ADDRESSING LEARNING GAPS IN ACID-BASE CHEMISTRY USING NOVEL THREE-DIMENSIONAL MODELS WITH LEARNING MODULE

by

Gabrielle Grimes

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ABSTRACT

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Teaching scientific concepts is very complex and includes the discussion and use of different models that support students' understanding of particle-level interactions and behavior of chemical phenomena. The presented research describes the development of three-dimensional acid-base models and an accompanying learning module to support students' understanding of the autoionization of water, acidic strength, pH, and K_a in aqueous acid-base chemistry. The model set includes acid and base models embedded with magnets and removable hydrogen atoms or hydroxide groups to model particle-level interactions. The magnetic models allow students to investigate particle-level processes with student-built models of aqueous acid and base systems. To asses student learning gains, this research discusses the development and validation process of a pre- and post-assessment and the results after the implementation of the learning module in an analytical chemistry course. In addition, follow-up interviews with participants were conducted to support the results of the analysis and clarify students' responses to assessment items.

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Chapter 1: Introduction and Background

1.1 Introduction

Research on model use in science education at the secondary and postsecondary level has shown models play an important role in learning and problem solving (Gilbert & Boulter, 1998a; Gobert & Buckley, 2000; Gilbert, 2007; Gilbert & Justi, 2016). Models in chemistry are an effective tool to visualize system changes, chemical phenomena, particle-level interactions, and physical structures; and aid in the understanding of particle-level interactions, relationships between components in a system, molecular structure, and three-dimensional special relationships (Gilbert, 2007; Khine, et al., 2011).

Models in science education exist in many different modes of representation. Models can be two-dimensional representations including diagrams, graphs, and drawings; three-dimensional physical representations that can be touched and manipulated, computer simulations, virtual models, mathematical models, verbally expressed models, and gestural models (Gilbert & Justi, 2016). Gilbert and Justi (2016), define the difference in the use of models for *"model-base teaching"* vs. *"modeling-based teaching"*. Model-based teaching consists of an instructional process using instructor provided models, such as models shown in textbooks, and are more exploratory in use where students work with a provided model. Modeling-based teaching is a learning process requiring students be actively involved in the modeling of a given phenomenon or entity in which students make their own models based on their own ideas, reflections, and revisions to their model (Gilbert & Justi, 2016).

In the constructivist learning theory, knowledge does not pass from the teacher to the learner with coherence. Instead, the learner constructs their own understandings and knowledge through active participation and connections to prior learning and experiences (Charmaz, 2014). Social constructivism theories emphasize the importance of social interactions and experience in the acquisition of knowledge (Schunk, 2020). There are a variety of student-centered and active-learning activities that reflect the main principles of constructivism, including discovery learning, collaborative learning, case studies, research projects, flipped classroom models, and modeling-based learning (Clark, 2018).

Scientific literacy includes understanding the processes of science, the knowledge that supports these understandings, and the ways in which science is communicated (Gilbert & Justi, 2016;). Research on model use in science education has shown models play an important role in the development of students' scientific literacy and help in the formation of hypotheses, the creation and validation of scientific knowledge, the explanation of scientific phenomena, and that models are a key component of scientific literacy. (Gilbert & Boulter, 1998a, 1998b; Gobert & Buckley, 2000; Khine, et al., 2011; Chittleborough et al, 2005; Gilbert & Justi, 2016). Gilbert and Justi (2016, p. 11-12) describe four roles of modeling in education for scientific literacy. 1) *Modeling can provide a way to reconstruct established scientific models*. If students can relate to the models reconstructed to provide explanations to their own experiences it allows them to more readily inquire into other everyday phenomena and engage in problem solving. 2) *Modeling will be recognized as a core component in the conduct and validation of science and technology*. Students that recognize the important role of models in the creation and validation of scientific knowledge will better interpret and evaluate scientific claims. 3) *Modeling can be a route to the development of general mental skills*. Understanding the scientific language used in modeling is an essential skill to acquire scientific literacy. Modeling can foster the ability to communicate scientific ideas and phenomena. 4) *Modeling entails a further development of personal values concerning the world-as-experienced*. Students that view scientific knowledge as the outcome of scientific debate and agreement are more aware of issues related to the conduct of science, their applications, and their consequences.

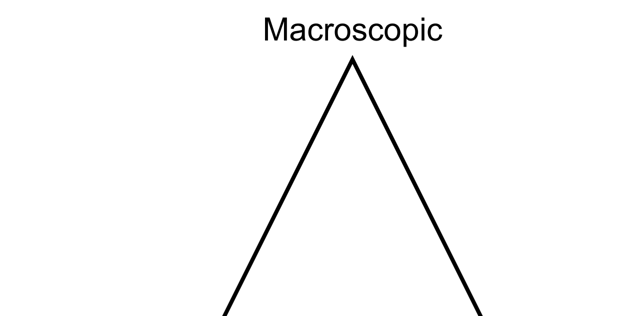
The use of models in teaching is an important part of secondary and postsecondary education. The Next Generation Science Standards includes *A Framework for K-12 Science Education* that identifies seven crosscutting concepts. Each crosscutting concept is identified to *'bridge disciplinary boundaries, uniting core ideas throughout the fields of science and engineering*' (NGSS Release, 2013). *Systems and system models* are recognized as one of the seven crosscutting concepts and an important educational tool in various science disciplines. NGSS describes models that can be physical, mathematical, or computer models and used to simulate systems and interactions in science. In addition, developing and using models is one of the eight Science and Engineering Practices identified in the *Framework for K-12 Science Education* (NGSS Release, 2013). Although the Next Generation Science Standards are written for K-12 students, the design committee reviewed the College Board Science Standards for College Success and state that '*engaging in these* *practices help students become successful analytical thinkers and prepared for college and careers.*' (NGSS Release, 2013).

1.2 Literature review

1.2.1 Johnstone's triangle

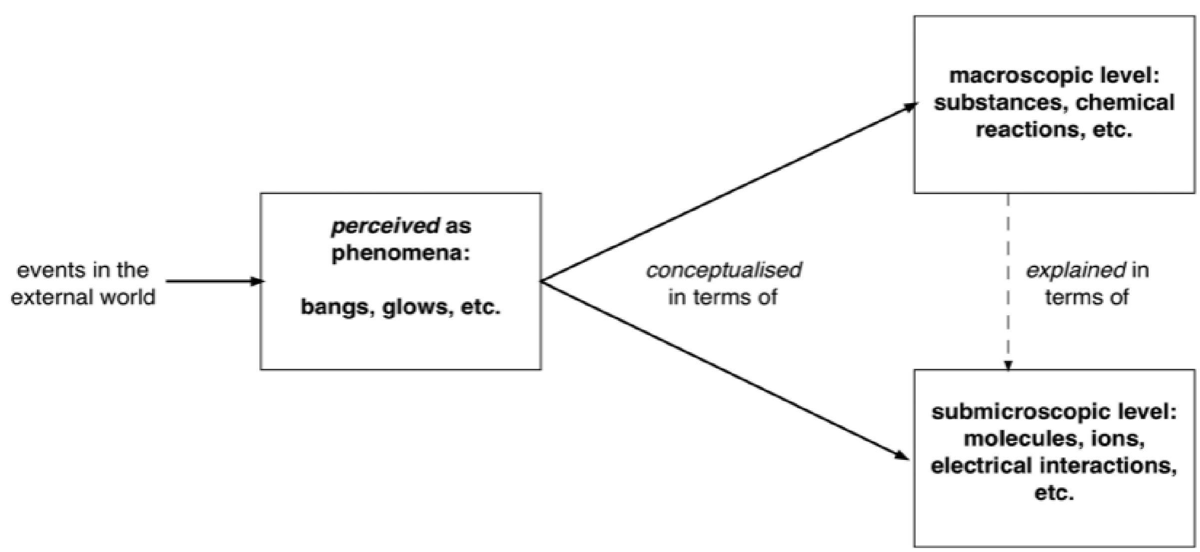
The ability to visualize chemical phenomena and processes at the particle-level and connect particle-level interactions to the symbolic language of chemistry are key to a sound understanding and the ability to critically think and solve problems in chemistry (Johnstone, 1982, 1993). A.H. Johnstone focuses on three representations of chemistry, the macroscopic, symbolic, and sub-micro (or particle-level), now referred to as Johnston's triangle (Johnstone, 1993). Johnstone's triangle is shown in **figure 1.1**.

Figure 1.1: Johnstone's triangle



Today, Johnstone's triangle is a well-known and accepted instructional framework for learning chemistry, and the ability to translate and make connections between representations is an important part of understanding chemical concepts (Vilardo, et al., 2016; Petillion & McNeil, 2020; Ryan & Herrington, 2014). It has been modified by other researchers to clarify and expand on each of the three representations. For example, Taber (2013), modified Johnstone's triangle to explain that chemical phenomena experienced by students are conceptualized at the macroscopic and submicroscopic levels. This representation is shown in **figure 1.2,** and connects the macroscopic level to the submicroscopic or particle-level interactions. Johnstone's representations have been widely researched in chemical education and used as a structural framework to guide chemistry curriculum and instruction (Galloway, Stoyanovich, & Flynn, 2017; Petillion & McNeil, 2020; Philipp, Johnson, & Yezierski, 2014; S. Taber, 2013; Sanchez, 2018; Schmidt, 2021; Vilardo, MacKenzie, & Yezierski, 2016).

Figure 1.2: Modified representation of Johnston's triangle (Taber, 2013)



There have been many attempts to help students connect the different representations of chemistry in Johnstone's triangle. Vilardo, MacKenzie, and Yezierski

(2016) developed and implemented a modeling-based teaching guided-inquiry activity for high school chemistry students (N=58) related to the classification of matter to help students connect the macroscopic concept of air to the particle-level and symbolic representations. The activity focused on students' understanding before and after a laboratory activity using different colored circular magnets as physical 3-dimensional models representing matter that makes up air. Prior to the activity with the magnetic models, students drew their interpretation of air and participated in small-group student-led discussions, followed by a teacher-led large group discussion. Next, students built models of the matter that makes up air based on six different symbolic representations and answered a set of guided questions. In the post-activity, students drew a second picture of air based on their new understanding and reflected on their revised drawings. Researchers analyzed and categorized the pre- and post-activity drawings into categories from one to ten to capture changes in students' understanding. A category one indicated the lowest conceptual understanding and a category ten indicated the highest conceptual understanding. The results were validated by 10 high school chemistry teachers through collaboration and re-sorting of the drawings until they reached consensus. Results from the pre-lab images showed 31% of students drew air in the particle-level domain before the activity using mostly non-bonding small circles. After the activity, 72% of students used particle-level representations to draw air and 71% of the particle-level drawings included bonding particles and diatomic elements. This increase suggested an improvement in students' particle-level understanding of air even though students had little experience learning the particle-level domain in chemistry prior to the activity. This study suggests that modeling-based teaching using

3-dimensional physical models are an effective tool to help students visualize matter that cannot be seen. When asked to compare their first and second drawings, one student responded, "*At first I didn't draw anything because you can't see air but now I know it is a mixture of multiple atoms and molecules*." (Vilardo, MacKenzie, & Yezierski, 2016).

A study by Petillion and McNeil in 2020 developed a flipped-classroom design with a series of videos using Johnstone's triangle as an instructional framework. Each video included three segments with each segment representing one of the three representations of chemistry. Molecular animations conveyed the particle-level interactions, narrated screencasts displayed symbolic representations, and laboratory demonstrations shown on video were used for the macroscopic level. The video format could be easily viewed by each student with the benefit of watching animations more than once or pausing the video as needed. To assess student learning three-question pre-video and post-video quizzes were given on three different topics: chemical bonding (pre-quiz N=527, post=quiz N=469), resonance structures (pre-quiz N=506, post-quiz N=456) and intermolecular forces (pre-quiz N=480, post-quiz N=428). Results showed that students performed significantly better ($p < 0.001$) on all three quizzes and on each individual quiz question except for one (Petillion & McNeil, 2020). Results support the use of instructional activities connecting Johnstone's domains to improve students' understanding.

Ryan and Herrington (2014) developed and implemented a modeling-based teaching activity using physical 3-dimensioanl models of ionic compounds to support students understanding of the particle-level processes when ionic compounds dissolve.

To investigate the impact of the activity on students' understanding of particle-level representations and connections to the symbolic representations, pre- and post-tests was administered. Students used the models to work through a series of questions separated out into two parts. For each part students manipulated the models, drew pictures, and wrote symbolic equations to record their observations. In part A, students used the models to show the solvation of ionic compounds formed from +1 and -1, +2 and -1, and +1 and -2 monoatomic ions and answered a series of related questions. Part B was similar to part A, but the compounds included polyatomic ions. The polyatomic ion models were held together in plexiglass to remain a discrete unit and focus on the behavior of polyatomic ions when dissolved. Next, students responded to analysis and discussion questions, followed by a class discussion about the main ideas and the limitations of the models. The activity was implemented in three sections of a non-major college chemistry course (N=47, N=45, & N=44). All three groups showed large percent gains on the pre- and post-test for drawing dissolved ionic compounds (30% pre – 94% post, 27% pre – 100% post, 27% pre – 93% post), and for the correct symbolic representations (26% pre – 83% post, 9% pre – 89% post, 18% pre – 82% post). Researchers did not include statistical analysis to show the significance of their findings. However, this work suggests that modeling-based teaching with magnetic models improved students' understanding of the process of dissolving ionic compounds at the particle-level, polyatomic ions as discrete chemical units, and connections to the symbolic representations (Ryan & Herrington, 2014).

1.2.2 Modeling in science education

The use of models in science far outdates any literature included in this review. This review focuses on examples in recent literature investigating the use of models in science education and their influence on learning and understanding science.

A two-year study with 11th grade chemistry students (N=210) investigated the benefit of modeling-based teaching using physical models on students' understanding of particle-level and mathematical representations of acid-base solutions. Students were divided into two groups that performed the same laboratory experiments and had the same discussion prior to each laboratory experiment. The treatment group (N=110) included a discussion following each experiment to explicitly connect the experimental data to building a physical three-dimensional model to explain the ion concentration in a solution. Students developed the physical models of acid and base solutions with given model sets of water molecules that broke apart into the hydrogen and hydroxide ions and guiding questions focused on how ions in solution changed during the experiment. Analysis was done using validated guided inquiry open-response questions prior to the laboratory experiments and a final summative multiple-choice assessment implemented with the control and treatment group. Results showed that 29% of the treatment group versus 7% of the control group, were able to connect mathematical representation to a visual model of ions in solution, and 78% of students in the treatment group showed improvement in the summative assessment compared to 51% in the control group. These results support the use of student-built acid-base models to improve students' knowledge of aqueous acids and bases (Hale-Hanes, 2015).

Bain, et al (2006) developed 3-dimensional models of biomolecules to improve students' ability to recognize structural features of proteins and identify particular details within the protein complexes. This research was conducted over four years with more than 400 students (exact number of participants was not published) as a laboratory activity in the second semester of general chemistry. The laboratory activity included four sets of models developed at the Center for BioMolecular Modeling in Milwaukee, Wisconsin. The week before the laboratory activity, students completed three sets of online tutorials and had two hours of lecture reviewing and expanding on the material covered in the laboratory modeling activity. The activity was divided into four modeling stations (A-D) completed in groups of 3-4 students. Station A concentrated on alpha-helices and beta-sheets, and required students to identify the N-terminal and partially sequence each structure. Station B modeled the zinc finger motif and required students to answer questions about features of the model. Station C consisted of two proteins with a focus on the different backbones shown in the models. In station D, students built layers of DNA using DNA model kits with pieces that attach via magnets set into sockets keyed to only allow for the correct assembly of the backbone.

Survey results showed that the majority of students felt their understanding improved after completing the modeling activity. The researchers report students had a statistically significant improvement in scores on the post-test compared to the pre-test scores (Bain, et al. 2006). This work suggests students' learning may be supported by the use of physical 3-dimensional models as a laboratory activity.

