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Reasoning about Reactions in Organic Chemistry: Starting It in General Chemistry

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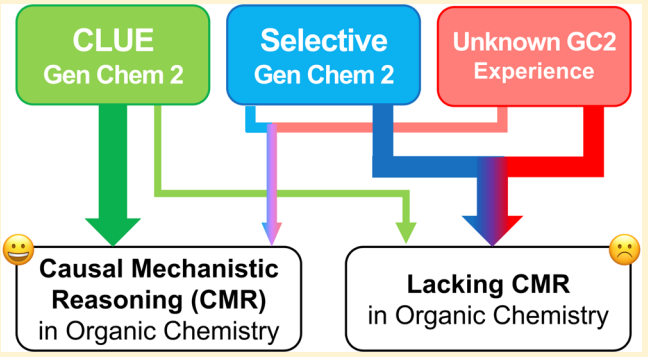
Supporting Information

ABSTRACT: The study presented here is a follow-up to a previous report in which we investigated how general-chemistry students in a transformed curriculum reason about simple acid−base reactions. In the present study, we use and adapt the previously developed coding scheme for a longitudinal study in which we follow students from general chemistry through organic chemistry. We find that (i) generally, the manner in which students reason about acid−base reactions increases in sophistication over the course of a two-semester sequence of organic chemistry; (ii) there is little difference in reasoning between students at the end of a transformed general-chemistry course and a similar cohort at the beginning of organic chemistry; (iii) the nature of a student's general-chemistry experience has a profound effect on the sophistication of their reasoning in that students from a transformed general-chemistry course are more likely to provide causal mechanistic explanations for simple acid−base reactions than students with other general-chemistry experiences; and (iv) the type of acid−base reaction that the students discuss impacts the type of reasoning they exhibit. We find that when asked to explain a Lewis acid−base reaction, students are less likely to invoke electrostatic ideas.



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INTRODUCTION

Acid−base chemistry is fundamental to understanding a wide range of chemical reactions: from simple Brønsted proton transfer to nucleophilic substitutions to the role of Lewis acids in catalysis. In organic chemistry, it is generally acknowledged that to develop expertise, students must:

1. understand the central role of acid−base chemistry,
2. be able to identify acids and bases,
3. be able to predict the products of acid−base reactions,
4. move flexibly among the various models chemists use to describe such reactions.

Nevertheless, there are numerous studies on the problems associated with student conceptual understanding of the nature of acid and bases.[1−8] For example, it has been shown that students struggle to identify acids and bases both at the high-school chemistry level[1−3] and at the undergraduate level.[4−8] We also know that students do not necessarily leave chemistry degree programs with an operational understanding of acid−base reactions.[9] For example, chemistry graduate students in the midst of their dissertation research can wrestle with determining the acidity of simple alcohols.[9]

Much of the prior work on acid−base understanding at the college level has tended to focus on the nature of acids and acidity, rather than on the acid−base reaction itself. For example, McClary and Talanquer identified types of naive heuristics, or rules of thumb, that general-chemistry students may be using when reasoning about relative strengths of acidity.[10,11] These findings were operationalized by Bretz and McClary in the development and validation of an instrument to help organic-chemistry instructors identify incorrect ideas about acid strength that their students may hold.[6] Other researchers have focused on how students use acid−base models. For example, Cartrette and Mayo found that most students tend to use the Brønsted acid−base model, even in cases where it is not appropriate.[7] Although many educators

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agree that a firm grip on the use of the Lewis acid−base model of reactivity is important for organic chemistry, there are few indications that most students who emerge from a general-chemistry course are prepared to use it to reason about organic reactions. Because of this, most commercially available organic-chemistry textbooks include early chapters dedicated to acid−base chemistry that are intended to refresh and build on students' knowledge of acid−base reactions from general chemistry.[12,13] These chapters typically offer definitions and examples for Brønsted acid−base theory and Lewis acid−base theory and provide examples of acid−base reactions of various types.

We have previously reported our findings about how students who were enrolled in a transformed general-chemistry course reason about the simple Brønsted acid−base reaction in which HCl reacts with H_2O.[14] In this earlier study we showed that student reasoning about acid−base reactions can be elicited by appropriately designed prompts and that students who were able to provide causal mechanistic explanations (discussed below) for acid−base reactions were also more likely write correct mechanistic arrows that correlate with electron movement during such reactions. Here we extend that study to (1) investigate the evolution of student causal mechanistic explanations and mechanistic-arrow drawings of Lewis acid−base reactions over two semesters of organic chemistry; (2) investigate, via a longitudinal study, the effects of different general-chemistry preparation on student causal mechanistic reasoning as they move through organic chemistry; and (3) apply this methodology to student understanding of a simple Lewis acid−base reaction.

DEFINING CAUSAL MECHANISTIC REASONING

Although it has been noted that causal mechanistic reasoning is an important goal in science education, there are a number of different ideas about just what this phrase means. Some have argued that mechanistic reasoning is inherently causal and frequently use the terms "causal mechanistic reasoning" and "mechanistic reasoning" interchangeably.[15−18] Russ et al. emphasized the need to identify the components of the system that are "doing" the phenomenon when they stated that "mechanisms account for observations by showing that underlying objects cause local changes in the system by acting on one another."[18] The key term in this passage is the "underlying objects". The mechanistic piece of a causal mechanistic explanation must have defined underlying objects or entities that are at least one scalar level below the phenomenon of interest. In a similar vein, Krist, Schwarz, and Reiser have proposed a framework of epistemic heuristics to support students' development of mechanistic thinking, which involves (i) thinking across scalar levels, (ii) identifying and unpacking relevant factors, and (iii) checking how well the underlying mechanisms fit the observed phenomenon.[19] Indeed, Talanquer states that mechanistic reasoning is necessary in chemistry as "the organization of components can take place at various levels, and properties of a system at a given level often emerge from the properties, interactions, activities, and organization of the subcomponents defined at a sublevel."[20]

In our work on causal mechanistic reasoning to explain chemical phenomena we have separated the causal and mechanistic pieces, because our analysis shows that students can provide causal explanations, without a mechanistic piece involving objects at a scalar level below the phenomenon of interest, and vice versa.[14,21] For example, in discussing how London dispersion forces arise, students may give a causal description that involves transient positive and negative charges being attracted without discussing how those transient charges arise. The mechanistic aspect of the explanation arises from a discussion of electron movement creating the transient charges.[21] In this case, the level below the observed phenomenon includes electrons or other subatomic particles. An explanation that involves the movement of electrons to produce transient charges that result in attraction between particles is classified (by us) as a causal mechanistic explanation of London dispersion forces.[21]

Similarly, in characterizing acid−base reactions, we were able to separately identify causal explanations, mechanistic explanations, and causal mechanistic explanations.[14] Causal explanations generally invoke an electrostatic interaction between the reacting species, whereas mechanistic explanations include the idea that electrons are moving as bonds break and form. Causal mechanistic explanations include both these ideas. For acid−base reactions, the situation is further complicated by the theories that students use to explain the reactions. For example, when asked to explain the reaction HCl + $H_2O \rightarrow H_3O^+ + Cl^-$, some general-chemistry students simply provide us with a description.[14] For example, Heather writes, "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^+." This explanation was coded as "Brønsted Descriptive" because the student used the Brønsted acid−base model and simply described what happened, but did not explain why or how the reaction occurred. However, when we refined the prompt to ask both *what* is happening and then separately *why* it is happening, many more students were able to provide a causal mechanistic explanation.[14] For example, Francis wrote, "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." This description invokes the Lewis acid−base model because the student invokes the involvement of the lone pair and provides a causal mechanistic explanation for why the reaction occurs and was therefore classified as "Lewis Causal Mechanistic". The full coding scheme that is used in the prior work[14] and in this study of the investigation of HCl and H_2O is provided in the Data Analysis section, below.

