As students become more expert in this process, the explanation step will be omitted, but if students are never asked to explain as they learn, they will tend to draw arrows without understanding their meaning.

(3) Instructors should think carefully about the structure of the prompts that they use to elicit student thinking. It is quite common to ask students to explain their thinking, but if we do not provide students with some structure about what we expect them to include in their response, it can be confusing. As noted earlier, there is a fine balance between providing enough scaffolding to indicate to students what is expected and providing too much scaffolding so that students do not really have to construct their own response. Over-prompting can

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result in the same kind of overestimate of student understanding that has been reported with some multiple choice questions. We have found that it is particularly helpful to separate the prompts so that students understand that they should both describe what is happening and why it is happening.

FUTURE WORK

Since we believe that our characterizations correspond to levels of sophistication in student reasoning, it is possible that by administering the tasks to students at different places in the curriculum we may be able to identify student trajectories over time. We intend to monitor student responses by following cohorts of students throughout the curriculum. We will also investigate how students reason about more complex acid−base reactions; for example, the reaction of an amino acid with water may serve as a "transfer task". It may also be possible to use the task to evaluate the effects of interventions within a particular course, such as investigating the effect of introducing a Lewis acid−base module into a more traditional course structure. In addition, we plan to expand this type of assessment to other classes of reactions to investigate whether similar approaches can improve student mechanistic reasoning for other more complex reactions. We have a great deal of past data on how students, who have not been asked to provide mechanistic and or causal reasoning, draw mechanisms, and it will be interesting to investigate whether changes (improvements) can be made for future cadres of students by helping them articulate their understanding in words.

LIMITATIONS OF THE STUDY

A limitation of this study is that the student participants were enrolled in a transformed general chemistry curriculum, and it may well be that students in a more traditional curriculum do not respond to the prompts in the same way. In the transformed curriculum, mechanistic reasoning is emphasized and students are asked to draw and write responses to open-ended homework tasks on a regular basis. Acid−base chemistry also plays a prominent role. For example, the topic of equilibrium is introduced in the context of acid−base chemistry rather than in the context of gas-phase reactions, and the course ends with discussions of how networked acid−base reactions regulate blood pH. Students from traditional general chemistry programs who are not expected to support their assertions with reasoning may have trouble providing normative explanations for chemical phenomena. Lastly, students in the CLUE general chemistry curriculum are also taught to draw simple reaction mechanisms for acid−base reactions using curved arrows. Therefore, our results are almost certainly not typical. However, as previously noted, the construction of scientific explanations is one of the few pedagogies that has been shown to be strongly correlated with deeper learning, and the tasks we have developed may help other instructors monitor students' achievement as they design new curricular approaches.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.6b00417.

Student populations who were administered the assessment task during the development process of the assessment; student demographic information for the two comparative groups of students SP12 and SP15 (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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