A study by Luxford and Bretz in 2013 used Johnstone's levels of representation as a structural framework to investigate students' understandings of ionic and covalent bonding through the use of student-generated physical models. Data was collected using student interviews (N=24) after the topic of bonding had been taught and tested by their instructors. To ensure the inclusion of a wide range of student abilities, students from a secondary physical science course (N=8), a secondary chemistry course (N=3), and first year university chemistry course (N=13) were included in the sample (Luxford & Bretz, 2013). In each interview the researchers asked students what came to mind when they heard the words '*chemical bonding*' and to explain and clarify different terms used in their explanation. After this initial investigation, students used colored pens, paper, playdoh, and toothpicks to build multiple physical models to show covalent and ionic bonding and describe the differences between them. Results showed that students' models did not always match their definitions and suggested that having students build just one type of model may not be adequate to investigate understanding. Seven of the 24 students built more than one type of model to represent one type of bonding and express additional characteristics that were not included in their initial model. The researchers state, "*Asking students to create their own models should prove useful in future research studies and it gives the researcher access to students' ideas beyond memorized definitions. Furthermore, asking students to generate more than one type of model may reveal inconsistencies, contradictions, and misconceptions.*" (Luxford & Bretz, 2013, p. 221). This work highlights important implications for modeling-based teaching and shows multiple student-develop models to represent the different characteristics and nuances of the system or phenomena being studied may be needed.

1.2.3 Student misconceptions in acid-base chemistry

Acid-base chemistry is included in high school and undergraduate chemistry courses and introduces students to the different models for acids and bases, acid-base reactions, and acid-base laboratory experiments (Hale-Hanes, 2015; Nurisa & Arty, 2019). Acid-base chemistry is important in undergraduate chemistry courses and understanding acid-base concepts and related calculations are a key component in undergraduate analytical chemistry courses. However, some concepts such as acid-base strength and acid-base reactions are challenging for many high school and general chemistry students (McClary & Bretz, 2012; Cooper, Kouyoumdjian & Underwood, 2016) and can continue to be a struggle for upper-level chemistry students (Orgill & Sutherland, 2008).

A study by Czysz, Schroeder, and Clark in 2020 looked at undergraduate organic chemistry and biochemistry students' understanding of acid-base chemistry by designing a laboratory exercise in each course with an emphasis on connecting the macroscopic level and particle-level representations to symbolic and mathematical representations. Study participants (N=24) completed a general chemistry prerequisite course that included equilibrium, acid-base chemistry, and buffers. Before the laboratory exercise, students were given an example with particle-level images and corresponding titration curves for different time points of the titration of acetic acid and sodium hydroxide. Next, students completed a pre-lab assignment that included writing the reaction for the dissociation of a weak acid in water and the reaction of the weak acid with sodium hydroxide, followed by drawing particle-level images for different time points during the titration and a corresponding titration curve. After the pre-lab, students completed a titration of a weak acid with sodium hydroxide to demonstrate the macroscopic level and make connections to their particle-level drawings. Students reflected on their particle-level drawings at different time points during the titration and had the opportunity to redraw their particle-level representations and titration curves after completing the laboratory experiment. Finally, students were asked to explain why they changed their pre-lab particle drawings after completing the laboratory experiment using the titration data collected.

Results from both semesters were analyzed using constant comparative methods and qualitative coding and showed that most students from both semesters (81% & 88%) were able to write the correct symbolic chemical reaction for the titration. Results indicated it was a challenge for most students to draw particle-level images corresponding to different time points during the titration. While students showed improvement in their images for both semesters, only the spring 2018 semester showed a significant improvement in particle-level images (p=0.0018). Results suggest students may need additional practice connecting molecular, symbolic, and macroscopic representations of acid-base concepts. Qualitative results show students struggle with the inverse relationship between pH and hydronium ion concentrations, and hold a misconception that a rapid pH change correlates to the reaction suddenly taking place instead of the weak acid buffer reducing the pH change as strong base is added (Czysz, Schroeder & Clark, 2020).

Misconceptions about acid-base solutions and buffer problems were identified by Orgill and Sutherland (2008). Students from a general chemistry course, analytical chemistry course, and biochemistry course participated in this study (N=26). Students were interviewed about their understanding of pH, acid-base solutions, and buffer problems. The interviewer asked students to describe buffers, the Henderson-Hasselbalch equation, buffer ratios, ionization constants, and the relationship between pK_a and K_a and pH and $[H^+]$, and draw an image of what they think a buffer solution looks like on a particle-level. Next, participants were asked to think aloud while solving buffer problems and reflect on the prompts to identify important or misleading information. Results showed some students were not able to correctly distinguish weak and strong acids and bases. One misconception identified is the belief that buffers can consist of any acid or base in any proportion. Another misconception found was that acid-base solutions are static instead of at a dynamic equilibrium, describing solutions as non-interacting acids and bases. Most analytical and biochemistry students could use the Henderson-Hasselbalch equation to solve problems, but could not describe how buffers maintain pH or the particle-level interactions between components (Orgill & Sutherland, 2008). This work shows that general, analytical, and biochemistry students struggle with understanding particle-level interactions of acid-base solutions and highlights the need for more instructional support in acid-base chemistry.

McClary and Bretz developed a diagnostic tool to identify organic chemistry students' misconceptions related to acid strength. The instrument consisted of nine items and was given to second semester organic chemistry students (N=89). Analysis showed two significant misconceptions. An incorrect response selected by at least 30% of the participants indicated a misconception. The first misconception, '*functional group determines acid strength*', found that students overgeneralize structural features to determine acid strength without considering implicit, electronic properties that may better predict chemical behavior. The second misconception found, '*stability determines acid strength*', showed students rely on the prior knowledge about stability of the acid to determine strength instead of identifying that an acid with a more stable conjugate base is a stronger acid (McClary & Bretz, 2012). This research shows more than 50% of upper-level chemistry students continue to struggle with the concept of acid strength and the different structural features that determine strength.

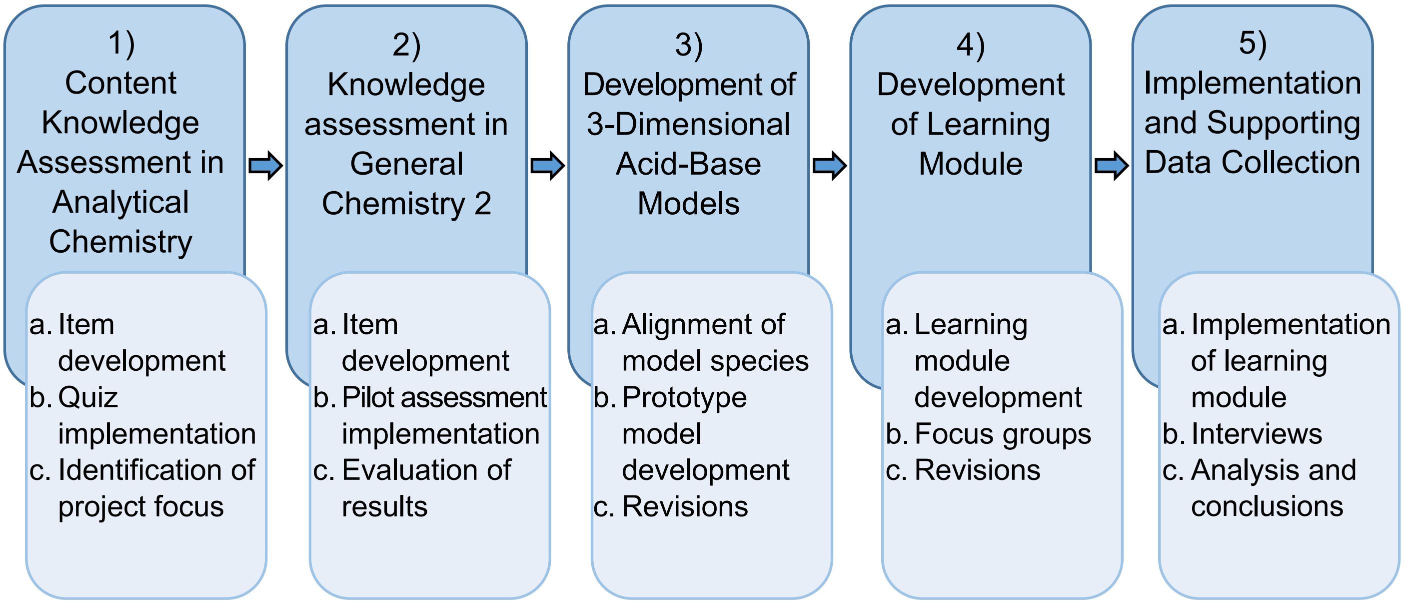
1.3 Research Questions

This research seeks to answer two questions:

1. Does an acid-base learning module using the novel acid-base models impact students' performance on acid-base content questions using a pre- and post-assessment?
2. Does an acid-base learning module using the acid-base models impact students' understanding of the autoionization of water, acidic strength, pH, and K_a?

The research process used to answer these questions is shown in **figure 1.3.**

Figure 1.3: Research process



Chapter 2: Investigation of Analytical Chemistry Students' Knowledge Level of Laboratory Content and Particle-Level Processes

2.1 Introduction

This study began by investigating analytical chemistry students' knowledge level of the particle-level interactions and processes in laboratory experiments. The initial investigation included multiple concepts applied in laboratory experiments. All experiments used acid or base reagents and most experiments required the application of acid-base concepts to understand the particle-level processes. Due to the extensive coverage of acid-base chemistry in the laboratory experiments and the results of the qualitative analysis, the focus of this research was narrowed to the investigation of students' understanding of aqueous acid-base chemistry.

2.2 Methods

Data reported in this study was collected under IRB approval #19.073. Only data from students that gave their consent to be part of this study are included. Investigatory laboratory quizzes in an undergraduate analytical chemistry course were implemented to assess students' knowledge level of phenomena and processes in laboratory experiments. **Figure 2.1** shows the research process designed to investigate students' knowledge level of laboratory content and determine the focus of the project.

Figure 2.1: Research process

a. Item development
- Alignment with laboratory experiments
- Focus on particle-level processes

b. Quiz implementation
- Following weekly laboratory experiments
- Fall 2018 (N=28)
- Spring 2019 (N=33)

c. Identification of project focus
- Categorization of items
- Analysis of acid-base items

2.2.1 Elementary Quantitative Analysis course details

To investigate students' knowledge level of the processes occurring in laboratory experiments, weekly investigatory quizzes were administered in a 200-level undergraduate analytical chemistry course: *Elementary Quantitative Analysis* at a large Midwestern R1 research university. The prerequisite for this course is General Chemistry II with a grade of C or higher. Quizzes were administered in the fall semester of 2018 (N=28) and the spring semester of 2019 (N=33). The same instructor taught the course both semesters and has taught this course for many semesters prior to this study. The course consisted of two 50-minute lectures given by the course instructor and two, 2-hr and 50-minute lab sessions with a teaching assistant per week. The first lab period each week was focused on performing the experiment. The second lab period each week allowed students time to complete the laboratory experiment if unfinished, review material, and take a laboratory quiz. It was typical that the second lab session each week ended prior to the scheduled end time allowing time to administer the research laboratory quizzes without disruption to the course schedule.

2.2.2 Item development

Quiz items were written each week to investigating students' knowledge level of the particle-level processes in laboratory experiments as opposed to questions focused on calculations. Each quiz was one page (two-sided) with approximately six to ten questions that align with each experiment. The researcher attended all course lectures to take notes about analytical processes, concepts, and connections to laboratory work covered during lecture and used the course textbook, student laboratory manual, and teaching assistant manual as resources to write quiz items. Some fall 2018 items were reviewed and revised with the principal investigator before implementation. After an initial review of responses from the fall 2018 quiz items and feedback from experts (the course instructor, analytical laboratory teaching assistants, and principal investigator) items were revised, removed, or added to align with the spring 2019 semester. The spring 2019 semester included an additional laboratory experiment and the order of the experiments was slightly different than the fall semester. The schedule of laboratory experiments and lab quizzes for both semesters are listed in **Appendix A**.

2.2.3 Quiz implementation

In the fall 2018 semester (N=28) seven quizzes were administered during the second lab period each week there was a new laboratory experiment and during the final week of classes during laboratory check-out. A total of nine different laboratory experiments were required in the fall 2018 semester. Quiz administration began during did week six with laboratory experiment four due to pending IRB approval .

In the spring 2019 semester (N=33) ten quizzes were administered during the second lab session each week there was a new experiment and during the final laboratory check-out period. However, inclement weather cancelled classes early in the spring 2019 semester causing an altered schedule for the first and second laboratory experiments. Both labs one and lab two were completed in the same week (week 2) requiring the entire time of both lab sessions that week. Quiz implementation in the spring 2019 semester began during week three.

Laboratory teaching assistants administered the quizzes and instructed students to work independently without notes. The teaching assistants collected the quizzes and returned them to the researcher to be graded. Quiz items were graded on completion with a score of zero for any items not attempted. Quiz grades were given to the course instructor at the end of each semester and students received extra credit points for all items completed.

2.2.4 Qualitative analysis methods

This research uses a mixed methods approach to analyze laboratory quiz data. To identify the content areas covered in each item's stem, deductive coding was used. Deductive coding employs the application of predetermined codes to the data (Bingham et al, 2022). Quiz items were coded for seven content areas covered in the laboratory experiments. The seven content areas are acid-base chemistry, complexation reactions, gravimetric analysis, hydrolysis, redox reactions, spectroscopy, and titration.

Inductive qualitative data analysis was guided by the coding practices described by Charmaz (2014). Inductive qualitative research is a “bottom up” approach that uses the data, in this case student responses, to construct themes from individual student’s data and develop codes inductively. Codes emerge from the data analyzed through a two-step iterative process. First, initial coding focuses on topics and themes in the data. This requires the researcher to become very familiar with the data and repeatedly interact with the data on a line-by-line basis. This line-by-line (each individual student response) coding allows the data to be sorted analytically and detected patterns. The data is continually compared with the data, and the influence of the researcher’s own beliefs, prior ideas, or bias can be minimized by creating initial codes based on common terminology and phrases present in the data (Charmaz, 2014). These initial codes are revised, combined, or expanded as patterns emerge to sort and analyze the data in the most meaningful way. For example, the codes ‘*proton*’ and ‘H^+’ were two initial codes that matched the terminology used in students’ responses, but were later combined into a single code of ‘*proton/H+*’. This process defines possible analytic paths to follow in the next step of coding.

The second step is focused coding, or concept coding, using the initial codes as an organizational guide. Charmaz (2014) describes focused coding as considering the most significant and frequent initial codes to begin to deeper analyze large amounts of data. This requires the categorization of the data by making decisions about which initial codes establish the strongest analytic directions. Inductive qualitative analysis systematically analyzes data by continually going back and forth between the data collected and analysis using constant comparative methods. The codes developed impose a framework for a more cohesive analysis of the data (Charmaz, 2014).

Following the inductive coding of item responses, students' open-response answers were deductively coded for the level of understanding expressed in the response based on specific criteria for each item developed through the analysis and organization of the inductive coding. Four levels of understanding codes were used: sound understanding, correct with partial understanding, incorrect with partial understanding, and no understanding.

2.2.5 Coding of quiz item stems into content areas

To identify the laboratory content areas, each item stem was coded through group consensus between two graduate researchers and the principal investigator for all content areas that fit that item. The seven laboratory experiment content areas and number of items fitting each code are shown in **table 2.1**.

Table 2.1: Number of items coded in each content area by quiz

	Acid-base	Complexation reactions	Gravimetric analysis	Hydrolysis	Redox reactions	Spectroscopy	Titration
Fall 2018 Quiz 1	5		2				2
Fall 2018 Quiz 2	5				1		4
Fall 2018 Quiz 3	1				1	4	1
Fall 2018 Quiz 4	1	2		2		3	
Fall 2018 Quiz 5	1	3				4	
Fall 2018 Quiz 6						6	
Fall 2018 Quiz 7	4	2			1	6	5

Total Fall 2018	17	7	2	2	3	23	12
Spring 2019 Quiz 1	12						6
Spring 2019 Quiz 2			4				5
Spring 2019 Quiz 3	5		2				2
Spring 2019 Quiz 4	5				1		4
Spring 2019 Quiz 5	1				1	3	1
Spring 2019 Quiz 6	1			2		4	
Spring 2019 Quiz 7	1	2		2		1	
Spring 2019 Quiz 8	1	4				3	
Spring 2019 Quiz 9						6	
Spring 2019 Quiz 10	4				1	5	5
Total Spring 2019	30	6	6	4	3	22	23

Most items on the spring 2019 quizzes were the same as the fall quizzes starting with quiz 3. This was due to the fall 2018 quizzes starting later in the semester due to pending IRB approval compared to the spring 2019 semester. Quiz 1 in the spring semester was two quizzes combined due to the cancellation of classes the week before from inclement weather and was all new questions. Quiz questions were most frequently coded as acid-base, spectroscopy, and titration. Ten items in the fall semester and 12 items in the spring semester were coded as titration and acid-base. All laboratory experiments in both semesters used acid-base reagents, indicators, or refer to acids or bases in the laboratory directions. Three labs were acid-base titrations, two additional labs specifically described the importance of controlling the pH during the experiment in the laboratory directions, and two experiments had to be carried out in a buffer solution. Due to this heavy focus on acid-base chemistry in laboratory experiments, extensive coverage in lecture, and students' responses indicating learning gaps in understanding acid-base concepts, acid and base questions that were given in both semesters were analyzed to investigate students' knowledge level of acid-base chemistry and became the focus of this research.