It should be noted that causal mechanistic reasoning in the sense described above is not the same as mechanistic reasoning in organic chemistry as exemplified by the drawing of curved arrows. Although in a national survey of 103 organic-chemistry faculty, 77 experts agreed with a definition of mechanistic reasoning that requires one to represent electron movement on the basis of previously established knowledge of chemical reactivity,[22] this does not *necessarily* include the idea of pushing electrons from a source (a region of high electron density) to a sink (a region of lower electron density) but perhaps involves something more akin to pattern recognition on the part of the student. Ideally one might hope that as students draw mechanistic arrows, they are mindful that the arrows represent the movement of electrons from a source of electrons to a sink. However, there is ample evidence that many students do not use their knowledge of chemical reactivity to do this but rather rely on pattern recognition and memory to answer questions

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J. Chem. Educ. 2019, 96, 213−226

about mechanisms.[23,24] Triangulation of data from both written responses and drawn mechanisms can provide us stronger evidence of student understanding then either data source alone.

It is somewhat problematic that the terminology, definitions, and meanings of mechanistic reasoning are easily conflated and can create confusion about what is expected of students and how we will know if they have met those expectations. For the purposes of this paper and on the basis of our previous work with acid−base reactions and our work in other contexts, we define causal mechanistic reasoning as a type of explanation of a phenomenon that identifies the causal factors and the physical entities underlying a phenomenon and uses both the causal factors and the activities of the underlying entities (electrons) to provide a stepwise account of the phenomenon from start to finish.

Reasons for Engaging Students in Causal Mechanistic Reasoning in Organic Chemistry

In an investigation of the utility of mechanistic thinking for organic students at the end of second-semester organic chemistry (OC2), students were asked to draw mechanisms and predict products for both familiar and unfamiliar reactions.[25] Just as in other studies,[23,24] the number of students who were able to use mechanistic arrows productively was rather disappointing. For the unfamiliar tasks, where the students could not recall the answer from memory, students who drew mechanisms were significantly more likely to predict the correct products than the students who did not use mechanisms.[26] This is certainly evidence that students' use of reaction mechanisms can be a powerful predictive tool if used appropriately. However, it is common for organic instructors to assess student learning by asking them to draw the product of a reaction or even a mechanism without justifying their prediction or mechanistic proposal, believing (erroneously) that this is evidence of students' ability to reason about organic chemistry. Indeed, in a small survey of organic exams given at the nation's elite universities, little explicit evidence of reasoning was required from students.[27]

There is an extensive literature on the benefits of having students answer deep explanatory questions. For example, the construction of deep explanatory accounts of phenomena is cited in the IES report *Organizing Instruction and Study to Improve Student Learning: IES Practice Guide* as one of only two instructional strategies that are supported by strong evidence as improving learning.[28] We propose that helping students to engage in causal mechanistic thinking is an important and useful variant of this idea.[29] The process requires that students reflect on and connect the sequence of events underlying a phenomenon and the causal drivers involved. That is, the act of constructing a causal mechanistic explanation should help students learn. Indeed, in our earlier study on acid−base reactions, we found that students who constructed causal mechanistic explanations also had the highest success in drawing an appropriate curved-arrow mechanism.[14]

■ VALUE OF LONGITUDINAL STUDIES IN CER

When students advance into organic chemistry and beyond, instructors expect that they are bringing foundational general-chemistry knowledge with them and expect that they will know when and how to invoke this knowledge. In fact, colleges and universities structure degree-plans in many disciplines in such a way that entry-level courses are prerequisite to the advanced upper-level courses. This is especially true in chemistry, where most courses past general chemistry have prerequisites. Although it makes sense that students must learn basic concepts first so that they can build on them to learn more complex ideas in later courses,[30,31] there is scant research on how students carry basic ideas forward to the next set of courses. Similarly, whereas much work has been done on characterizing student alternate ideas or misconceptions, we know little about how these ideas change as students move throughout the curriculum. That being said, what research there is seems to indicate that even graduate students in chemistry may have persistent and problematic understanding of chemistry ideas.[23,32] For example, Bodner and Bhattacharyya report that chemistry graduate students are unable to use electron-pushing arrows in a predictive manner.[23] In our work on drawing Lewis structures, we found that organic-chemistry students were little better than general-chemistry students at drawing structures and that upper-level and graduate students were no more likely to understand that structures can be used to deduce information about physical and chemical properties.[32]

In fact, the lack of longitudinal studies was noted in the National Academies report on discipline-based education research (DBER), along with the need for more such studies.[33] Well-constructed longitudinal studies have the potential to elicit evidence of long-term impacts of curriculum, interventions, or other factors, because these impacts may only become apparent weeks, months, or years later.[34] White and Arzi define a longitudinal study as "a study in which two or more measures or observations of a comparable form are made of the same individuals or entities over a period of at least one year."[34] The chemistry-education-research (CER) community is responding to the call for more longitudinal studies that follow cohorts of students through two semesters of a given course and gather data via a pretest and post-test.[35−37] However, because of student-enrollment patterns, it is far less common and much more difficult for researchers to continue studying a phenomenon for two or more years. Typically, one must begin with a very large initial cohort to have a chance of retaining enough students for meaningful study by the end of the project.[38−41]

In our own prior work, we have explored how student understanding of structure−property relationships[42] and intermolecular forces (IMFs)[43] changes over two years from the beginning of general chemistry to the end of organic chemistry. We were able to show that students who learned general chemistry in a transformed general-chemistry curriculum were much more likely to make connections between a chemical structure and its macroscopic properties and that this difference was maintained throughout organic chemistry.[42] Similarly, in a study on student understanding of IMFs, students from the transformed courses were significantly more likely to represent IMFs as forces operating between molecules compared with students from a traditional curriculum, and this difference was maintained through another year of organic chemistry.[43]

Longitudinal Information about Student Reasoning Provided by Polytomous Assessments

Most assessment instruments used at the college level are dichotomous; that is, the answer is scored as either right or wrong, which means that many of the nuances of student understanding are lost. Particularly when students are

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Table 1. Research Design Comparing Data from Students in Four Cohorts on Several Demographic and Academic Measures

Description of Cohort			Semester Data Gathered[a]		
Identifier in Paper	Course Students in the Group Completed	*N*	End of GC2 (Spring 2015)	Start of OC1 (Fall 2015)	End of OC2 (Spring 2016)
CLUE-GC	CLUE−general-chemistry-2 course	107	×	—	—
Cohort A	CLUE−general-chemistry 2 course	92	—	×	×
Cohort B	More selective general-chemistry-2 course	48	—	×	×
Cohort C	None[b]	54	—	×	×

[a]All analyses were performed using SPSS. The full statistical data are provided in the Supporting Information. [b]These students transferred general-chemistry-2 credit from another institution or did not take a general-chemistry-2 course.

constructing explanations and arguments, the types of responses can vary widely, as do the ideas and mechanisms invoked. The analyses of student responses to the Brønsted−Lowry acid−base prompt used in this paper allow us to differentiate among the ideas and mechanisms used in the responses, and as such, the characterizations represent increasingly sophisticated explanations of acid−base reactions. There are several possible codes; therefore, these assessment instruments are polytomous. By using this approach (rather than items that are scored right or wrong), we are able to investigate how students' ideas change over time.