2.2.6 Concept identification of acid-base quiz items

Due to the small class size each semester, analysis was done on acid-base items that were given both semesters to analyze a greater number of responses (N=61). This included 14 items with 3 of the 14 items consisting of multiple parts. The acid-base items were coded to identify acid-base concepts covered in the 14 items by the researcher and principal investigator. Six acid-base concepts were identified: conjugate pairs, acid-base indicator, pH, proton or H^+, acid-base strength, and titration. **Table 2.2** shows the concepts identified for each item. For the complete subset of acid-base items analyzed see **appendix B**.

Table 2.2: Acid-base concept areas identified by item

Item number	Conjugate pairs	Acid-base Indicator	pH	Proton/H^+	Acid-base strength	Titration
1		✓	✓	✓		
2			✓	✓		
3	✓			✓	✓	
4		✓	✓		✓	✓
5	✓			✓		
6						✓
7			✓		✓	✓
8			✓			✓
9			✓		✓	✓
10						✓
11			✓		✓	✓
12			✓			✓
13			✓		✓	✓
14			✓		✓	✓
Totals	2	2	10	3	7	10

2.2.7 Qualitative analysis of students' responses

To investigate student knowledge, possible misconceptions, and learning gaps held by analytical chemistry students in acid-base chemistry, transcriptions of student responses and student images were uploaded into ATLAS.ti Version 8 Qualitative Analysis software. Multiple-choice questions were coded as correct or incorrect. Titration image items asking the student to draw an arrow to the equivalence point were coded for the location of the arrow on the titration curve. If the student drew an arrow on the vertical part of the curve it was coded as "equivalence point", if the arrow was above or below the vertical part of the curve it was coded as top or bottom of curve.

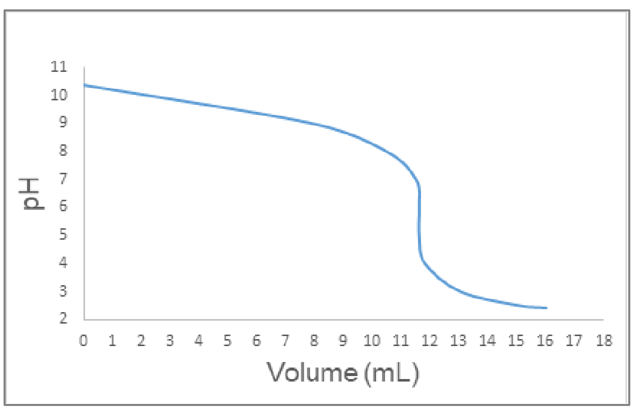
Students' responses to open-response items were inductively coded for themes and concepts. Using the inductive codes, specific guidelines were developed for each item by the researcher and reviewed by the principal investigator, to deductively code each response for the level of understanding expressed. Four level of understanding codes were used to identify the range of knowledge expressed in students' answers. The code *sound understanding* was used for open-responses items that expressed the most understanding and were identified by being coded with multiple correct concept codes. A *correct with partial understanding* code was applied to responses that were coded with fewer correct concept codes but still expressed understanding. An *incorrect with partial understanding* code was used for responses that were coded with correct inductive concept codes, but used or described the concept incorrectly. The code *no understanding* was used for responses that did not show any understanding a were not coded with any correct concept codes. Examples of the qualitative codes used with the code's description is shown in **table 2.3**. A description of the codes used for all items can be found in **appendix C.**

Table 2.3: Examples of acid-base item coding

Item 2) What is pH?

Concept code	Description
Mathematical definition	pH=-log[H^+] or pH equals the negative log of the hydrogen/H^+ concentration
Range or scale definition	Describes a logarithmic scale, pH scale, or pH range (low/high pH is acid/basic).
General definition	Describes general measurement of acidity, basicity, or H^+
Concentration definition	Describes measurement of concentration of H+, must state *concentration*
Power of hydrogen	Uses the specific phrase "power of hydrogen" in response.
Level of understanding	**Description**
Sound understanding	Correctly defines pH using 2 or more concept codes other than power of hydrogen
Correct with partial understanding	Correctly defines pH using just one concept code other than power of hydrogen
Incorrect with partial understanding	Incorrectly describes pH using a concept code (i.e. a high pH is acidic or pH ranges from 1-7)
No understanding	Does not describe pH, or only uses phrase "power of hydrogen"

Item 4) Draw an arrow pointing to the equivalence point on the titration curve below.



Concept code	Description	Code	Description
Equivalence point	Arrow points to the vertical section of graph	Correct	Coded as equivalence point
Top of curve	Above the vertical section of graph	Incorrect	Coded as top of curve
Bottom of curve	Below the vertical section of graph	Incorrect	Coded as bottom of curve

2.3 Results

2.3.1 Interrater agreement

The support the reliability of the qualitative coding results, all responses for 75% of the open-response items were coded by a second coder for percent interrater agreement. The second coder was either a chemistry education graduate student or the principal investigator. The researcher described all codes in detail using examples, any questions were discussed, and responses were coded independently. After an initial round of independent coding any discrepancies were discussed in a group with all coders and codes were revised independently. The researcher's final codes after discussion and revisions were used for the analysis.

Percent interrater agreement was calculated by taking the sum of responses with matching codes between raters and dividing it by the total number of responses coded. There is no single accepted standard for percent agreement between two coders for reliability, but Lombard et al. (2002) suggests that a percent agreement of 90% or greater indicates good agreement and 80% or greater is acceptable (Lombard et al., 2002). Results for the percent interrater agreement are listed in **table 2.4**.

Table 2.4: Percent interrater agreement

Item	% Interrater agreement for level of understanding	% Interrater agreement for concept codes
1	89.9	88.9
2	94.8	91.4
3	92.2	87.9

2.3.2 Qualitative analysis of item responses

Only students who were present and provided an answer are included in the results for each item. Results are shown in **table 2.5**. Results for all codes are shown in **appendix D**.

Table 2.5: Results of level of understanding codes for quiz items

Item (N)	Code	# of responses	percent
1 (N=54)	Sound understanding	12	22.2
	Correct with partial understanding	15	27.8
	Incorrect with partial understanding	15	27.8
	No understanding	12	22.2
2 (N=58)	Sound understanding	27	46.6
	Correct with partial understanding	26	44.8
	Incorrect with partial understanding	3	5.2
	No understanding	2	3.4
3 (N=58)	Sound understanding	14	24.1
	Correct with partial understanding	14	24.1
	Incorrect with partial understanding	17	29.3
	No understanding	13	22.4
4 (N=56)	Correct	40	71.4
	Incorrect	16	28.6
4a (N=58)	Correct	29	50.0
	Incorrect	29	50.0
4b (N=57)	Correct	34	59.6
	Incorrect	23	40.4
5 (N=55)	Sound understanding	33	60.0
	Correct with partial understanding	16	29.1
	Incorrect with partial understanding	5	9.1
	No understanding	1	1.8
6 (N=54)	Correct	45	83.3
	Incorrect	9	16.7
7 (N=55)	Correct	29	52.7
	Incorrect	26	47.3
8 (N=55)	Sound understanding	16	29.1
	Correct with partial understanding	12	21.8
	Incorrect with partial understanding	14	25.5
	No understanding	13	23.6
9 (N=58)	Correct	48	82.8
	Incorrect	10	17.2
10 (N=48)	Correct	42	87.5
	Incorrect	6	12.5
11 (N=54)	Correct	35	64.8
	Incorrect	19	35.2
12 (N=54)	Sound understanding	19	35.2
	Correct with partial understanding	8	14.8
	Incorrect with partial understanding	14	25.9
	No understanding	13	24.1
13 (N=54)	Correct	47	87.0
	Incorrect	7	13.0

Item (N)	Code	# of responses	percent
14 (N=54)	Correct	48	88.9
	Incorrect	6	11.1

Results from item two, '*What is pH?*' identified five different student definitions for pH. One definition that was used by three students (5.2%) was "power of hydrogen". This definition is not found in the course material or textbook and was considered incorrect. Students coded with a definition code (i.e., range or scale) but explained or used the definition incorrectly were coded as incorrect with partial understanding to distinguish those responses from responses that were not coded for any definition and showed no understanding. **Table 2.6** shows example student responses for item 2 matching each code.

Table 2.6: Examples of student responses and codes for acid-base quiz item two

Student response	Code(s)
pH is the value that tells whether the reaction occurs or not.	No understanding
pH= -log[H$^+$]	Mathematical Correct with partial understanding
pH is the [H+] ion concentration that is inside a solution. It is calculated using the -log of this value in order to determine its strength from 1-14, 1 being the most acidic while 14 is the most basic.	Concentration Mathematical Range or scale Sound understanding
pH is 'power of the hydrogen' It is the -log of the concentration of hydrogen ions.	Power of hydrogen Mathematical Correct with partial understanding
The acidity of a solution ranging from 1-7. 7 being most basic and 1 being most acidic	Range or scale Incorrect with partial understanding

Results showed that most students (91.4%) knew at least one correct definition for pH. When students were asked to explain why pH was important to control in their laboratory experiment only 22.2% were coded with a sound understanding and 27.8% were coded as correct with partial understanding. Most students describing the species being measured as H^+ (63.8%). However, four students coded as correct used the term proton, one student wrote H_3O^+, and one student responded with *'hydronium ion'*. showing a need to further investigate students' understanding of the different symbolic representations and terms used in acid-base chemistry.

Student responses to the two items relating to conjugate acid-base pairs showed students could identify conjugate pairs in an equation more often than they could describe the relationship between pairs and give an example on their own. When given two equations showing conjugate acid-base pairs, 60.0% of students were able to correctly identify and label all pairs, and 29.1 % of responses correctly identified pairs but did not label all species. When asked "*What is a conjugate acid-base pair? Please explain with as much detail as possible using an example.*" (item three), 44.8 % of students were able to give a correct example, but only 24.1% of students showed a sound understanding by correctly explaining the relationship between pairs and providing a correct example.

Student responses coded as incorrect with partial understanding or no understanding most frequently gave a neutralization reaction as an example. This code *neutralization* was specific to responses that formed a salt and water. Eight students (13.8%) drew a neutralization reaction between a strong acid and a strong base with the most common neutralization reaction between hydrochloric acid and sodium hydroxide. A neutralization reaction showing formation of a salt and water does not match the definition of a conjugate acid-bas pair used in the analytical course or textbook, which specifically states that "*Conjugate acids and bases are related to each other by the gain or loss of one H^+.*" (Harris, 2013, p. 168)

Analysis of items 9, 13, and 14 investigated students' understanding and possible misconceptions related to pH trends at the equivalence point and the species responsible for the trend. The equivalence point pH for a strong acid-strong base titration was correctly identified by 96.6% of students and 82.8% of students were able to correctly identify the pH at the equivalence point for all three titration types (item 9). These results are supported from analysis of items 13 and 14. The three items are shown below. Results of these items are shown in **table 2.7.**

9. Complete the table below by circling the correct pH in each box in column 2. Then explain how you made your choice in column 3.

Titration type	**pH at the equivalence point**	**Explain your choice. (Excess of what species leads to this pH?)**
strong acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak base – strong acid	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	

13. A strong acid/weak base titration will have a pH **greater / less** than 7 at the equivalence point?

14. A weak acid/strong base titration will have a pH **greater / less** than 7 at the equivalence point?

Table 2.7: Results of items 9, 13, and 14

Titration type	% Correct Question 9	% Correct Question 13	% Correct Question 14
Strong acid-strong base	96.6		
Weak acid-strong base	82.8		88.9
Weak base-strong acid	82.8	87.0	

Analysis of students' explanations from item 9 suggests that despite the majority of students knowing the pH trend for different types of titrations only 5% of students (3 out of 58 responses) used the term '*conjugate*' or described the conjugate of the weak species as responsible for the pH trend at the equivalence point. Qualitative coding showed 36.8% of students explained the pH trend of the weak-strong titrations was due to an excess of the strong species and 21.1% described the strong species as 'dominating' or 'overpowering' the weak species at the equivalence point.

2.4 Conclusions

The investigation of students' understanding of particle-level processes in analytical chemistry experiments identified acid-base concepts and processes as extensively covered in the laboratory experiments and focused this research to specifically investigate processes occurring in aqueous acids and bases. Analysis of the 14 acid-base items showed gaps in students' understanding of acid-base chemistry and identified concepts where more instructional may support students' understanding.

Qualitative coding of the 14 acid base quiz items identified six acid-base concepts covered in the quiz items: Acid-base strength, proton/H^+, pH, titration, conjugate pairs, and acid-base indicators. No items investigated students' knowledge level of acidic strength related to particle-level processes and differences in ionization, showing a need to collect more data to investigate students' understanding of acidic strength. An understanding of acidic strength is necessary for a deeper understanding of some aqueous acid-base processes occurring in laboratory experiments. For example, an understanding of acidic strength is necessary to explain the particle-level processes and species present at different time points in acid-base titrations.

Results from questions probing student understanding of pH trends at the equivalence point of different types of titrations shows most students know the pH trend for the three titration types, but students may hold a misconception that the strong species in a weak-strong titration is still present at the equivalence point to influence the pH. Additional instruction focusing on the conjugate of the weak species and its influence on pH at the equivalence point may improve students' understanding of particle-level processes occurring in different types of titrations.

Item 4 showed a titration curve and asked students to write the approximate pH at the equivalence point. Half of the responses included a pH in the correct range. The most common incorrect response (24.1%) was a pH=7, interestingly 64.3% of the students that responded with pH=7 at the equivalence point also marked the titration curve near the top of the curve directly across from a pH=7 on the graph. This suggests students hold a misconception that acid-base reactions always have a pH =7 at the equivalence point. Sheppard (2006) identified a similar misconception held by high school chemistry student that an indicator in a titration would always change color at a pH=7 (Sheppard, 2006).

Analysis of students' drawings and descriptions for conjugate acid-base pairs showed a difference between students' ability to identify conjugate acid-base pairs and explain them on their own or provide an example. This indicates students may rely on a memorized definition of conjugate acid-base pairs but may not have a deeper understanding of the relationship between pairs. Without a deeper understanding students may have difficulty understanding buffers and the species responsible for the equivalence point pH of different titration types.

All acid-base concepts identified from the quiz items are also taught in the prerequisite course, General Chemistry II. An investigation of General Chemistry II students' understanding of aqueous acids and base can help determine if additional instruction in acid-base chemistry would support General Chemistry II students' understanding and better prepare them for Analytical Chemistry.

2.5 Limitations

Item response analysis was investigatory in nature and the results cannot be generalized to other student populations. The laboratory experiments may not represent laboratory experiments performed in other analytical chemistry courses or other chemistry courses that include acid-base laboratory experiments and do not represent all processes occurring in the experiments. Items do not represent all acid-base concepts covered in the analytical chemistry laboratory experiments or the course and do not identify all learning gaps related to the processes in the laboratory experiments.

Chapter 3: Knowledge Assessment in General Chemistry II

3.1 Introduction

Data reported in this chapter was obtained from IRB approval #14.404. Only students who gave consent are included in this research. To collect additional data on students' understanding of acid-base strength, an online acid-base assessment was used in General Chemistry II after acids and bases were covered and tested in the course. Students in the General Chemistry II course were selected because it is a prerequisite course for Analytical Chemistry and provided an opportunity to investigate the need for more instructional support in acid-base chemistry before beginning Analytical Chemistry where acid-base concepts are applied in laboratory experiments. An assessment with General Chemistry II students also allowed data collection from a larger sample size. General Chemistry II curriculum includes the Arrhenius, Bronsted, and Lewis definitions, acid-base properties of water, pH, acid and base strength, ionization constants, conjugate acid-base pairs, molecular structure, buffers, acid-base titrations, and acid-base equilibria.