The present study is an extension of our previously published research on reasoning about acid−base reactions with general-chemistry students where we (i) developed a causal-mechanistic-reasoning framework, (ii) developed a prompt structure to elicit causal mechanistic responses, and (iii) developed a coding scheme that allowed us to identify increasingly sophisticated responses.[14] In this study, using this causal-mechanistic-explanation framework and the prompt structure, we investigate how organic-chemistry students respond to the same prompt and to a new prompt that asks about a Lewis acid−base reaction that does not involve the more familiar proton transfer.

The research questions that were guided this study were the following:

1. How does student reasoning change over time from the end of general chemistry to the end of organic chemistry for both Brønsted and Lewis acid−base reactions?
2. What is the effect of students' prior general-chemistry experience on their reasoning and ability to draw mechanistic arrows?

METHODS

Student Participants

These studies were performed at a large Midwestern research intensive university. All students were informed of their rights as human research subjects, and all data was obtained and handled in accordance with the Institutional Review Board.

There are four groups of student participants in this study: their backgrounds and the times of data collection are summarized in Table 1. All students were recruited via email as approved by the relevant instructor of record and completed the assignment for extra credit.

CLUE-GC (N = 107) students were enrolled in a transformed general-chemistry-2 course (Chemistry, Life, the Universe, and Everything: CLUE[44]) in 2015. The data presented here were discussed in our prior work[14] and are used here to show a progression of reasoning from the end of general chemistry 2 (GC2) through organic chemistry 2 (OC2). These students are representative of the whole CLUE cohort, but in spring 2015, the assessment item was only administered to these 107 students.

The other three groups of students reported in this study were enrolled in and completed both semesters of a traditional sophomore-level organic-chemistry course (using a published text[13] and homework) during the fall 2015 semester (OC1) and the spring 2016 semester (OC2). Out of the 674 students who completed both assessment items administered at the beginning of OC1 and at the end of OC2, 200 students were randomly selected. These students were then characterized by the nature of the GC2 course they completed, and three main GC2-coursework pathways emerged for these students. Almost half of the students had completed the CLUE transformed general-chemistry course for their GC2 coursework (N = 92). That is, they were enrolled in the same course as the CLUE-GC group who were the focus of our previous paper.[14] Although these students are not the same subpopulation of students as that in CLUE-GC, they are comparable using various academic and demographic measures (see Tables S2 and S3 in the Supporting Information). These students will be referred to as Cohort A (N = 92).

Originally, we envisaged that the remaining students would form a single cohort, but on further analysis we saw that there were two different groups of students: Cohort B (N = 48) had been enrolled in a more selective general-chemistry sequence. These students include honors students, chemistry majors, and students who were enrolled in a self-selected residential-college program. Cohort C (N = 54) was composed of students who either transferred credit for GC2 (and we therefore did not know what type of general-chemistry experience they had been exposed to) or had not taken GC2 (at this institution, GC2 is not a prerequisite for OC1). There were also six students who had taken a previous version of general chemistry several years earlier. Because these six students did not readily fall into any group, we did not use their data for this study, leaving us with 194 total students in our comparison groups.

Summaries of all statistical analyses of demographic and academic measures are reported in Sections S2 and S3 of the Supporting Information. Comparisons of the background information among all the cohorts showed that except for the instances discussed below, there were no significant differences. Cohort A had earned somewhat higher grades than CLUE-GC in GC2 (means of 3.3 vs 2.9, U = 3617.0, z = −3.202, p = 0.001, r = 0.23; small effect size). As one might expect, students who continued on into organic chemistry were more successful in general chemistry. A comparison of the three organic-chemistry cohorts, A, B, and C, showed that Cohort B had slightly higher ACT scores than Cohort A (U = 1555.5, z = −2.548, p = 0.011, r = 0.22; small effect size) and Cohort C (U = 900.0, z = −2.145, p = 0.032, r = 0.21; small effect size). Because Cohort A had elected to take more selective general-chemistry courses, one might expect that they

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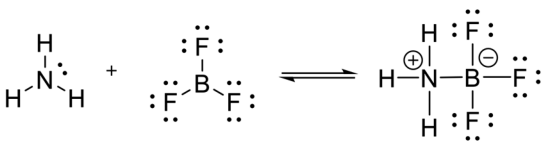
would have higher incoming ACT scores. Cohort C had a significantly lower GPA at the start of OC1 than Cohorts A and B, with medium effect sizes. At the end of OC2, Cohorts B and C also differed in terms of their OC2 grades, with a small effect size (see Table S2 in the Supporting Information). Cohorts A and B did not differ in terms of their final OC2 grades.[45,46]

Description of Assessment Tasks

The assessment prompt was designed specifically to elicit student causal mechanistic reasoning about a given acid−base reaction. In this paper, we report on student responses to the previously reported reactions of HCl with H_2O and the Lewis acid−base reaction of NH_3 with BF_3, which has not been previously reported. As in our earlier study, we structured each assessment task into four parts. First, students were presented with Lewis structures of the reactants and the products for the given reaction and asked to classify the reaction and explain their classification (Figure 1a). Next, students were asked to



a) How would you classify this reaction? Please explain why you chose that classification.
b) Can you 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) For the following reaction, please draw arrows in the BLUE box to indicate how the reaction occurs.

Figure 1. Assessment prompts administered using *beSocratic* for the reaction of BF_3 with NH_3. An identical prompt structure was used for the reaction of HCl with H_2O.

describe what was happening at the molecular level (Figure 1b). The prompt then asked students to explain why the reaction occurred using a molecular-level explanation (Figure 1b). Finally, the students were provided Lewis structures of the reactants and products and asked to draw the mechanistic arrows to indicate how the reaction occurred (Figure 1c). It is important to note that the prompt asking students to describe what is happening and the prompt asking students to explain why the reaction occurs are separated in the prompt structure and students are provided two separate boxes to respond to these prompts separately. On the basis of our previous work,[14] we know that by asking these questions separately, students recognize that *explaining why* is different than *describing what*.

Data Collection

Data analyzed in this study were collected via the online homework and research platform *beSocratic*.[43,47−49] These data were in the form of written student explanations and drawn mechanistic arrows. The same prompt structure was used to elicit student knowledge about two acid−base reactions: the reaction of HCl with H_2O, which has been previously reported for CLUE-GC,[14] and the reaction of NH_3 with BF_3, reported here for the first time. These prompts were administered to CLUE-GC at the end of GC2 in spring 2015 and to students in the organic-chemistry sequence, once at the start of OC1 in fall 2015 and once at the end of OC2 in spring 2016, as shown in Table 1. Both reactions were administered each time, and the prompts were identical in each administration. It should be noted that although the students answered these prompts at the start of OC1 and again at the end of OC2, the answers were not provided to them. The activity was administered to 107 CLUE-GC students in spring 2015, 763 OC1 students in fall 2015 with an 83% response rate, and then again to OC2 to 674 students in spring 2016 with a 92% response rate. Data from 194 randomly chosen organic-chemistry students who completed both assignments were analyzed, and these students made up organic-chemistry Cohorts A, B, and C. The student responses were anonymized and coded without knowledge of which cohort they belonged to.

DATA ANALYSIS

Prompt 1: HCl and H_2O

The written student responses to the HCl−H_2O prompt were analyzed using the published causal-mechanistic-reasoning coding scheme (Table 2).[14] Student responses that only discuss the observation that a bond was breaking or forming were characterized as "General Descriptive" (GD). Some descriptive explanations were closely aligned with the Brønsted acid−base definition (e.g., they identified the proton donor or proton acceptor and explicitly identified the reaction species) but still did not discuss electrostatic interactions or explicit electron movement. We characterized these types of responses as "Brønsted Descriptive" (BD). Responses that provided Brønsted acid−base causal reasoning, including discussion of polarity and electrostatic interactions, were characterized as "Brønsted Causal" (BC). Responses that provided a Lewis acid−base explanation that included discussion of electron activities were characterized as "Lewis Mechanistic" (LM) and often incorporated a Brønsted-like explanation as well. Ideally, students would provide Lewis acid−base casual reasoning discussing both polarity and electron movement, which were characterized as "Lewis Casual Mechanistic" (LCM).

Two of the authors (M.M.C. and H.K.), who were involved in the development of the scheme and had previously coded responses for the earlier report,[14] both coded randomly chosen responses that were not part of the data set and obtained a Cohen's kappa of 0.9. Next, one author (H.K.) coded 388 explanations for the HCl−H_2O prompt collected from organic students (194 for OC1 and 194 for OC2). Spot checks of 20 randomly chosen responses by other authors showed 100% agreement. As with our previous work on this reaction and coding scheme, the student responses for "describe what is happening" and "explain why" were analyzed together because students sometimes responded to the why question in the what textbox and vice versa. Student responses to "classify this reaction" were only analyzed when additional context was needed to make sense of student responses to "describe what" and "explain why". Student mechanistic arrows were reviewed separately from the written responses and were coded as described in the previous work: (i) the first arrow should have

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Table 2. Published[a] Characterization Scheme for the Reaction of HCl and H_2O

Characterization Scheme		Example
No Response (NR)	No answer was provided, or the explanations were unreadable or incomprehensible.	Viktor: "I do not really have a reasoning."
Non-normative (NN)	Students provided non-normative or unrelated explanations. In addition, students did not recognize it as an acid−base reaction and instead attributed the mechanism to other types of reactions or other macroscopic observations.	Raymond: "The hydrogen on the HCl is donating its electrons to the oxygen on the water."
General Descriptive (GD): what	Students provided scientifically simplistic descriptions and may have discussed bonds breaking or forming.	Catherine: "The acid is reacting with the base and the acid is a proton donor while the base is a proton acceptor."
Bronsted Descriptive (BD): what	Students provided Brønsted acid−base explanations, including identification of the acid and base and discussion of proton transfer.	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^+."
Bronsted Causal (BC): what and why	Students provided Brønsted acid−base causal reasoning that included 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 (LM): what and how	Students provided Lewis acid−base explanations including the role of the lone pair. (These may have also encompassed the Brønsted explanation.)	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."
Lewis Causal Mechanistic (LCM): what, how, and why	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 HCl. The H−Cl bond is broken and forms a new bond with oxygen. The reaction occurs because the partial negative charge on 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."

[a]See ref 14.

been drawn from the lone pair on the oxygen in water to the hydrogen in HCl, and (ii) the second arrow should have been drawn from the bond between the hydrogen and the chlorine atom in HCl to the chlorine atom. Any other variations of arrow drawings were coded as incorrect.

Prompt 2: NH_3 and BF_3

Because student reasoning about the reaction of NH_3 with BF_3 should be similar to that of HCl−H_2O, a modification of the previously established HCl−H_2O coding scheme was developed (Table 3). As with HCl−H_2O, we were able to identify different ways in which students responded to the prompt, with the difference being that only the Lewis model of acid−base reactivity is appropriate for the reaction. Responses that simply described what was shown in the reaction scheme were categorized as "Descriptive General" (DG). These responses identified the formation of the bond between the nitrogen atom and the boron atom but did not discuss electron movement nor provide any causal reason about why the reaction occurs. Aaron displayed this type of reasoning when he wrote, "Two compounds come together to make one new compound." Responses that discussed the electrostatic attraction between the nitrogen and the boron but omitted any discussion of electron movement were characterized as "Descriptive Causal" (DC), as exemplified by Casey: "The boron is electron deficient and is attracted to the nitrogen."

Responses that displayed evidence of understanding that the lone pair of electrons on nitrogen form a bond with boron but did not discuss electrostatic attraction were characterized as "Descriptive Mechanistic" (DM) because students were invoking the Lewis acid−base model of reactivity in their reasoning. Tony's reasoning fit this characterization when he said, "I believe that is because the boron has an available space/orbital around it that will allow the lone pair from the nitrogen to bond. Because N and B are both neutral, the bonding causes the nitrogen to have a positive charge, and the boron negative charge." Finally, responses that included reasoning about the mechanism in terms of electron movement and also explicitly discussed the attraction of the lone pair to the boron atom were characterized as "Causal Mechanistic" (CM). Timothy's response, "The lone pair of electrons on the nitrogen attacks the partial positive boron which creates a new shared bond between them", includes both of the necessary elements. The characterization scheme of student reasoning for the reaction of BF_3 with NH_3 is shown in Table 3.

Three of the authors (M.M.C., H.K., and O.M.C.) coded a random sample of 20% of the 388 student responses (194 from OC1 and 194 from OC2) to establish inter-rater reliability, resulting in pairwise Cohen's kappa values above 0.7 to establish the coding scheme. To finish coding the other 80% of the data, one of the authors (O.M.C.) worked to train two undergraduate coders. Each trained coder obtained Cohen kappa values ranging from 0.69 to 0.93 with the author (O.M.C.). These two trained coders coded sets of 75−100 responses, and their results were compared with each other to ensure accuracy. In the case of any discrepancies between the two trained undergraduate coders, the author (O.M.C.) and the two trained coders would discuss until consensus was reached.

The mechanistic arrows for the reaction of NH_3 with BF_3 were coded in a similar way to that previously described in the HCl−H_2O prompt. The mechanistic arrow was considered correct if the arrow began at the lone pair on nitrogen and

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J. Chem. Educ. 2019, 96, 213−226

Table 3. Characterization Scheme for the Reaction of NH_3 with BF_3

	Characterization Scheme	Student Examples
No Response (NR)	Student did not provide an answer, or the explanation was unreadable or incomprehensible.	—
Non-normative (NN)	Student attributed the mechanism to other types of reactions or to other macroscopic observations.	Kate: "The acid, the NH_3 is accepting electron pair from BF_3 then they come together due to ionic bond."
Descriptive General (DG): what	Student provided a scientifically simplistic description of bond formation.	Rachel: "The nitrogen bonds to the boron to make the new complex."
Descriptive Causal (DC): what and why	Student provided an explanation that discussed the electrostatic attraction of the species.	Casey: "The boron is electron deficient and is attracted to the nitrogen." Andrew: "The partially negative nitrogen is pulled to the boron."
Descriptive Mechanistic (DM): what and how	Student provided a Lewis acid–base explanation that explicitly discussed electrons and their movement.	Tony: "I believe that is because the boron has an available space/orbital around it that will allow the lone pair from the nitrogen to bond. Because N and B are both neutral, the bonding causes the nitrogen to have a positive charge, and the boron negative charge." Michelle: "Boron has a vacant orbital in which the lone electrons on the N can form a bond."
Causal Mechanistic (CM): what, why, and how	Student provided a causal and a mechanistic explanation for the reaction.	Mary: "The lone pair in the NH_3 is able to give its electrons to the B in BF_3. It acts as a nucleophile and is partially negative while the B is partially positive." Timothy: "The lone pair of electrons on the nitrogen attacks the partial positive boron which creates a new shared bond between them."

ended at the boron. Drawings that included backward arrows or any extraneous arrows were considered incorrect.