3.2 Methods

The online quiz was offered to all General Chemistry II students for extra credit in the spring 2021 semester online in Canvas. Both lecture sections of General Chemistry II were taught by the same instructor in a hybrid format that gave students the option to attend lectures in person or virtually. Students attended laboratory sessions in-person following all university policies and procedures for face-to-face instruction during Covid-19. Acids and bases were covered in the course during weeks 6-9. The assessment was administered during week 12 and 88 students completed the survey and consented to have their data included in this research. All items included the follow-up question, "*In your opinion, is the question above clearly worded and you knew what you were asked to do?"* to collect reliability data. Students could select *yes* or *no* for each follow-up item. Responses from 80% of the open-response items were coded by a second coder for percent interrater reliability. All codes were discussed in detail with the second coder before coding each response independently.

3.2.1 Assessment item development

Assessment items were written to investigate students' knowledge and particle-level understanding of acidic strength and different symbolic representations used in acid-base chemistry. Acidic strength was identified as an important acid-base concept applied in the analytical laboratory experiments. Implementation of the assessment items with General Chemistry II students after acids and bases had been covered and tested in the course provided an opportunity to investigate students' knowledge before beginning the analytical chemistry course. Nine items were developed by the researcher and revised through collaboration and discussion with the principal investigator.

3.2.2 Response analysis

To analyze the correctness of each response, a coding scheme specific to each item was developed by the researcher and discussed with the principal investigator. Responses to multiple-choice items were coded as correct or incorrect and responses to most open-response items were coded as correct, partially correct, or incorrect to better assess the range or students' knowledge. For items that included particle-level images, the percent of students that chose each image was calculated to further investigate students' understanding of particle-level representations and possible misconceptions. The percentage of students that responded "*yes*" for an item they found clearly worded was calculated for each item as a measure of the item's reliability. All items are shown in the next section with a discussion of the results for each item.

3.3 Results

Item one investigated students' understanding of different symbolic representations used for the ionization of a strong acid and was coded as correct or incorrect. Item one is shown below.

1) Consider the follow reactions

I. $HCl(aq) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$

II. $HCl(aq) \rightarrow H^+(aq) + Cl^-(aq)$

Please answer the following questions:

a) Do these equations represent different reactions?
b) Describe in your own words the similarities or differences of the two equations.

Both symbolic representations for the ionization of HCl are used in the general chemistry and analytical chemistry courses and textbooks. Responses that described the reactions as the same were coded as correct. For example, some students described the reactions were the same because the second reaction shows a simplified version of the first reaction. Other correct responses explained the reactions are the same because aqueous means water is present and $H^+(aq)$ is equivalent to $H_3O^+(aq)$. An example of a response coded as correct is below.

"These equations do represent the same reaction, however the second one is simply written in a simpler notation, that focuses more on the hydrogen ion rather than the interaction it has with water to make hydronium."

Responses coded as incorrect stated and described the reactions as different. Some responses coded as incorrect showed no understanding of the (aq) symbol and explained water was not present in reaction 2. Other responses described the reactions as showing different processes. An example of a response coded as incorrect is shown below.

"Yes. One equation will make hydrochloric acid, while another makes per chloric acid."

The results for item one are shown in **table 3.1.**

Table 3.1: Results of item one

Code	%	% yes to follow up item	% interrater agreement
Correct	56.5	92.0	92.9
Incorrect	43.5		

These results show that only about half of the General Chemistry II students recognize these two common symbolic representations for the ionization of HCl in water as equivalent and some students do not understand the meaning of the (aq) symbol using in symbolic chemical reactions.

Item two investigated students understanding of equivalent terms used in acid-base chemistry. **Table 3.2** shows the results for item two with a description of the codes used and an example response fitting each code. Item two is shown below.

2) In acid-base chemistry, the H+ ion is also referred to as the proton. Explain why these terms are equivalent.

Table 3.2: Results of item two

Code	Description	Example response	%	% yes to follow-up	% Interrater agreement
Correct	Clearly explains that the H^+ ion is a single proton	*The hydrogen ion, H^+, has only a single proton with no neutrons or electrons which is why the terms are equivalent.*	33.0	94.3	92.0
Partially correct	Identifies the same charge without clearly identify the H^+ as a single proton	*It has a +1 charge like a proton.*	33.0		
Incorrect	Does not make connection between proton & H^+ or charge	*The ion is transferred from a cation to an anion.*	34.0		

Results indicate many students may not have a sound understanding of why H^+ is equivalent to a proton. This could cause confusion for some students when the symbolic representation, H^+, is referred to as a proton in class or in print.

Item three uses particle-level images to investigate students' understanding of the ionization of a strong acid in water. The response options included two particle-level images that correctly represent the ionization of HCl and one incorrect image showing no ionization. The two correct options were used to probe students understanding of the symbolic representation of the species formed when the H^+ ion interacts with a water molecule. However, this was not clearly stated in the item stem and students were not able to select both beakers showing the correct ionization or explain why they selected one of the correct images as the best representation of the species in solution.

This item is shown below. The results are shown in **table 3.3**

3) When hydrochloric acid, HCl, ionizes in aqueous solution, which image best represents the species that are in solution aside from the H_2O molecules? (Water molecules have been removed for clarity.)

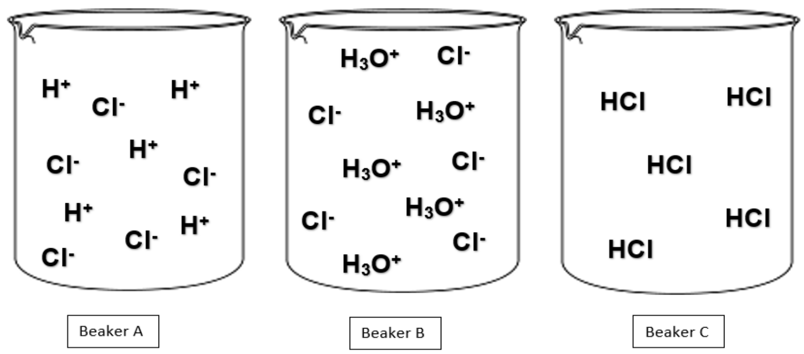


Table 3.3: Results of item three

Response	code	%	% yes to follow-up
Beaker A	Correct	52.3	
Beaker B	Correct	42.0	88.6
Beaker C	Incorrect	5.7	

The results from item three shows that 94.3% of students select an image that correctly shows the ionization of HCl in water. These results only indicate that the majority of students recognize a particle-level image of the ionization of a strong acid and that both symbolic representations, H^+ and H_3O^+, are recognized as species present in solution. The results do not show how many students recognized both images as correct and cannot be used to investigate students' understanding of the species present when a H^+ ion interacts with a water molecule.

Item four used an open-response format to investigate students' level of understanding of the particle-level interaction between the H^+ ions and water molecules in solution. Item four is shown below. The results are shown in **table 3.4** with a description of each code and an example response fitting that code.

4) When an acid is dissolved in water and ionizes into H^+ ion and an anion, how do the H^+ ions interact with the water molecules in solution? Please describe in your own words.

Table 3.4: Results of item four

Code	Description	Example response	%	% yes to follow-up	% Interrater agreement
Correct	Describes formation of H_3O^+, hydronium ion, or attraction/bonding between H^+ and water	*The H+ ions interact with water to form hydronium because H+ alone does not occur in water.*	53.4		
Partially correct	Describes an interaction between species, but does not clearly describe attraction/bonding between H^+ and water, formation of H_3O^+, or hydronium ion	*They interact by forming a new ion.*	18.2	86.4	93.0
Incorrect	Incorrectly explains interaction, or forms an incorrect species	*They pair with the other H molecules*	28.4		

Results show 28% of General Chemistry II students were not able to describe the interactions between water and the H^+ ion in solution or the species formed after acid-base chemistry had been taught and tested in the course.

Item five used a multiple-choice format to investigate if students could identify the correct definition for a strong acid. Item five is shown below. The results are shown in **table 3.5**.

5) What does it mean when we describe an acid as strong? Select the statement that you agree with most.

a) A strong acid will ionize into ions completely in solution
b) A strong acid contains more hydrogen atoms in its chemical structure than a weak acid
c) An acid is strong if it is highly concentrated in a solution
d) A strong acid is any acid that reacts with water to produce the hydronium ion.

Table 3.5: Results of item five

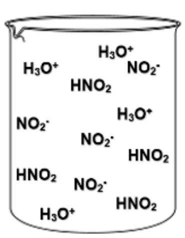
Response	code	%	% yes to follow-up
a	Correct	88.6	96.6
b, c, or d	incorrect	11.4	

Results show most students can select the correct definition for a strong acid after acid-base chemistry had been covered in General Chemistry II. These results support the results from item three that showed 94% of students selected a correct particle-level image for a strong acid.

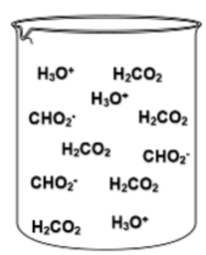
Item six investigated students' understanding of the relative strength of weak acids using particle-level images showing different amounts of ionization. Students were asked to rank the acids from strongest to weakest based on the amount of ionization shown in each image. Item six is shown below.

6) Comparable molar amounts of four different acids (HNO_2, H_2CO_2, $HClO$, HCN) are shown below in solution. Based on these images, rank the acids from the strongest acid (1) to the weakest acid (4).

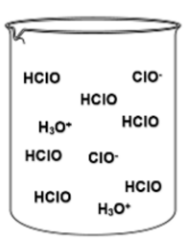
Solution 1: $HNO_2\,(aq) + H_2O\,(l) \Longleftrightarrow H_3O^+\,(aq) + NO_2^-\,(aq)$



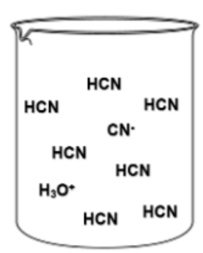
Solution 3: $H_2CO_2\,(aq) + H_2O\,(l) \Longleftrightarrow H_3O^+\,(aq) + HCO_2^-\,(aq)$



Solution 2: $HClO\,(aq) + H_2O\,(l) \Leftrightarrow H_3O^+\,(aq) + ClO^-\,(aq)$



Solution 4: $HCN\,(aq) + H_2O\,(l) \Leftrightarrow H_3O^+\,(aq) + CN^-\,(aq)$



Student's that ranked all four solutions correctly were coded as correct with all other responses coded as incorrect. The results for item six are shown in **table 3.6.**

Table 3.6: Results of item six.

Code	%	% yes to follow-up
Correct	37.5	79.5
incorrect	62.5	

Results show only 37.5% of students were able to correctly rank all four images from the strongest to the weakest acid using the particle-level images. Analysis of responses showed that 24% of students selected solution three, the chemical structure with the most hydrogens, as the strongest acid. The chemical formula used for formic acid in solution three was H_2CO_2 instead of the more common formula HCOOH. The use of this formula may have been misleading to students and caused more students to incorrectly rank the four weak acids.

Item seven used particle level images to further investigate students' understanding of the ionization of a strong acid in solution. Item seven is shown below. The results for item seven are shown in **table 3.7.**

7) Generally, the reaction of a strong acid in aqueous solution can be shown as:

$$\mathbf{HA(aq) + H_2O(l) \rightarrow H_3O^+(aq) + A^-(aq)}$$

Which image best shows a strong acid in aqueous solution?

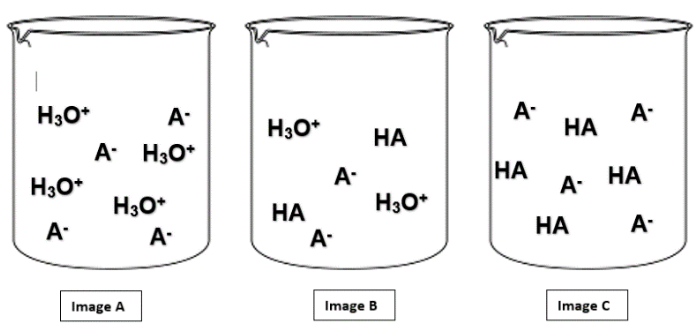


Table 3.7: Results of item seven.

Response	Code	%	% yes to follow-up
Image A	Correct	68.2	
Image B	Incorrect	20.4	94.3
Image C	Incorrect	11.4	

Results show 31.8% of students selected an incorrect particle-level image for the ionization of a strong acid in solution. Fewer students selected the correct particle-level image for this item (68.2%) compared to item 3 (94%). This difference may be due to item three including only one incorrect response leading to more correct guesses. Item seven also included an image showing partial ionization of a strong acid and, which was not included in item three, which may have made item seven more difficult.

Item eight investigated students' understanding of the structures and effects influencing acidic strength. Item eight is shown below. The results are shown in **table 3.8** with a description of each code and an example response fitting that code.

8) HF and HCl are both binary acids, both containing a hydrogen and a halogen. Despite these similarities, HF is considered a weak acid because it only ionizes partially in solution, while HCl is a strong acid, completely ionizing in water.

Explain what, in your opinion, might cause these different behaviors. Please do not explain what it means for acids to ionize partially or completely, instead, base your answer on structures and effects within the HCl and HF molecules.

Table 3.8: Results of item eight

Code	Description	Example response	%	% yes to follow-up	% Interrater agreement
Correct	Describes the difference in bond strength, may describe the size difference or bond length difference and correctly relate it to strength.	*The 2 factors of bond enthalpy and polarity are the determining factors. although HF is more polar, the fact that HCl has lower bond enthalpy (which is the predominant factor) makes HCl stronger.*	18.2		
Partially correct	Describes correct features or competing factors without explaining relationship to strength	*What might cause this is bond enthalpies and electronegativity.*	31.8	76.1	97.7
Incorrect	Describes polarity or electronegativity decreasing strength, explains dissociation, or incorrect statement	*F is more electronegative than Cl making it a weaker acid when bonded with H*	50.0		

The results show that most students could not correctly describe the differences between the two acids that causes the change in acidic strength. Most students with an incorrect response describe the difference in electronegativity as the reason HF is a weak acid and HCl is a strong acid. This indicates many students may not have a sound understanding of how electronegativity influences acidic strength or the other factors that contribute to acidic strength.

Item nine is a follow-up item to item eight asking students which acid, HF or HCl, has the stronger hydrogen-halogen bond. Item nine is shown below. The results are shown in **table 3.9**.

9) Following up on your response to the previous question, which acid must contain a stronger hydrogen-halogen bond, HF or HCl?

I. HF
II. HCl

Table 3.9: Results of item nine

Code	%	% yes to follow-up
Correct	70.5	97.7
incorrect	29.5	

Results show that most students correctly identify HF as having the stronger hydrogen-halogen bond. The different results from items eight and nine may indicate that some students understand how electronegativity influences bond strength but may not understand the other competing factors or structural features that contribute to the acidic strength.

The results of the nine items show many students may need additional support to better understand the different symbolic representations used in acid-base chemistry, interpreting particle-level images showing acid ionization, and the factors that contribute to acidic strength.

3.4 Conclusion

Item one investigated students' understanding of equivalent symbolic representations of aqueous hydrochloric acid and showed 56.5% of students correctly identified the two equivalent equations as the same. Results from item two asking students to explain why H^+ is also referred to as a proton suggests that the equivalent terms often used in acid-base chemistry may not be clearly understood by all students. More direct instruction regarding equivalent symbolic representations, such as $H^+(aq)$ and $H_3O^+(aq)$, and equivalent terms may benefit students understanding of the symbolic representations used in acid-base chemistry and support connections between the symbolic and particle-level. Modeling-based learning, discussed in the literature review, has been shown to help students make connections between the particle-level and symbolic representations.