RESULTS

We have organized our findings by our two research questions: (i) How does student reasoning change over time from the end of general chemistry to the end of organic chemistry? (ii) What is the effect of prior general-chemistry experience on student reasoning? We will address the results for each type of reaction ($HCl + H_2O$ and $NH_3 + BF_3$) within each research question.

Research Question 1

How does student reasoning change over time from the end of general chemistry to the end of organic chemistry for both Brønsted and Lewis acid–base reactions?

Finding 1a. All three organic cohorts improved throughout the two semesters of organic chemistry.

$HCl + H_2O$. In general, all students' reasoning, regardless of general-chemistry preparation, became more sophisticated over the course of two semesters of organic chemistry. Figure 2 shows the classification of student reasoning for Cohorts A, B, and C both at the start of OC1 and at the end of OC2. Because we are comparing how reasoning changed from one time point to the next for the same group of students, a McNemar test for repeated measures[45] was used to analyze the change in the proportion of students who transitioned from a non-LCM characterization to an LCM characterization from the start of OC1 to the end of OC2. For Cohort B and Cohort C, there is a noticeable shift from GD responses to LCM ones by the end of OC2. At the start of OC1, only 15% of Cohort B and 11% of Cohort C gave LCM responses. By the end of OC2, 40% of the students in both of these cohorts gave LCM responses. These shifts from non-LCM to LCM responses from the start to the end of organic chemistry were significant for Cohorts B and C ($p = 0.012$ for Cohort B and $p = 0.001$ for Cohort C). Students in Cohort A improved from 43% of students giving LCM responses at the start of OC1 to 58% at the end of OC2 ($p = 0.043$). Recall that these students all completed the same organic-chemistry course with the same instructor, and the primary difference between these three cohorts is their general-chemistry preparation. We will report our observed effects from general-chemistry-course experience in the Research Question 2 section.

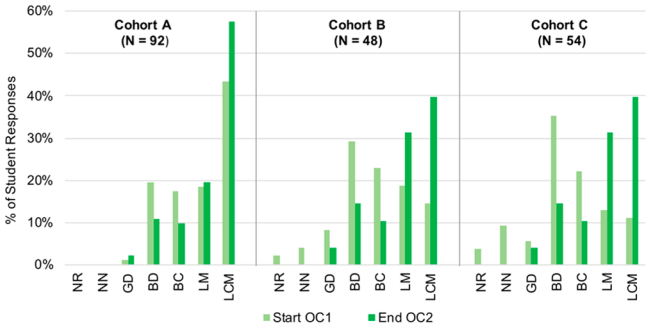

Figure 2. Characterization of student explanations for HCl + H_2O for Cohorts A, B, and C at the start and end of organic chemistry. Exact percentages are listed in Section S4 in the Supporting Information. No Response (NR), Non-normative (NN), General Descriptive (GD), Brønsted Descriptive (BD), Brønsted Causal (BC), Lewis Mechanistic (LM), Lewis Causal Mechanistic (LCM).

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J. Chem. Educ. 2019, 96, 213–226

NH_3 + BF_3. As shown in Figure 3, a similar but less marked pattern emerges for the reaction of NH_3 + BF_3. All of the

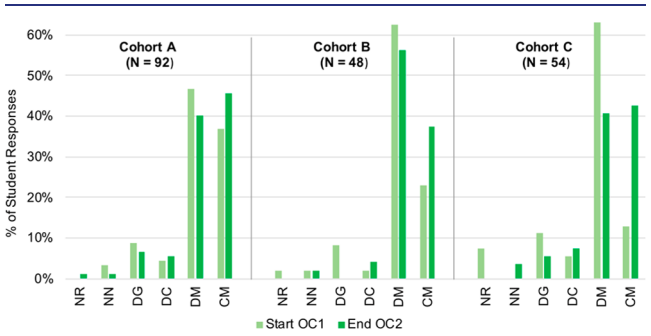

Figure 3. Characterization of student explanations for NH_3 + BF_3 for Cohorts A, B, and C, at the start and end of organic chemistry. Exact percentages are listed in Section S10 in the Supporting Information. No Response (NR), Non-normative (NN), Descriptive General (DG), Descriptive Causal (DC), Descriptive Mechanistic (DM), Causal Mechanistic (CM).

cohorts shift from a descriptive explanation to a causal mechanistic explanation, but only the change for Cohort C is significant ($p < 0.001$).

Finding 1b. A comparison of the pattern of responses for the two reactions shows that students are more likely to provide a mechanistic explanation for NH_3 + BF_3 than for HCl + H_2O even at the start of OC1.

Although the coding schemes are somewhat different for the two reactions, there are some comparisons that can be made. At the start of OC1, for Cohorts B and C, the most prevalent type of explanation for HCl + H_2O is simply a description of what is happening: that is, a proton is being transferred from the acid to the base (BD). This is followed by the BC explanation, where students indicate why the interaction occurs. Together these account for over 50% of Cohort B and C explanations, whereas explanations that invoke the movement of electrons (LC and LCM) account for between 20 and 30% of the explanations. For Cohorts B and C at the beginning of OC1, this reaction does not seem to activate ideas about the involvement of electrons. In contrast, for the Lewis acid−base reaction, over 80% of students invoke the involvement of electrons (DM and CM) during the reaction for all three cohorts.

By the end of OC2 for all cohorts, the explanations for HCl + H_2O have shifted to between 70 and 80% mechanistic (LC and LCM), similar to the NH_3 + BF_3 responses. At the end of OC2 the responses for Cohorts B and C are comparable for the two reactions. That is, enrollment in organic chemistry appears to help students use mechanistic (but not necessarily causal mechanistic) thinking. We will discuss the differences among Cohorts A, B, and C in the results for Research Question 2.

Finding 1c. CLUE students retain their reasoning ability from the end of general chemistry to the start of organic chemistry.

HCl + H_2O. We have previously reported findings on causal mechanistic reasoning for students at the end of a CLUE general-chemistry course (CLUE-GC), and here we compare those findings to the results from Cohort A. As shown in Figure 4, there is little difference between these two groups despite the fact that there was a several-month gap between collection of the two data sets. As shown in Figure 4, the major

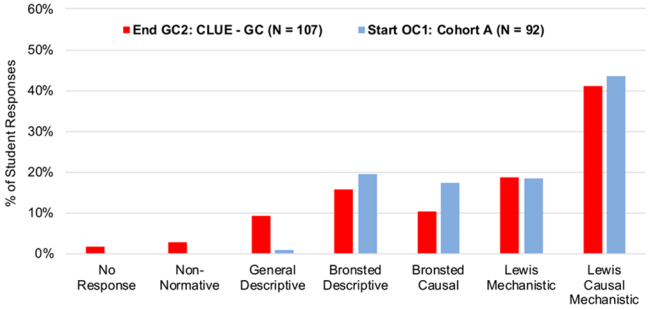

Figure 4. Classification of student explanations for the reaction of H_2O + HCl. These students were enrolled in a CLUE-GC2 course but were given the assessment item at different times.

category of explanation at both time points was LCM, and the pattern of responses was quite similar: 41% of students in the CLUE-GC cohort and 43% of students in Cohort A provided LCM explanations ($\chi^2(1) = 0.113$, $p = 0.737$). These data from CLUE-GC students seem to belie the common complaint from faculty that student knowledge tends to decay over the summer and valuable time must be wasted at the start of OC1 to review GC material.

We also compared the number of students who could draw the correct mechanistic arrows at both time points (Table 4).