Results showed that most students could select the correct definition of a strong acid in a multiple-choice format and the correct particle-level image of a strong acid in solution. However, Correct responses dropped dramatically when students were asked to rank the relative strengths of weak acids according to particle-level images and the number of particles ionized in solution. These results suggest that most students know the definition of a strong acid and can easily distinguish between simple particle-level images (complete ionization vs. no ionization). However, interpretation of images showing partial ionization are more challenging. The most common incorrect response when ranking the relative strengths of weak acids was the selection of formic acid as the strongest acid by 23.9% of students out of the four images (HNO_2, H_2CO_2, HClO, HCN) even though the particle-level image of nitrous acid (HNO_2) shows greater ionization. These results may have been influenced by the formula used for formic acid (H_2CO_2). The formula used for formic acid should be changed HCOOH or HCO_2H in any future items using the symbolic representation for formic acid.

Item eight and nine investigating students' understanding of the different factors that contribute to acidic strength. The results indicate many students may need additional instructional support to understand the effect of electronegativity on acidic strength and other particle-level structural features, such as atomic size and bond length, that contribute to acidic strength.

Reliability data collect from the follow-up item, "*In your opinion, is the question above clearly worded and you knew what you were asked to do?"* Showed 86-99% of students responded "yes" to seven out of nine items. Less than 80% of students responded "yes" to this follow-up question in two items, item six (79.5%) and eight (76.1%). The lower reliability in items six and eight may be due to the difficulty of the items as both items scored below 50% correct. Percent interrater agreement for all items coded by a second coder was between 92-93% agreement after any discrepancies were discussed and codes were revised independently. This is considered good percent agreement for content analysis (Lombard, Snyder-Duch, Bracken, 2002).

3.5 Limitations

The data for this analysis was collect from general chemistry II students and not analytical chemistry students. General Chemistry II is a prerequisite for Analytical

Chemistry; however, results from the data collected from General Chemistry II students cannot be generalized to analytical chemistry students. Although these results may not represent students' understanding of acid-base chemistry in other student populations, they do suggest more instructional support in General Chemistry II may enhance students' understanding of the symbolic representations and particle-level interactions of acid-base chemistry and better prepare students for Analytical Chemistry.

Student's interpretation of the items and reliability follow-up question was not studied. It is unknown if students interpreted the follow-up question as intended. Lower reliability scores on items that scored lower suggest that some students may have interpreted the question *"In your opinion, is the question above clearly worded and you knew what you were asked to do?"* as relating to their understanding of the question instead of its clarity.

Chapter 4: Pre- and Post-Assessment Item Development

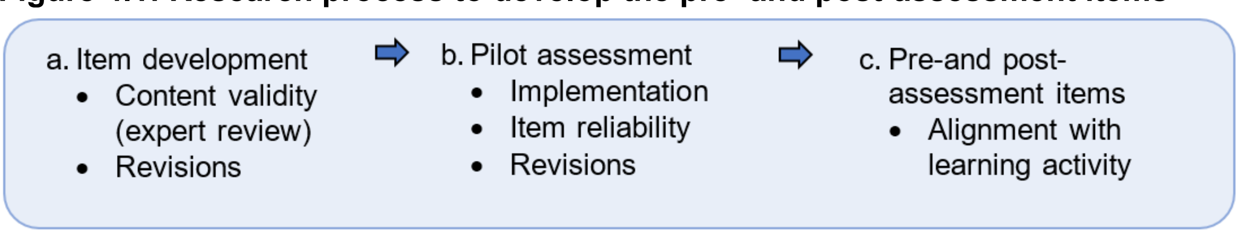
4.1 Introduction

The results of the qualitative analysis of the analytical chemistry laboratory quiz items and general chemistry II items identified learning gaps in students' understanding of the particle-level interactions between species in solution, symbolic representations, pH, and acidic strength. To address these gaps, a learning module using the acid-base models was being developed for implementation in an analytical chemistry course (discussed in chapter 6). To measure analytical chemistry students' learning gains after implementing the learning module, assessment items were developed for use on a pre- and post-assessment. A detailed description of the item development is included in the Methods.

4.2 Methods

The research process to develop the pre- and post-assessment items is shown in figure 4.1.

Figure 4.1: Research process to develop the pre- and post-assessment items

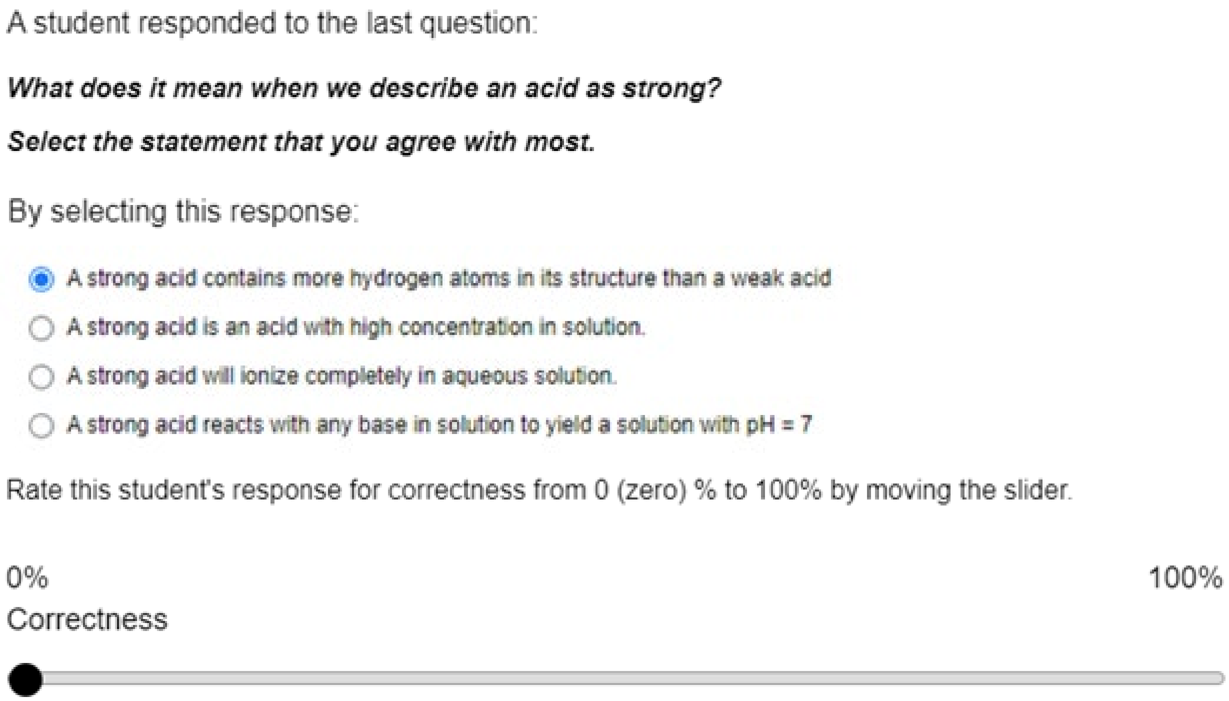


4.2.1 Item development

During the spring 2022 semester 40 assessment items were developed to align with the learning module and measure students' understanding of the particle-level interactions between species in solution, symbolic representations, autoionization of water, acidic strength, pH, and K_a. Some items were based on previous items from the analytical chemistry laboratory quizzes and general chemistry II assessment. Some new items were developed that include pH calculations, K_a expressions, and students' understanding of the autoionization of water. Calculations and K_a expressions are a large part of the analytical chemistry laboratory expectations and course exams and were included in the learning module to help students connect particle-level interactions to symbolic expressions and mathematical equations. The autoionization of water is fundamental to understanding the particle-level behavior of aqueous acids and bases and is covered in General Chemistry II and Analytical Chemistry.

The items were written in Qualtrics XM, a web-based survey instrument, and included follow-up questions to collect validity data. Items included either a follow-up text box below the question for students to explain their reasoning or a prompt to evaluate another student's response for correctness to the same question the student had just answered using a sliding scale from 0-100%. To avoid students changing their own response after seeing another student's answer in the follow-up item, students were unable to go back and change their response. An example of a follow-up item to evaluate another student's response is shown in **figure 4.2**.

Figure 4.2: Example of follow-up item to evaluate another student's response


A student responded to the last question:

What does it mean when we describe an acid as strong?

Select the statement that you agree with most.

By selecting this response:

- A strong acid contains more hydrogen atoms in its structure than a weak acid
- A strong acid is an acid with high concentration in solution.
- A strong acid will ionize completely in aqueous solution.
- A strong acid reacts with any base in solution to yield a solution with pH = 7

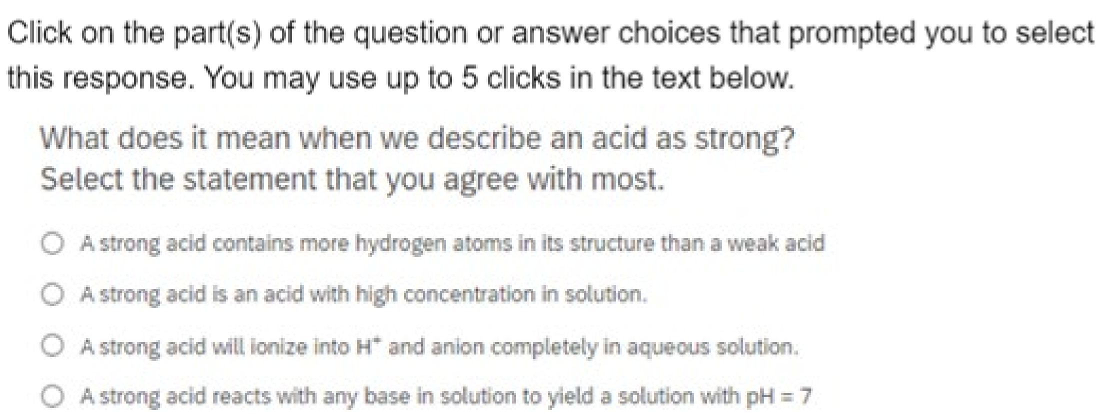
Rate this student's response for correctness from 0 (zero) % to 100% by moving the slider.

0% 100%

Correctness

For additional validity data, all items included a Qualtrics XM heat map follow-up item. Heat map items used an image of the question stem and response options and allowed students to click on the information in the question they focused on when selecting their response. Heat map items were used to indicate any items where students may not be focusing on the intended information to answer the item and indicates a validity threat. An example of a heat map item is shown in **figure 4.3.**

Figure 4.3: Example of a heat map item


Click on the part(s) of the question or answer choices that prompted you to select this response. You may use up to 5 clicks in the text below.

What does it mean when we describe an acid as strong?
Select the statement that you agree with most.

- A strong acid contains more hydrogen atoms in its structure than a weak acid
- A strong acid is an acid with high concentration in solution.
- A strong acid will ionize into H^+ and anion completely in aqueous solution.
- A strong acid reacts with any base in solution to yield a solution with pH = 7

All items were reviewed by content experts to assess content validity and guide revisions. Content experts included two general chemistry II instructors and one analytical chemistry instructor. Review by content experts is one way to show evidence of content validity and supports that the items validly represent the construct being measured (American Educational Research Association, 2014). Content experts reviewed item stems, follow up items, item images, and multiple-choice options.

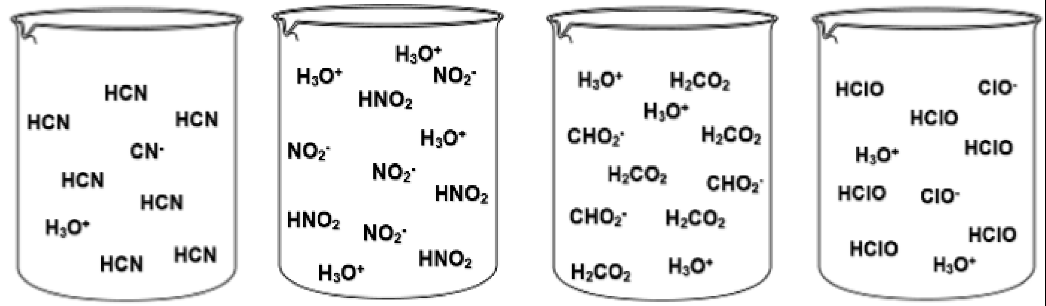
4.3 Revisions

Expert reviewers noted common student errors for calculation and multiple-choice items to use as distractors for multiple-choice options. Some Items needed to be revised for clarity. For example, the question, "*In acid-base chemistry, the* H^+ *ion is also referred to as a proton. Explain why these terms are equivalent.*" was revised to, "*Explain why an* H^+ *ion can also be referred to as a proton*." And "*Interpret the equilibrium expression for water,* $K_W = [H_3O^+][OH^-]$*, using your own words.*" was revised to, "*What does the equilibrium expression for water,* $K_W = [H_3O^+][OH^-]$*, mean in your own words?"* Four items were noted to be repetitive or confusing and were removed.

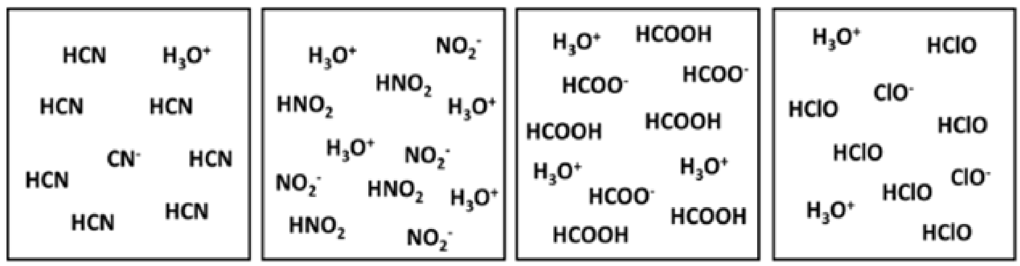
Expert reviewers noted particle-level images should not show beakers and to avoid promoting any possible misconceptions related to the size of particles compared to a size of a beaker. All particle-level images were revised to boxes instead of beakers. The chemical formula for formic acid was also revised to be consistent with the other acid formulas. An example of particle-level image and formula revisions is shown in figure **4.4**.

Figure 4.4: Example of original and revised images and formula (The original formula used for formic acid is shown in the third beaker from the left, the revision is shown in the third box from the left)

Original images



Revised images



The original heat map follow-up items developed included an image of only the question stem. Expert feedback suggested heat map items should include the question stem and response options to collect more validity data and indicate any item stems or response options that may be of concern. Revisions included adding response options to heat map items to allow students to click where they focused on in the response options or question stem. Wording of heat map items was revised to include the number of clicks allowed and be specific to text or images, stating '*Click on the part(s) of the question that prompted you to select your response.*' or '*Click on the part(s) of the image that prompted you to select your response.*'.

Follow-up items with prompts for students to evaluate another student's response for correctness and completeness on a sliding scale between 0-100% originally include a correctness and completeness scale. These items were revised to included only a correctness scale from 0-100%. It was unknown how student would interpret the completeness scale and analysis of this scale would not be meaningful.

The remaining 36 assessment items with follow-up items to collect validity data were implemented with general chemistry II and analytical chemistry students to determine the final items used on the pre- and post-assessment. All 36 items are shown in **appendix E.**

4.4 Assessment implementation

Due to the length of the assessment, the items were split into two assessments to avoid student fatigue. Both assessments were offered to all General Chemistry II and Elementary Quantitative Analysis students through Qualtrics XM for extra credit during weeks 14 and 15 of the spring 2022 semester. Students were recruited by the course instructors in lecture and a QR code and assessment link was posted on Canvas. A total of 115 student participated in assessment one and 81 student participated in assessment two. Students that did not give consent (N=21) or did not complete the assessment (N=27) were removed from the data set. The final data set included data from 87 participants for assessment one and 61 participants for assessment two.