Table 4. Comparison of Percentages of Correct Mechanistic-Arrow Drawings for the Reaction of H_2O + HCl

		Answers, %	
Cohort	Time	Correct	Incorrect
CLUE-GC (N = 107)	End of GC2	71	29
Cohort A (N = 92)	Start of OC1	59	41

At the end of general chemistry, 71% of students (CLUE-GC) were able to draw both arrows of the mechanism correctly, whereas at the beginning of OC1 the percentage fell slightly to 59%. The difference between these two sets of data at different time points is not significant ($\chi^2(1) = 3.321$, $p = 0.068$); that is, there was little decline in students' mechanistic-arrow-drawing abilities.

NH_3 + BF_3. A comparison of the data from CLUE-GC with that of Cohort A for NH_3 + BF_3 again showed that there was little difference between the end of GC2 and the start of OC1 ($\chi^2(1) = 0.394$, $p = 0.530$; Figure 5). Students in CLUE-GC were already quite successful at drawing the correct

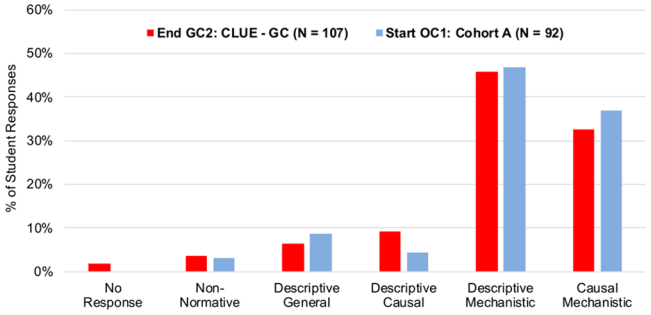

Figure 5. Classification of student explanations for the reaction of NH_3 + BF_3. These students were enrolled in a CLUE-GC2 course but were given the assessment item at different times.

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J. Chem. Educ. 2019, 96, 213−226

mechanistic arrows for this process (77% correct), and that percentage grew to 87% at the end of OC2 ($\chi^2(1) = 3.481$, $p = 0.062$; see Table 5).

Table 5. Comparison of Percentages of Correct Mechanistic-Arrow Drawings for the Reaction of NH_3 + BF_3

Cohort[a]	Time	Answers, %	
		Correct	Incorrect
CLUE-GC (N = 107)	End of GC2	77	23
Cohort A (N = 92)	Start of OC1	87	13

[a]These students all took CLUE for GC2 but were given the assessment item at different times.

Research Question 2

What is the effect of students' prior general-chemistry experience on their reasoning and ability to draw mechanistic arrows?

Finding 2a. Cohorts B and C gave similar responses regardless of general-chemistry-2 course experience.

An inspection of Figures 2 and 3 shows that the pattern of responses for Cohorts B and C are similar to each other. At the start of OC1, the most common response for HCl + H_2O for both Cohorts B and C was BD (29 and 35%, respectively). The similarity between Cohorts B and C also extends to the other types of reasoning: BC (23 and 22%, respectively), LM (19 and 13%, respectively), and LCM (15 and 11%, respectively). Indeed, the difference in proportions of LCM responses compared with non-LCM responses for Cohorts B and C at the start of OC1 is not significant ($\chi^2(1) = 0.275$, $p = 0.600$). These data suggest that students who took a "selective" GC2 course (Cohort B), had higher ACT scores, and higher OC1 and OC2 grades actually began organic chemistry with a similar ability to explain a simple Brønsted acid−base reaction as that of students who did not take a GC2 course at all or transferred an equivalent credit into the university (Cohort C). Similarly, by the end of OC2, these cohorts did not appear different in their ability to reason about a simple proton transfer ($\chi^2(1) = 0.014$, $p = 0.905$; Figure 2). It is encouraging that both cohorts improved their ability to reason about the reaction over two semesters of organic chemistry; however, Cohort B did not outperform Cohort C as one might have expected. We observed the same pattern of performance between Cohorts B and C for the reaction of NH_3+ BF_3 at the start ($\chi^2(1) = 1.732$, $p = 0.188$) and end ($\chi^2(1) = 0.274$, $p = 0.601$) of organic chemistry. We therefore combined Cohorts B and C to simplify data visualization and statistical comparisons from this point on. From now on we refer to this combined cohort as Cohort B+C (N = 102).

Finding 2b. Students in Cohort A were more likely to provide causal mechanistic reasoning than those in combined Cohort B+C.

HCl + H_2O. At the beginning of OC1, we see that the performance of Cohort A is quite different from that of combined Cohort B+C (Figure 6). The major response category for Cohort A is LCM, whereas for Cohort B+C, the major category is BD (Figure 6). Combining Cohorts B and C allowed us to compare the two groups Cohort A (N = 92) and Cohort B+C (N = 102) using a χ-square analysis. We first compared the percent of LCM codes to the sum of all the other codes (all other non-LCM codes). These analyses indicate that there are significant differences between the two

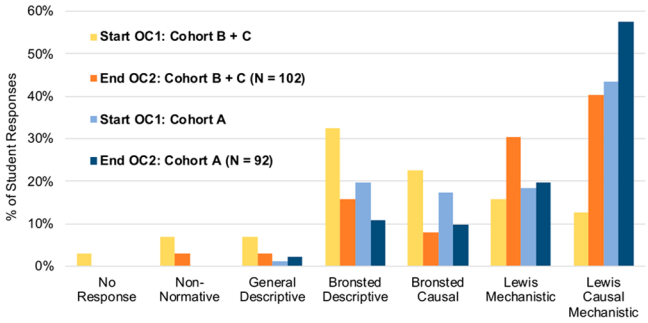

Figure 6. Classification of student explanations for the reaction of H_2O + HCl. These students had different GC2 experiences but were given the assessment item at the start of OC1 and the end of OC2.

groups both at the start ($\chi^2(1) = 23.010$, $p < 0.001$) and at the end ($\chi^2(1) = 5.872$, $p = 0.015$) of the two semesters of organic chemistry. By the end of OC2, the percentage of students providing an LCM response from Cohort A (58%) was still higher than that for Cohort B+C (40%). In fact, the percentage of students from Cohort B+C providing LCM responses is lower at the end of OC2 than the percent from Cohort A at the beginning of OC1 (43%).

To compare the change over time from the start of OC1 to the end of OC2, a McNemar test for repeated measures was used to analyze the proportion of students who transitioned from a non-LCM (43%) to an LCM (58%) response. This was significant both for Cohort A (43−58%, $p = 0.043$) and for Cohort B+C (13−40%, $p < 0.001$).

Students in Cohort A were also more likely to explicitly reason about electron movement at the start of OC1, meaning they gave LM (19%) or LCM responses (43%). Less than 30% of Cohort B+C reasoned about electron movement at all at the start of organic chemistry. This difference is significant ($\chi^2(1) = 20.713$, $p < 0.001$, Cramer's $V = 0.327$, medium effect size[45,46]) but fades by the end of OC2 ($\chi^2(1) = 1.411$, $p = 0.235$). Although it is encouraging that Cohort B+C began to incorporate more mechanistic thinking into their reasoning, their lack of causal reasoning seems to be a defining difference between these two groups by the end of OC2. This is particularly interesting as all students in Cohorts A, B, and C had the same organic-chemistry course and instructor.