4.5 Coding of assessment items

Students’ responses to open response items and select all multiple-choice items were coded as correct, partially correct, or incorrect using a detailed description for each code. Single response multiple-choice items and calculations were coded as correct or incorrect. **Table 4.1** shows examples of student responses with codes**.**

Table 4.1: Examples of coding with student responses

Code	Description	Example
Item 1) Describe how water behaves as a solvent when the solute hydrogen chloride (HCl) is added to the water to make a solution. Explain how the particles interact with each other.		
Correct	Describes solvation of HCl and interaction with water due to polarity, formation of bonds, H_3O^+, or the hydronium ion	*When HCl is added to water, the water molecules make the HCl dissociate into its ions (H^+ and Cl^-). In this case, water acts as a hydrogen acceptor and becomes H_3O^+. This decreases the pH of the water and becomes more acidic.*
Partially correct	Describes solvation of HCl but does not describe the interaction between species	*The molecules of HCl dissolve and dissociate into Hydrogen ions and Chloride ions. Since this is a strong acid, it dissociates completely.*
Incorrect	Does not answer the question, incorrectly explains interaction, or provides an incorrect species formed	*The water molecules will dissociate the HCl molecules and will compose H2 and Cl-*
Item 17) In acid-base chemistry, the H+ ion is also referred to as a proton. Explain why these terms are equivalent.		
Correct	Clearly explains that the H^+ ion is a single proton	When hydrogen becomes an ion it loses an electron so all that's left is a proton
Partially correct	Identifies the same charge for H^+ and a proton, but does not clearly identify the H^+ as a single proton	Protons are positively charged and H+ has a charge of 1+
Incorrect	No connection between proton and H+, irrelevant or incorrect information	Proton and electron both have to be a part of an ionic equation

4.6 Item validity

Items asking students to rate another student's response for correctness were analyzed for item validity. Due to the variability in students' correctness ratings, all correctness responses were categorized as either a high, middle, or low percent rating to assess the validity of the item and identify any items that may be a validity threat.

The categories were determined through discussion and consensus between the researcher and principal investigator. **Table 4.2** shows the precents included in each category.

Table 4.2: Percent correctness rating categories

Category	Percent rating
High	67-100
Middle	34-66
Low	0-33

If the student's selected response matched the follow-up response to score, it's expected that the student would rate the correctness with a high percent correctness to show agreement with their response. If a student's selected response did not match the student response to score, it's expected that the student would rate the correctness with a low percent to show disagreement. In both of these cases the correctness score provided evidence of item validity and the correctness rating was given a score of 1. If a student gave a rating between 34-66% and their selected response either matched or did not match the student response to rate, they were given a score of 0.5 for validity. Students that gave a low percent correctness when the follow-up response scored matched their selected response or gave a high percent correctness when the response scored did not match their selected response, the correctness rating was given a score of zero to indicate a possible validity threat. The correctness rating scores for an item were summed and divided by the total number of responses to determine a validity score for the item. In addition, all open-response items were coded by the researcher and a single second coder independently, any discrepancies were discussed, and codes were revised to determine the percent interrater agreement to support the validity of the scores.

4.7 Results

Results for the 36 assessment items are shown in **table 4.3**.

Table 4.3: Results for assessment items

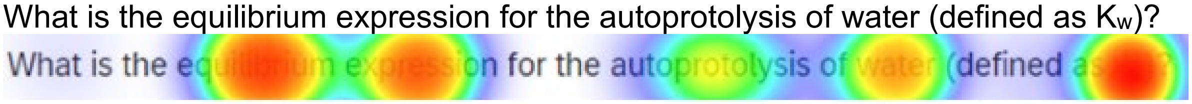
Item	Code	%	% Interrater agreement	Validity score
1	Correct Partially correct Incorrect	29.9 51.7 18.4	95.4	81.2
2	Correct Partially correct Incorrect	48.3 44.8 6.9		87.4
3	Correct Incorrect	77.0 23.0		72.4
4	Correct Partially correct Incorrect	39.1 39.1 21.8	90.8	75.3
5	Correct Incorrect	91.6 8.4		92.0
6	Correct Incorrect	73.0 27.0		95.4
7	Correct Incorrect	66.7 33.3		84.8
8	Correct Incorrect	29.9 70.1		85.3
9	Correct Incorrect	58.6 41.4		83.9
10	Correct Incorrect	69.0 31.0		77.0
11	Correct Incorrect	58.6 41.4		81.6
12	Correct Incorrect	56.9 43.1		93.1
13	Correct Incorrect	42.5 57.5		81.6
14	Correct Incorrect	56.4 43.6		85.5
15	Correct Incorrect	69.8 30.2		96.6
16	Correct	66.7		90.8

Item	Code	%	% Interrater agreement	Validity score
	Incorrect	33.3		
17	Correct Partially correct Incorrect	40.2 12.6 47.5	94.3	83.8
18	Correct Incorrect	98.9 1.1		87.0
19	Correct Incorrect	70.1 29.9		75.9
20	Correct Incorrect	67.8 32.2		69.8
21	Correct Incorrect	85.1 14.9		85.4
22	Correct Incorrect	60.9 39.1		97.7
23	Correct Incorrect	39.1 60.9		82.3
24	Correct Incorrect	29.9 70.1		96.6
25 strong acid	Correct Incorrect	39.3 60.7		83.9
25 weak acid	Correct Incorrect	52.5 47.5		83.9
26 (OR)	Correct Partially correct Incorrect	26.2 31.4 42.4	93.4	Included only heat map follow-up
26 (MC)	Correct Incorrect	68.9 31.1		Included only heat map follow-up
27	Correct Incorrect	6.6 93.4		64.5
28	Correct Partially correct Incorrect	52.5 27.9 19.6	100	80.4
29	Correct Partially correct Incorrect	54.1 29.5 16.4	100	86.6
30	Correct Partially correct Incorrect	60.7 13.1 26.2	96.7	67.8
31	Correct Incorrect	67.2 32.8		80.4
32	Correct Partially correct Incorrect	75.4 13.1 11.5	98.4	Included only heat map follow-up

Item	Code	%	% Interrater agreement	Validity score
33	Correct Incorrect	67.2 32.8		76.8
34	Correct Incorrect	93.4 6.6		87.1
35	Correct Incorrect	65.6 34.4		81.1
36	Correct Incorrect	54.1 45.9		80.85

Results from the heat map items show a color-coded density map to indicate the areas of the item students most frequently clicked on. All heat map images were reviewed for areas of concern. Areas of concern would show a high density of clicks on an irrelevant part of the question such a white area or words that do not contain information needed to answer the item. A valid item should have the highest density of clicks (shown in red) on the most important information needed to correctly answer the item. No heat map images showed areas of concern indicating students focused on the information the researcher intended to respond to the item. These results support the validity of the items. Examples of heat map results are shown in **table 4.4**.

Table 4.4: Examples of heat map results

Item with heat map results
What is the equilibrium expression for the autoprotolysis of water (defined as K_w)? 
Calculate the concentration of H_3O+ in water when the $[OH^-] = 2.90 \times 10^{-7}$ M. ($K_w = 1.0 \times 10^{-14}$) 

Areas with the highest density of students' clicks is shown in red, yellow indicates a moderate number of clicks, green indicates areas with the lowest density of clicks, and white indicates no students selected that area.

4.8 Conclusion

To determine the final pre- and post-assessment items, items that had an 80% validity score or higher were determined to have acceptable validity for use on the pre- and post-assessment. There is no set standard for validity scores determined through evaluation of another student's response and was at the discretion of the researchers. Using the guidelines from Lombard et al. (2002), items with a score less than 80% were considered for revisions or removal. Repetitive items or items that that did not alignment with the learning module were removed. For example, item 29 was removed because the item assessed students' understanding of K_b which is not covered in the learning module. Assessment items that were revised or removed, the reason for the change, and the items included in the final pre- and post-assessment are shown in **table 4.5.**

Table 4.5: Revisions and final pre- and post-items

Assessment Item #	Included in pre- and post-assessment	Revisions		Reason for revision or removal
		Original item	Revised item	
1	Yes	Open response	Multiple-choice	Student's responses used for multiple-choice options
2	Yes	None		
3	Yes	Multiple-choice	Open response	Low validity score
4	No	Removed		Low validity score
5	Yes	Multiple-choice with 2 options	Multiple-choice with 4 options	Repetitive – made into a single multiple-choice item
6	Yes	Multiple-choice with 2 options		
7	No	Removed		Poor alignment with learning module
8	Yes	None		
9	Yes	None		
10	No	Removed		Low validity score
11	Yes	None		
12	Yes	None		

Assessment Item #	Included in pre- and post-assessment	Revisions		Reason for revision or removal
		Original item	Revised item	
13	Yes	None		
14	Yes	Multiple-choice with 6 options	Multiple-choice with 4 options	Removed 2 least selected options
15	Yes	Do these equations represent different reactions	Do these equations below represent different processes?	Revised wording for clarity
16	Yes	Which equation is a more realistic representation of HCl solution?	Which equation represents an aqueous HCl solution more realistically?	Revised wording for clarity
17	Yes	In acid-base chemistry, the H^+ ion is also referred to as a proton. Explain why these terms are equivalent	Explain why an H^+ ion can also be referred to as a proton.	Revised wording for clarity
18	Yes	None		
19	Yes	What does it mean when we describe an acid as strong? Select the statement you agree with most	Select the statements that are true for a strong acid	Low validity score
20	No	Removed		Low validity score
21	Yes	None		
22	Yes	Calculation question with autoionization follow-up	Separated into two successive items	Individual numbering of each item
23	Yes	None		
24	Yes	Multiple-choice item with autoionization follow-up	Separated into two successive items	Individual numbering of each item
25	Yes	The same concentration of four different acids are shown below in aqueous solution. Based on these particle images, which acid is the strongest and which acid is the weakest?	The same concentration of four different acids are shown in the images below. Judging by the images, which acid is the strongest and which acid is the weakest?	Revised wording for clarity
26	Yes	Open response with multiple-choice follow up	Separated into two successive items	Individual numbering of each item

Assessment Item #	Included in pre- and post-assessment	Revisions		Reason for revision or removal
		Original item	Revised item	
27	Yes	Compare the structures of the three acidic molecules shown below. Rate the molecules form most acidic (1) to least acidic (3)	Compare the structures of the three acids below. and rate the acids from most acidic (1) to least acidic (3)	Revised wording for clarity
28	No	Removed		Poor alignment with learning module
29	No	Removed		Poor alignment with learning module
30	No	Removed		Poor alignment with learning module
31	Yes	None		
32	No	Removed		Poor alignment with learning module
33	Yes	Select the statement that is incorrect about the fraction of dissociation.	Select all the statements that are incorrect about the fraction of dissociation.	Revised wording for clarity
34	No	Removed		Poor alignment with learning module
35	Yes	None		
36	Yes	Multiple-choice item with multiple choice follow-up	Separated into two successive items	Individual numbering of each item

The final pre- and-post-assessment consisted of 30 items in the areas of the autoionization of water, acidic strength, pH, and K_a. The pre- and post-assessment items are shown in **appendix F.**

4.9 Limitations

Some acid-base concepts included in the learning module, such as the ionization of a strong base in solution and the relationship between pH and pOH, are not covered in the pre- and post-assessment items. Learning gains in these areas cannon be measured with the final 30 assessment items. Additional data to establish response process validity of the items, such as response process interviews, was not collected.

Chapter 5: Development of Novel 3-Dimensional Acid-Base Models

5.1 Methods

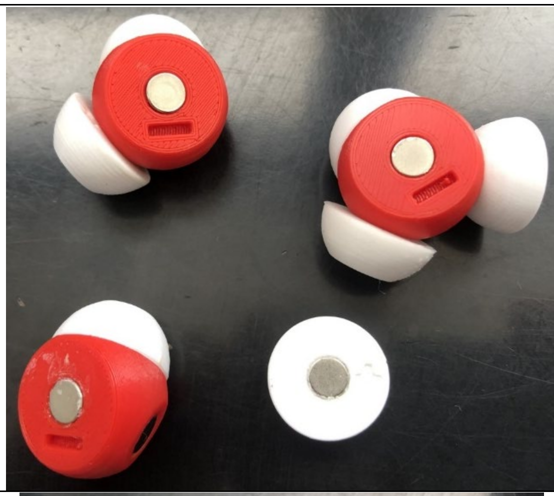
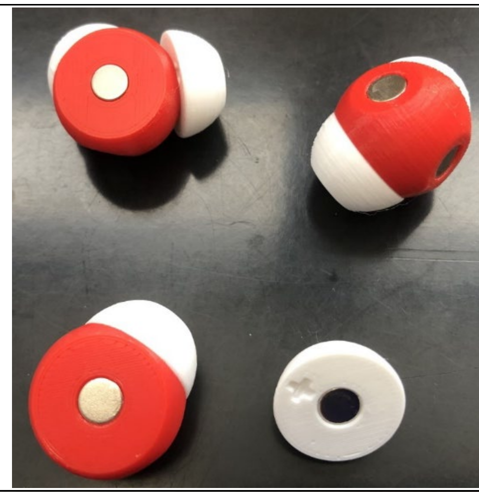
Following the determination to focus on acid-base chemistry, the researcher listed acid and base species used in the analytical laboratory experiments. Different processes occurring in the laboratory experiments were discussed with the principal investigator (i.e., strong and weak acid ionization, acid-base indicator function, and interactions with water molecules) to brainstorm which species should be used to model particle-level processes and interactions. The principal investigator already had magnetic water molecules embedded with magnets to model the attraction between water molecules, but these pieces did not easily come apart in hydrogen and hydroxide ions. Model pieces embedded with magnets to show the movement of the proton between species and the ionization of aqueous acid and base molecules would allow students to build their own models of acid and base solutions for modeling-based teaching.

A meeting was held with model design experts from 3D Molecular Designs in Milwaukee, Wisconsin (formerly the Center for BioMolecular Modeling), the researcher, and the principal investigator to discuss the development of the novel 3-dimensional acid-base model set using 3D printed pieces with removable parts embedded with magnets.

Using the online software, Molecule Maker from 3D Molecular Designs, virtual space-filling 3-dimensional models were built for all desired molecules and species to be included in the model set. These virtual representations were sent to 3D Molecular Designs where a prototype set of models were 3D printed and embedded with magnets. The prototype model set included acidic, basic, and amphiprotic species. Models were printed with a plus sign on each hydrogen atom that would become visible when the hydrogen was removed to indicate charge. After removal of a hydrogen atom from a water molecule a negative sign was visible on the oxygen atom. Nickel coated neodymium magnets of the same strength and size were placed in all atoms except for chlorine in HCl and sodium in NaOH, which were embedded with very weak ceramic disk magnets to model a difference in acidic or basic strength.

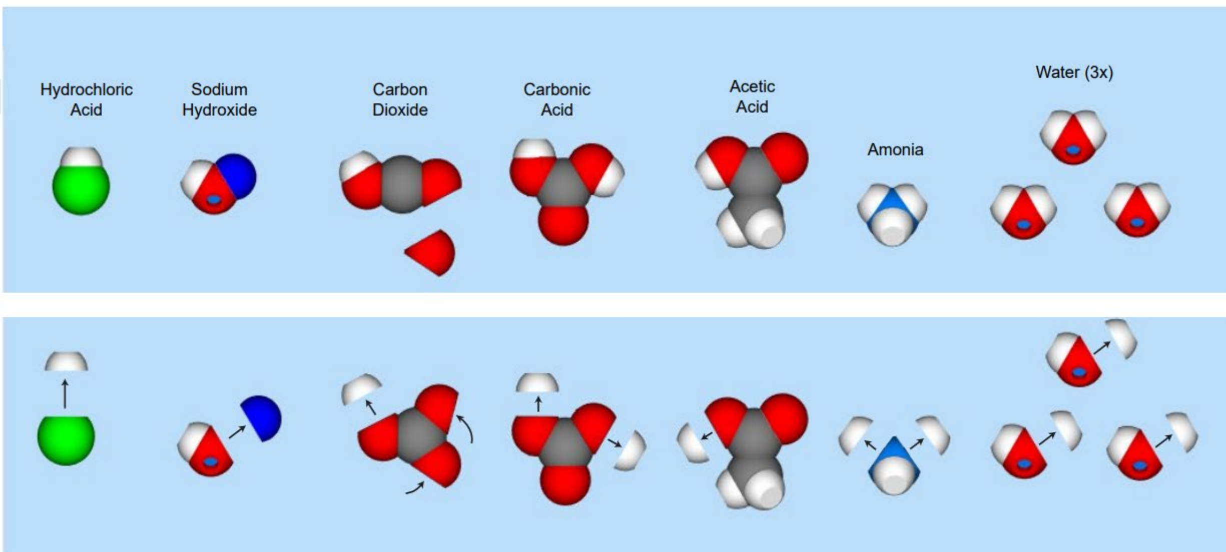
Experimentation with the model prototype was done to investigate how they functioned to modeled interactions between particles and any model pieces that did not function as expected were noted. Another meeting was held to discuss revisions to the prototype. Revisions included the addition of an indicator molecule to align with laboratory experiments and the removal of the negative sign on the oxygen atoms. The negative sign on the oxygen atom was removed to eliminate any possible confusion about charge. A hydrogen atom could be attached to any free magnetic spot on a water molecule, allowing a model of a neutral water molecule showing a negative sign to be made or an H_3O^+ model with a negative charge still visible on the oxygen atom. An image of this can be seen in **figure 5.1**. To indicate the charge left after ionization of HCl and NaOH, a negative sign was added to the chlorine atom and a positive sign to the sodium atom that was only visible after the removal of the hydrogen or hydroxide group. It was found that the weak ceramic magnets in the chlorine and sodium atoms were too weak in comparison to the nickel coated neodymium magnets causing the hydrogen to fall off or separate unintentionally. The revised strong species were embedded with smaller nickel coated neodymium magnets that would still model a difference in strength but were strong enough to keep the HCl and NaOH models together until the hydrogen or hydroxide group were intentionally removed by the user. These revisions are shown in **figure 5.1**.

Figure 5.1: Prototype and revised model pieces. (Top images: prototype and revised models of water molecules showing removal of negative sign on the oxygen atom. Bottom images: prototype and revised models of chlorine and sodium atoms showing addition of negative and positive sign and change from ceramic magnet to small neodymium magnets.)

Initial model	Revised model
	
	

The revised list of modeling pieces was sent to the design experts at 3D Molecular Designs to be 3D printed and embedded with neodymium magnets. **Figure 5.2** show the virtual rendition of the three-dimensional models to be printed by 3D Molecular Designs.

Figure 5.2: Virtual rendition of three-dimensional models for 3D printing



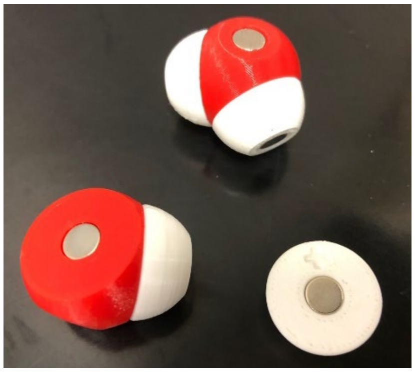
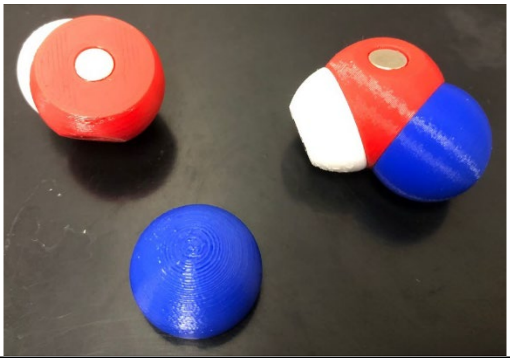
5.2 Model set design specifications

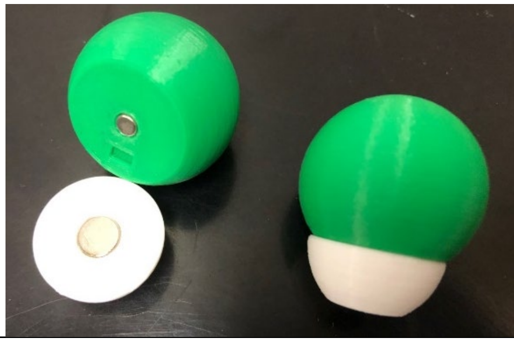
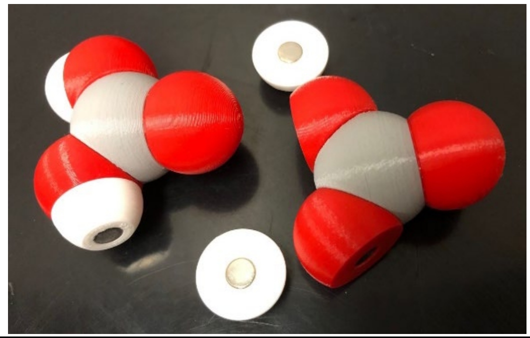
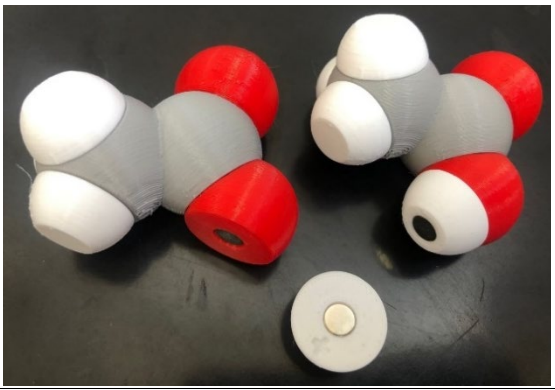
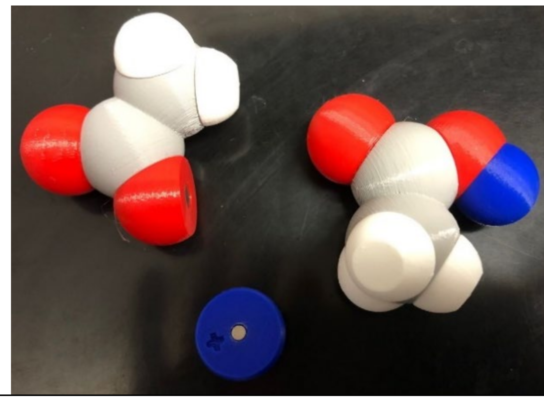
The model pieces were designed using two software programs: 1) Jmol, the open-source molecular visualization program (created by Bob Hanson at St. Olaf University) and 2) Materialize Magics, a 3D file editing CAD program from the company Materialize. The model set was built using PRUSA Mk3 printers with polylactic acid plastic (PLA) 3D printing filament. Model pieces were embedded with neodymium nickel-coated magnets using cyanoacrylate super glue, a thick gel glue.

5.3 Final model set

The final model set 3D printed and used for this study included nine acid-base species and extra hydrogen atoms. All hydrogen atoms and weak acids or bases were embedded with larger (stronger) neodymium nickel-coated magnets. Magnets were placed with the positive or negative side up to match the attraction between species. This allowed the protons to easily attach to a magnet in an oxygen, nitrogen, or chlorine atom and repel other positive species. The indicator molecules were made as rectangular prisms to represent a universal indicator and were embedded with stronger magnets with one end of the indicator molecule imbedded with the positive side of the magnet pointing out and the other end of the indicator molecule embedded with the negative side of the magnet pointing out to allow each indicator molecule to act as both an anionic and cationic species. **Figure 5.3** shows images of all species printed for the final model set.

Figure 5.3: Images of final acid-base model pieces

Model pieces	Model pieces
Water 	Sodium hydroxide 

Hydrogen chloride 	Carbonic acid 
Acetic acid 	Sodium acetate 
Carbon dioxide 	Universal indicator 
Ammonium 	

5.4 Limitations of model set

The two different strengths of the embedded magnets model only two different bonding strengths. This could potentially lead to a misconception that all weak or all strong species have the same bond strength instead of the range of bond strengths that exist in nature. The models can be used to build species that do not exist in nature. This could be both a benefit and limitation depending on how the model set is used to support learning. Instructor led or small group discussions of the student-built models may support students' understanding of the different characteristics and features that determines if a species can exist in nature.

Chapter 6: Development of Learning Module

6.1 Introduction

The learning module development was guided by the Understanding by Design Framework by Wiggins & McTighe, 2012. The Understanding by Design Framework is supported by research in cognitive psychology and student achievement studies. A key component of this framework is planning 'backwards' in three stages completed in order: 1) What are the desired results*? "What should students know, understand, and be able to do?"*, 2) What will be acceptable evidence of student understanding and learning? And 3) Plan learning activities and instruction (Wiggins & McTighe, 2012). Planning the instruction after identifying the learning goals (stage 1) is essential to plan the most appropriate learning activities to address the identified goals. Following the Understanding by Design framework structured the learning module and modeling exercises to align with the desired learning outcomes.

6.2 Methods

The learning module: *Autoprotolysis (autoionization) of water and acid-base strength,* was developed to be completed in small groups of 3-4 students in a laboratory or active learning classroom using the novel 3-dimensional acid-base models. The development of the learning module was based on three lesson goals following the Understanding by Design Template written to address learning gaps identified in the qualitative research. **Table 6.1** shows the three lesson goals for the learning module: *Autoprotolysis (autoionization) of water and acid-base strength*.

Table 6.1 The three lesson goals following the Understanding by Design Template

Lesson Goal(s)	Learning objectives	Evidence of learning
1) Apply the acid-base properties of water to explain the particle-level interactions between water molecules and the autoionization of water.	• Modeling the autoionization of water • Connect particle-level models and to symbolic representations • Apply the K_w expression to calculate H^+ or OH^- concentrations	• Particle-level images of student-built models of the autoionization of water • Responses to connection items after modeling the autoionization of water • Calculations using K_w
2) Calculate the pH of strong acids and bases, identify the species being measured, and connect the particle-level and symbolic representations of acid and base ionization.	• Modeling strong acid and base solutions • Connect a change in H_3O^+ concentration to a change in pH value • Apply the symbolic representations H^+ and H_3O^+	• Particle-level images of student-built models • Calculate the pH of strong acid and base solutions • Responses to connection items relating the student-built models to symbolic representations
3) Calculate the pH of weak acids, identify the particle-level features of strong and weak acids that influence acidic strength, and explain the relationship between acidic strength and K_a values	• Modeling the ionization of weak acids in solution • Apply the K_a value to pH calculations for weak acids in solution • Identify different structural features of strong and weak acids	• Particle-level images of student-built models of weak acid solutions • Calculate the pH of weak acid solutions • Responses after comparing the models of strong and weak acids

6.2.1 Learning module alignment with lesson goals

The learning module included six modeling activities that aligned with the three lesson goals. The six modeling activities developed are:

1. Modeling activity 1: Autoionization of water
2. Modeling activity 2: Strong acid solution
3. Modeling activity 3: Dilute strong acid solution
4. Modeling activity 4: Strong base solution
5. Modeling activity 5: Weak acid solution
6. Modeling activity 6: Comparison of strong and weak acids

The alignment of the three lesson goals with the modeling activities, evidence of learning, and the pre- and post- assessment items in the areas of the autoionization of water, acidic strength, pH, and K_a is shown in **table 6.2.**

Table 6.2: Alignment of lesson goals

Lesson Goal	Modeling activity alignment	Evidence of learning	Assessment item alignment
1	• Modeling activity 1: Autoprotolysis of water	• Particle-level drawings of the autoprotolysis of water • Symbolic expressions • Calculation table	• Autoionization • pH
2	• Modeling activity 2: Strong acid solution • Modeling activity 3: Dilute strong acid solution • Modeling activity 4: Strong base solution	• Particle-level drawings of a strong acid solution, dilute strong acid solution, and strong base solution • Symbolic expressions • Autoprotolysis and K_a connection items • Calculation tables	• Acidic strength • Autoionization • K_a • pH
3	• Modeling activity 5: Weak acid solution • Modeling activity 6: Comparison of strong and weak acids	• Particle-level drawings of a weak acid solution • pH calculation of a weak acid solution • Items comparing strong and weak acids	• Acidic strength • pH • K_a

The first modeling activity, the autoprotolysis of water, prompted students to use the models to investigate the autoprotolysis of water and different species present in pure water. After students built their model representing the autoprotolysis of water, follow-up items connected students' models to particle-level images by having each group draw a particle-level representation of the model they made. Additional items connected the particle-level image drawn by students to the symbolic representation, the K_w expression, and pH calculations. Students' particle-level images, symbolic representations of the autoprotolysis of water, and pH calculations using the K_w expression provide evidence of learning.

To address lesson goal 2, modeling activities 2, 3, & 4 focused on strong acid and strong base solutions. Students are prompted to model each type of solution and to draw particle-level images of their model, followed by the symbolic representation for the solution modeled. These particle-level images and symbolic representations are to support connections between the particle-level and symbolic representations and to provide evidence of learning. To address the learning objective: *Connect a change in H_3O^+ concentration to a change in pH value*, several tables were included in the learning module prompting students to solve for either pH, $[H_3O^+]$, or $[OH^-]$. The tables showed patterns between the concentration of H_3O^+, OH^-, and pH values to help students connect calculations to the particle-level process modeled.

Modeling activities 5 and 6 aligned with lesson goal 3 and focused on weak acid solutions and the differences between strong and weak acids. In modeling activity 5, students are prompted to model an acetic acid solution, draw a particle-level image of their model, write the K_a expression, and solve for pH using an ICE table. Modeling activity 6 focuses on the comparison of the different magnet strengths of the strong acid models (HCl) and the weak acid models (water, acetic acid, and carbonic acid), to support students' connections between the strength of the magnet embedded in the model to different bonding strengths in strong acid and weak acids. Due to the different strengths of the magnets in the models, students can feel the hydrogen atom is easier to remove from the model of HCl compared to acetic acid or water. Particle-level images and responses to follow-up items are to provide evidence of learning.

6.3 Revisions

The developed learning module was completed by the researcher using the model set to trial the modeling activities and check for clarity of item prompts, alignment with learning objectives, and identify any items that may need to be revised. For example, the six modeling activities prompted students to build their model on a magnetic whiteboard. However, after trialing the modeling activities with the whiteboard it was found that the models were easier to work with without the whiteboard. This allowed more space for students to make their model using more pieces to show different interactions and species, as well as, lessened the number of supplies needed to complete the learning module. Some repetitive calculations were removed from the calculation tables to reduce time spend on calculations and allow students more time to focus on the modeling activities and connections to the symbolic representations. The revised tables still included enough calculations to shown patterns between the concentration of H_3O^+, OH^-, and pH values. After initial revisions by the researcher, the learning module was reviewed by the principal investigator. The researcher and principal investigator discussed each modeling activity and all items to identify additional revisions needed to clarify prompts, make connections between the modeling activity and the particle-level and symbolic representations, and to ensure alignment with all learning goals.

6.4 Results

The revised draft of the learning module included six modeling activities that addressed all learning objectives identified for the three lesson goals using the Understanding by Design Framework. The number of items in each modeling activity, and the models students are expected to use to complete each activity are listed in **table 6.3.**

Table 6.3: Number of modeling activity items and expected model use

	Modeling activity					
	Autoprotolysis	Strong acid solution	Dilute strong acid solution	Strong base solution	Weak acid solution	Comparison of strong & weak acids
Number of items*	17	8	5	8	13	5
Expected model use	• Water	• Water • Hydrogen chloride	• Water • Hydrogen chloride	• Water • Sodium hydroxide	• Water • Acetic acid	• Water • Hydrogen chloride • Acetic acid • Carbonic acid

*Some items include multiple prompts

The learning module was developed to be completed in approximately 90 minutes; however, the total time needed and the time to complete each activity was unknown since the learning module had not been tested yet with students. Focus groups would be conducted to investigate the usability of the learning module items, the time needed to complete learning module, and guide item revisions. The revised version of the learning module that was tested by the focus groups is shown in **appendix G**.

Chapter 7: Learning Module Validation: Focus Groups

7.1 Introduction

To investigate the usability of the modeling activities, identify items for revisions, and validate the learning module, focus groups were conducted with general chemistry II students. The focus groups were conducted to investigate the five questions below about the learning module.

1) Do models function as intended and are used as expected?
2) What time is needed to complete the learning module?
3) Do students find the activities helped them understand acid-base chemistry?
4) Are the directions and questions clearly worded and functioned as intended?
5) What revisions should be made to the learning module before implementation?

7.2 Methods

Data reported from focus groups was collected under IRB approval #23.008. All participants consented and agreed to be audio and video recorded. To investigate the usability of the learning module (shown in appendix G), seven focus groups were conducted with a total of 25 participants in the summer 2022 semester with general chemistry II students. General chemistry II students were selected for focus groups because they were enrolled in the summer semester and had recently been instructed and assessed in all acid-base areas included in the learning module. The researcher and principal investigator recruited students using a short informational PowerPoint (about five minutes) presented at the beginning of their lecture. A request for volunteers was also posted by the course instructor online, and two additional recruitment emails were sent to students. Participants received a $20 gift card to the university gift shop for participating. Each focus group was scheduled for 90 minutes in a conference room and was audio and video recorded. All students that consented to be in a focus group were divided into groups of 3-5 participants according to their availability.