NH_3 + BF_3. Again, there was a larger percentage of Cohort A students who invoked a CM response involving electrostatic interactions relative to those in Cohort B+C (Figure 7). A χ-square analysis of responses from the two cohorts (A vs B+C) shows a significant difference between the two groups at the

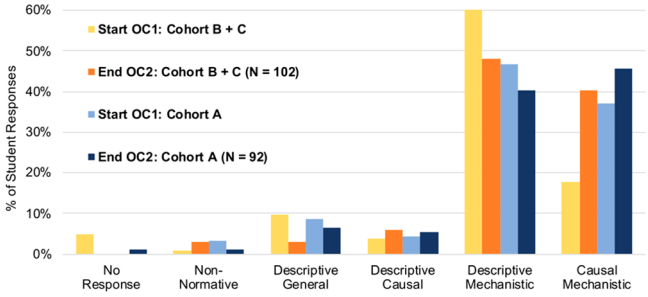

Figure 7. Classification of student explanations for the reaction of NH_3 + BF_3. These students had different GC2 experiences but were given the assessment item at the start of OC1 and the end of OC2.

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J. Chem. Educ. 2019, 96, 213−226

start of OC1 ($\chi^2(1) = 9.193$, $p = 0.002$, Cramer's $V = 0.218$, small effect size[45,46]). By the end of OC2, in contrast to the HCl and H_2O prompt, there is no significant difference between the cohorts of students ($\chi^2(1) = 0.588$, $p = 0.433$). As one might expect, the improvement of Cohort B+C from the start of OC1 to the end of OC2 was significant ($p < 0.001$), as it was for the HCl and H_2O reaction.

As discussed in Finding 1a above, almost all students from both cohorts invoked mechanistic reasoning (DM or CM) at the start of OC1 and the end of OC2 for this Lewis-only acid–base reaction. Comparing the proportion of mechanistic responses (DM and CM) to all nonmechanistic codes, we found no difference between Cohort A and Cohort B+C at the start of OC1 ($\chi^2(1) = 0.062$, $p = 0.804$) or at the end of OC2 ($\chi^2(1) = 0.241$, $p = 0.623$).

Finding 2c. Cohort A students were better at drawing mechanistic arrows.

HCl + H_2O. As recorded in Table 6, all students improved in their ability to draw mechanistic arrows over time, but Cohort A students were better at this task than Cohort B+C students, both at the beginning (59–15%; $\chi^2(1) = 40.845$, $p < 0.001$, Cramer's $V = 0.459$, a medium effect size[46]) and at the end of organic chemistry (88–75%; $\chi^2(1) = 5.044$, $p = 0.025$, Cramer's $V = 0.161$, a small effect size[46]). The gap between the cohorts narrowed over time but did not disappear. The difference between the two groups does seem to parallel the types of explanations that each provided. As in our earlier study, students who provide causal mechanistic explanations are more likely to be able to draw appropriate mechanistic arrows.

Table 6. Comparison of Percentages of Correct Mechanistic-Arrow Drawings for the Reaction of H_2O + HCl

Time	Cohort[a]	Answers, % Correct	Incorrect
Start of OC1	Cohort A ($N = 92$)	59	41
	Cohort B+C ($N = 102$)	15	85
End of OC2	Cohort A ($N = 92$)	88	12
	Cohort B+C ($N = 102$)	75	25

[a]These students had different GC2 experiences but were given the assessment item at the start of OC1 and the end of OC2.

NH_3 + BF_3. A comparison of the mechanistic-arrow drawings for NH_3 + BF_3 shows that there was little difference between students' drawings of mechanistic arrows (Table 7). Even at the start of OC1, the majority of all students are able to draw the one arrow that would indicate the formation of the Lewis acid–base complex, as shown in Figure 8. It is clearly a much easier task for most students than the Brønsted acid–base reaction.

Table 7. Comparison of Percentages of Correct Mechanistic-Arrow Drawings for the Reaction of NH_3 + BF_3

Time	Cohort[a]	Answers, % Correct	Incorrect
Start of OC1	Cohort A ($N = 92$)	87	13
	Cohort B+C ($N = 102$)	72	28
End of OC2	Cohort A ($N = 92$)	93	7
	Cohort B+C ($N = 102$)	88	12

[a]These students had different GC2 experiences but were given the assessment item at the start of OC1 and the end of OC2.

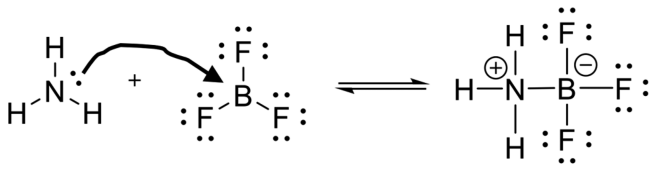

Figure 8. An example of a correct arrow drawing for the reaction of NH_3 + BF_3.

DISCUSSION

This study contributes to our overarching research goals that involve determining how student reasoning develops, how that reasoning can be elicited by appropriately designed prompts, and ultimately how a focus on causal mechanistic reasoning can support student learning in chemistry. In this study we were able to replicate our original finding (that students at the end of a CLUE general-chemistry course tend to provide Lewis causal mechanistic explanations)[14] with a different group of students (Cohort A) in the next course of the sequence. It is encouraging that many of these students were able to provide a sophisticated causal mechanistic explanation, even after a summer break. Often, faculty complain that students do not seem to remember material that they have learned in earlier courses, but in this case, we see little difference in the data collected at end of GC2 in spring 2015 and at the start of OC1 in fall 2015. We see a similar pattern in the same time period for the reaction of NH_3 and BF_3, which is clearly more recognizable as a Lewis acid–base reaction.

Because we did not have access to students from Cohorts B and C, during their general-chemistry experience, we must confine our remarks to what they know at the beginning of OC1. Although Cohorts B and C have had very different experiences in GC2, they look remarkably similar in their responses to questions of how and why HCl and H_2O react. That is, both students from highly selective courses and students who have had no GC2 experience tend to provide descriptions of the acid–base reaction using the Brønsted model rather than a causal mechanistic explanation that invokes a Lewis acid–base model. We believe that the difference between the CLUE cohort (Cohort A) and the others is a function of their general-chemistry experiences. Traditional general-chemistry courses typically do not include such scientific practices as the construction of models, arguments, and explanations, whereas the CLUE curriculum is built around such use of knowledge. Although it is unlikely that students would learn to use scientific practices without significant support and practice, it is encouraging that all the cohorts improved as they moved through the two semesters. That is, exposure to ideas about reaction mechanisms in an organic-chemistry context does improve students' ability to reason about simple acid–base reactions. However, there was still a significant difference between Cohort A and Cohort B+C at the end of OC2.

Similarly, student ability to draw mechanistic arrows for this simple reaction improved over the course of two semesters, although again Cohort A performed better both at the beginning and at the end of OC2 than the others. Just as in our prior studies,[14,26] the ability to draw mechanistic arrows seems to be correlated with the use of causal mechanistic

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J. Chem. Educ. 2019, 96, 213–226

reasoning to explain how the reaction occurs. There are numerous studies highlighting the difficulties that students have with drawing appropriate mechanistic arrows, and these findings seem to support the idea that causal mechanistic reasoning should be an explicit component of chemistry courses. It should be noted, however, that the ability to understand and draw mechanisms for simple acid−base reactions is not reflected in an increase in overall grades for Cohort A relative to those of Cohort B. One might imagine that the ability to explain and draw mechanisms would result in an improvement in organic-course grades. However, just as with many organic-course examinations (including the ACS examination and those in many "elite" chemistry departments), the examinations for this course did not explicitly address such mechanistic reasoning.[27] By the end of the second semester there was no difference in course grades for Cohorts A and B, although those of Cohort C were slightly lower. Whatever the course examinations are measuring, most students end up with equal facility regardless of their background. However, if an organic course were transformed such that students were explicitly required to engage in scientific practices such as constructing models, arguments, and explanations and to incorporate mechanistic reasoning, we might find that students who have already developed those habits of mind and approaches would be better prepared to engage with them. We are currently developing and testing such a transformed organic-chemistry curriculum and will report on our findings as we move forward.

The results from the reaction that is more recognizable as a Lewis acid−base reaction (NH_3 + BF_3) also show that students tend to move toward a causal mechanistic explanation over the two semesters of organic chemistry. It is interesting that a greater proportion of students in Cohort B+C tended to discuss the involvement of electrons from the beginning for this reaction than for the Brønsted acid−base reaction. Because the reaction of NH_3 with BF_3 is typically introduced in the context of Lewis acids and bases, it is likely that this prompt activates resources aligned with the Lewis acid−base model, which requires that students discuss the involvement of electrons. Clearly most of the students have grasped the idea of a Lewis acid−base reaction and are also able to draw an appropriate arrow to denote the mechanism.

IMPLICATIONS FOR TEACHING AND FURTHER RESEARCH

The results of this study show that students who have taken a curriculum that emphasizes causal mechanistic reasoning are indeed more likely to be able to employ such reasoning when prompted to do so and are also more likely to draw appropriate mechanistic arrows. Although an emphasis on causal mechanistic reasoning about phenomena may not be an explicit goal of most chemistry courses, it is certainly implicit for organic chemistry. Most organic faculty emphasize that the construction of an electron-pushing mechanism begins at a source and ends at a sink, but perhaps what is missing (or what students are unable to incorporate into their thinking) is an explicit emphasis on the cause of this electron movement. (Indeed, perhaps the arrow formalism should be renamed "electron pulling" rather than "electron pushing", to emphasize the attraction between electrophile and nucleophile). Numerous studies describe the difficulties that students have with drawing such mechanisms, but there are few that show improvements. Analysis of many organic examinations shows an emphasis on drawing a correct mechanism but not on reasoning about how and why that mechanism is drawn that way.[27]

We believe that an emphasis on asking students to articulate how and why a chemical phenomenon occurs provides them with the cognitive tools to use as they construct causal mechanistic explanations. These practices are emphasized in the CLUE curriculum, which has been extensively discussed elsewhere.[44] As the curriculum builds from interactions of atoms to networked biological reactions, students are asked to think about how and why these chemical phenomena occur. For example, questions such as "Why do neutral atoms attract each other?" and "Why do neutral molecules attract each other?" are used to drive instruction. Students are asked after almost every class to construct models and explanations using the online homework system *beSocratic* (as well as answer more traditional items such as calculations and skill development). Students become used to answering such questions, and we believe such repetition may help them to develop a set of cognitive tools that can be brought to bear on other problems. However, it may be that CLUE students simply are able to reproduce responses to familiar questions, rather than developing resources that might help them answer different questions. Clearly there is much work to be done in this area to determine whether students develop knowledge that is useful in other contexts, but there is some evidence from another study to support the idea that students are at least thinking about mechanisms more broadly.[50] Students who were concurrently enrolled in both a CLUE general-chemistry course and a molecular-biology course that was also undergoing transformation to focus on core ideas[51] were asked whether there were recurring ideas or "themes" in each course. In chemistry, one of the ideas that students discussed was "structure−property relationships", and for biology a similar theme was "structure−function". Of the 14 students interviewed, 9 students also spontaneously described a causal relationship in which molecular structure determines properties that determine function, despite the fact that this connection between the courses had not been made by the instructors. They saw that in biology there was often no explicit mechanism to link the structure to the function. One student said, "I think [the courses] worked together because I took what I learned in chemistry from structure determining properties, and was really able to apply that when I was thinking of structure going from properties and then that really changing the function, in biology." This finding has prompted us to further explore the impact of causal mechanistic reasoning across disciplines. We are also conducting more extensive studies on how causal mechanistic reasoning about more complex organic-chemistry reactions develops, and how this affects student construction of electron-pushing (pulling) mechanisms.

We believe that there is merit in helping students construct these kinds of explanations; however, many faculty are unable or unwilling to undergo a complete transformation such as would be required to adopt CLUE, and we have previously offered suggestions for those who would like to help students develop the "habit" of providing causal mechanistic reasoning. These include the idea that Lewis acid−base theory should be introduced in general chemistry and situated in a wider range of reactions so that students understand that this model can also be applied to Brønsted acid−base reactions. Students should be routinely asked both how and why chemical

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J. Chem. Educ. 2019, 96, 213−226

phenomena occur and asked to construct models (drawings) and explanations to accompany their answers. The construction of these questions can be quite difficult, because a prompt that is too vague may not activate the appropriate resources to answer the question, and a prompt that is too scaffolded may result in an overestimate of what students actually know.

Even if the general-chemistry course that precedes OC1 does not emphasize mechanistic reasoning and an understanding of how and when to invoke different acid−base theories, organic-chemistry instructors could expand the typically rather routine overview of acid−base reactions that most OC1 courses begin with to include the ideas described above and in our earlier publication. Additionally, an emphasis on *why* electrons move the way they do during a reaction, followed by activities in which students draw mechanisms and explain why electrons move from source to sink, may start to develop these kinds of reasoning skills. It is true that students do improve over the course of a year of organic chemistry, but it should be noted that Cohort A begins organic chemistry with a level of mechanistic reasoning and appropriate use of mechanistic arrows that the other two cohorts only achieve after a year of organic chemistry.

LIMITATIONS

There are several limitations to this study.

First, we do not know what knowledge Cohorts B and C had before they enrolled in organic chemistry; therefore, we do not make claims about what ideas they bring with them or how much they forgot over the summer. However, they do not seem to begin organic chemistry with the same level of facility that Cohort A has.

Second, the reactions studied are quite simple, and we do not know how students might fare with more complex tasks. However, it is our experience that we must begin studies by investigating simple systems to understand how students will respond in the best-case scenario. It can be very difficult to disentangle student reasoning if they do not understand the nature of the reaction. It bears noting that our goal is not to determine what students do not know, but rather to understand how students are able to construct and use explanations, arguments, and models. If we had begun these studies with the complex reactions typically taught in organic chemistry, it is unlikely that we would have been able to disentangle student reasoning about what was happening from other problematic ideas about structure, properties, and reactivity.[52] That being said, without studies on more complex systems, it is entirely possible that students from the transformed curriculum are simply repeating explanations and arrow-pushing mechanisms that they have memorized. That is, we may have exchanged one set of memorization tasks for another.

FUTURE WORK

Now that we have more understanding of how students from a range of backgrounds address simple acid−base reactions, our plan is to expand the methodology to more complex reactions: for example, nucleophilic substitutions and electrophilic additions. As reactions become more complex, we will investigate whether students are able to construct the same kinds of causal mechanistic explanations. We also plan to explore the correlation (or lack thereof) between sophistication of explanation and ability to draw mechanistic arrows as the system gets more complex.

FINAL THOUGHTS

There is a great deal of evidence to support the idea that many learners leave an organic-chemistry course without an understanding of the central concepts and skills that would make the course meaningful. The idea that organic chemistry is a course that can be mastered by memorization and pattern recognition is anathema to instructors, but yet we see many students using these strategies and being successful. It is our hope that by changing the emphasis of organic chemistry (and all chemistry courses) to emphasize the use of knowledge rather than the knowledge itself, organic chemistry will become a more useful and meaningful course to students. These studies on causal mechanistic reasoning provide us with some evidence about how to support students as they think through problems.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.8b00784.

Coding scheme for NH_3 + BF_3, statistical analysis of demographic and academic measures, and χ-square data tables (PDF, DOCX)

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Notes

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