Each focus group had one facilitator and one observer to take notes during the focus group. Observers were chemistry graduate students. Four observers were trained by the facilitator and one observer was present for the entire duration of each focus group. The facilitator brought all supplies, collect consent forms, and remained present to answer questions from participants, monitor the camera, and take notes. Focus group observers and the facilitator took notes using a focus group observation rubric. In addition, participants were given an exit survey to complete individually.

7.2.1 Focus group observation rubric

To collect additional data during the focus groups an observation rubric was written to align with each question in the learning module so observers could easily take notes. This rubric was developed using the guidelines outlined by the Enhancing Learning by Improving Process Skills in Stem project (ELIPSS) (Lantz et al., 2019). To keep track of the timeline, the observation rubric had a place to note the time each page of the learning module was started by the focus group. To collect data on any items students' needed clarification to complete or skipped and how often focus group participants interacted with the modeling pieces, the rubric consisted of specific criteria listed in a column next to each question: asked for clarification, skipped question, and interacted with modeling pieces, for the observer to easily check each criterion observed. An additional box was provided by each question for observers to note other important observations. A copy of the observation rubric is shown in **Appendix H.**

7.2.2 Focus group observer training

Prior to the focus groups, each observer was given a copy of the learning module and observation rubric to review and attended an online zoom training taught by the facilitator. The training familiarized observers with the modeling activities, the model pieces, and instructed observers how to document time, use the observation rubric, and the kind of notes that would be helpful. For example, if a student asked for help or clarification, observers were asked to note what was unclear and the question number. The facilitator was responsible to answered students' questions and provided clarity as needed during the focus groups to allowed observers to note unclear items and the students' questions while the facilitator interacted with participants to clarified the expectations of the item.

7.2.3 Focus group exit survey

A draft of the focus group exit survey was developed by the researcher using guidelines outlined by Morgan (1997, p. 23-29) and designed to capture students' comments on four aspects of the learning module based on individual participant feedback. The exit survey items were revised by the principal investigator to develop the final exit survey questions. Revisions included updated wording for clarity and the addition of a four-point Likert scale (strongly agree, agree, disagree, strongly disagree) to rate statements about the learning module. The four aspects investigated on the exit survey are listed below.

1) The use and function of the magnetic model pieces
2) If students felt the learning module helped them understand acid-base concepts and make connections to particle-level interactions, symbolic representations, and mathematical expressions.
3) If students thought completing the activity as a group was helpful.
4) The clarity of the instructions in the activity.

The final exit survey consisted of six statements with a 4-point Likert scale and three open-response items. The Likert scale did not include a neutral response for clearer analysis and instead included a space next to each statement for students to explaining why they selected that rating. The exit survey is shown in **appendix I.**

7.3 Focus group implementation

Each focus group was given 5 individual, unlabeled bags with models. One bag with 20 H_2O molecules and four additional bags each with eight models of HCl, NaOH, CH_3COOH, and H_2CO_3. A group learning module was completed by each focus group. After collecting consent forms from each participant and providing instructions, which took approximately 10 minutes, the first two focus groups worked through the modeling activities for 90 minutes. These two focus groups were not able to complete all activities in 90 minutes and participants stated they need to leave due to other obligations. Since the focus groups were schedule for 90 minutes and that time had already been exceeded, the first two focus groups did not complete the exit survey. The remaining focus groups were instructed which activities to complete to ensure data was collected from at least three focus groups for each of the six modeling activities. All participants in the remaining five focus groups completed the exit survey individually. All focus groups completed all or part of modeling activity 1, the autoprotolysis of water, to ensure they could answer connection questions in the other modeling activities. **Table 7.1** shows the model activities completed by each focus group.

Table 7.1: Modeling activity completion by focus group

	Group size	Activity 1: Autoprotolysis	Activity 2: Strong acid	Activity 3: Dilute strong acid	Activity 4: Strong base	Activity 5: Weak acid	Activity 6: Comparison of strong & weak acids
FG 1	4	1	1	1	1	0	0
FG 2	4	1	1	1	1	0	0
FG 3	3	0.75	1	1	1	0.5	0
FG 4	2	0.5	1	.5	1	0.5	1
FG 5	5	1	0	0	0	1	1
FG 6	4	1	0	0	0	1	1
FG 7	3	1	0	0	0	1	1
Total	25	6.25	4	3.5	4	4	4

A value of 1 indicates the group completed the activity, a 0.75 or 0.5 indicates the group completed about 75% or 50% of that activity, and a value of zero indicates the group did not complete any of the activity.

7.4 Results

7.4.1 Do models function as intended and are used as expected?

Review of the focus group videos and observation rubrics indicated the only issue experienced with the modeling pieces was a few magnets falling out of models. Review of the videos showed that no group used all the modeling pieces provided for any corresponding activity. For example, no group used all 20 water molecules to model the process of autoprotolysis. Groups that initially removed all 20 water molecules from the provided bag pushed some aside and used between 12-15 models, while other groups only removed 10-15 water molecules from the bag to complete the activity. To complete the other modeling activities, no group used greater than five models of HCl, NaOH, CH_3COOH and H_2CO_3. Some participants asked another group members or the facilitator what models were in different bags. These observations indicate fewer model pieces were needed to complete the learning module and labels on the bag of each model would be beneficial.

Items 7 and 8 on the exit survey asked participants about the use of the models. Item 7 asked students, '*What in your opinion, is the reason the models include magnets?*' Responses stated the magnets represented intermolecular forces, bonding, attraction, or to connect model pieces. Example responses are shown below:

Student 1: *"To connect different groups & magnets represent intramolecular forces."*

Student 2: *"The magnets demonstrated the strength of the bond attaching the hydrogen atom."*

Student 3: *"For better understanding of bonding."*

Item 8 asked, '*Did you experience any issues while using the modeling pieces? Please explain.*' 10 students (59%) responded "*no"* to this item. The remaining comments indicated the only issue was some magnets falling out of the model pieces. One student commented, "*Some magnets came off*." And another student wrote, "*Just some magnets coming lose.*"

These results show the magnetic models worked as intended, except for a few magnets needing more glue, and students understood what the magnets represented and were able to make connections between magnet strength and bond strength.

7.4.2 What time is needed to complete the learning module?

The time to complete each modeling activity was documented on the observation rubrics. This data helped determine the timeline for implementation with analytical chemistry students. **Table 7.2** shows the time (in minutes) for each group to complete each modeling activity and the average time (rounded to the nearest minute). (Only groups that completed the activity are included in this data.)

Table 7.2: Modeling activity completion times in minutes

	Intro page	Activity 1: Autoprotolysis	Activity 2: Strong acid	Activity 3: Dilute strong acid	Activity 4: Strong base	Activity 5: Weak acid	Activity 6: Acidic strength
FG 1	5	41	16	5	23		
FG 2	2	45	18	5	17		
FG 3	3		22	5	12		
FG 4	2		20		19		12
FG 5	2	34				14	15
FG 6	4	37				27	10
FG 7	3	30				27	12
Avg.	3	37	19	5	18	23	12

All groups took the most time to complete activity one. The first page of activity one, which included a table to draw different species possible from the autoprotolysis of water, took each group the most time in activity 1 (between 9-15 minutes). In modeling activity four, groups took the most time to complete the page with the calculation table (between 7-15 minutes). All groups completed modeling activity three in five minutes. Modeling activity three was the shortest modeling activity with the fewest items and calculations. None of the groups were able to complete the entire learning module in 90 minutes. It was expected that general chemistry II students will take more time to complete the learning module compared to analytical chemistry students because analytical chemistry students will have completed additional instruction and laboratory experiments in acid-base chemistry prior to implementation. The difference in the amount of time need to complete all activities between student populations is unknown. However, the average time for general chemistry II students to complete all activities was 117 minutes and indicates the need to reduce the time needed to compete the learning module. Results show revisions to modeling activity one and removal of repetitive calculations will reduce the total time needed to complete the learning module.

7.4.3 Do students find the activities helped them understand acid-base chemistry?

Exit survey item two investigated students' thoughts about the use of the models to make connections to particle-level and symbolic representations using a statement with a 4-point Likert scale and open-response explanation. Exit survey item two is shown below.

Circle how much you agree or disagree with the statement below.

2. *The modeling activities helped me to connect particle-level interactions to symbolic representations and/or mathematical expressions or calculations.*

Strongly agree
Agree
Disagree
Strongly Disagree

Indicate for which questions you think the models helped make important connections and solve problems.

Exit survey data showed 16 out of 17 students (94%) thought the modeling activities helped them make connections between the particle level and the symbolic or mathematical expressions, with 41% marking strongly agree and 53% marking agree. One student disagreed with this statement and provided no explanation for their response. Eight out of 12 students that provided an explanation for why they agreed with the statement indicated activity six, comparing strong and weak acids, for where the models helped them make important connections and solve problems. Other responses included modeling autoprotolysis, strong acids, weak acids, and bonding strength. Examples of student comments are shown below.

Student A: "*Modeling the autoprotolysis*."

Student B: "*The last questions, especially comparing HCl and acetic acid.*"

Student C: *"Towards the end I began to gain a better understanding of how a strong versus a weak acid interact with water on the particle level."*

Activity 6 was indicated to be helpful most frequently by students. This activity did not include any calculations, suggesting students were using the models to make connections between the modeling pieces (magnetic strength) and the particle-level behavior of weak and strong acids.

Exit survey questions 3 and 4 investigated if students thought the modeling activities helped them learn specific acid-base concepts using a Likert scale and open response explanation. Exit survey items 3 and 4 are shown below with their results.

3. *The modeling activity gave me a deeper understanding of interactions between water molecules in autoprotolysis.*

Strongly agree
Agree
Disagree
Strongly Disagree

Please explain what new information you have learned.

All but one student indicated that the modeling activity gave them a deeper understanding of autoprotolysis, with 7 students (41%) selecting *strongly agree* and 9 student (53%) selecting *agree*. One student selected disagree for this statement and provided no reason for their choice. Nine out of 16 students that strongly agreed or agreed provided an explanation. Two students indicated they learned the meaning of the word autoprotolysis. Some representative examples of other students' explanations are shown below.

Student 1: "*Water interacts with itself in more ways than I knew.*"

Student 2: "*The way a proton is transferred between H_3O^+, H_2O, & OH^-*"

4. *The modeling activity gave me a deeper understanding of acid and base strengths.*

Strongly agree
Agree
Disagree
Strongly Disagree

Please explain what new information you have learned.

Most students strongly agreed (24%) or agreed (65%) that the modeling activity gave them a deeper understanding of acid and base strength. Five students that strongly agreed or agreed explained that acidic strength is influenced by bond strength, other students explained that periodic table trends influence acidic strength or that the modeling activity helped them connect acid-base strength to the particle-level. Some examples of student responses are shown below.

Student 3: "*It helped visualize what's going on in the particulate level."*

Student 4: "*The influence of bonding character influences acid strength."*

Only 2 out of 17 students disagreed with the statement in item 4 and only one of these students provided and explanation stating, "*My chem prof. was awesome & this was a nice review."* The results and students' comments show most students feel the modeling activities helped them understand the autoprotolysis of water and acidic strength.

Since the learning module was written with the intent to be done in small groups of about 3-4 students, item 5 and 6 from the exit survey were analyzed. Items 5 and 6 are shown below with a discussion of their results.

5. *It helped me to complete the activity as a group.*

Strongly agree
Agree
Disagree
Strongly Disagree

Please explain your answer.

The majority of students, 14 out of 17 (82%), felt that completing the activity as a group was helpful. Three students selected agree and 11 students selected strongly agree. Seven out of 14 students that agreed or strongly agreed provided an explanation for their response. Explanations indicated that it was easier to learn as a group, the group knew more together than individually, or it was more fun as a group. Three students selected "disagree" with two students providing an explanation for their choice. Example responses are shown below, student A and B both thought completing the modeling activity as a group was helpful, student C and D selected disagree.

Student A: "*It was helpful building our ideas off of each other.*"

Student B: "*It was fun, and helps to talk through problems and brainstorm together.*"

Student C: "*I had different thoughts on some, but I felt the group wanted to quickly finish, so I can only keep going.*"

Student D: *"There was lowkey tension & I didn't want to argue."*

6. I could have completed the activity easily on my own.

Strongly agree
Agree
Disagree
Strongly Disagree

Please explain your answer.

Item six further investigated if students thought completing the activity as a group was helpful. Most students, 10 out 17 (59%), said they disagreed or strongly disagreed that the activity could have been easily completed on their own. Students explained that it was helpful to work as a group or that they did not remember enough acid-base chemistry to complete the activities on their own. One student wrote, "*I got a better understanding of a lot of concepts through listening to what peers had to say.*"

Out of the 7 students that agreed the activity could have easily been completed on their own, three students explained the reason for the response. The explanations provided by the three students that selected agree are shown below.

Student 1: "*If I was to use my phone as a resource.*"

Student 2: "*I could have completed it but not as well.*"

Student 3: "*I could have, but it's more fun as a group.*"

The results from items five and six support the intended use of the learning module as a group activity. All explanations from students that indicating they could have easily completed the activity on their own state that they would have need an additional resource, they would not have completed it as well on their own, or it was more fun to as a group, further supporting the intended use of the learning module as a small group activity.

7.4.4 Are the directions and questions clearly worded and functioned as intended?

7.4.4.1 Item validity

Item validity measures the extent to which each learning module item functions as the researchers intended. Do students complete the item by using the models expected, drawing particle-level images when prompted, writing symbolic representations, completing calculations, or providing reasoning? Analysis of individual responses provide evidence an item matches the intention of that item (American Educational Research Association, 2014). Responses for each item were analyzed. A variety of responses is expected, both correct and incorrect, but should match the intention of an item. Students' particle-level drawings, work shown, and explanations of reasoning provide evidence the item was interpreted as intended by the researchers.

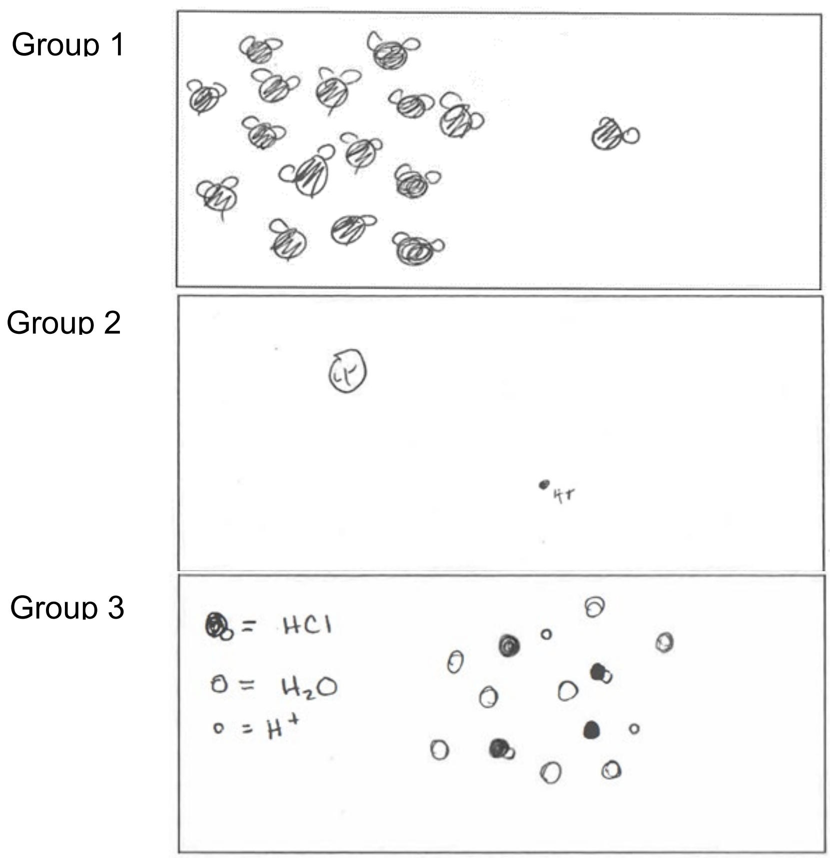
Item one in modeling activity one was intended to prompt students to use only water molecules to model the autoprotolysis of water and show different species that exist due to this process. Several groups asked for clarification of how to complete the table in item one and two groups used modeling pieces other than water molecules including NaOH, HCl, and CH_3COOH. This shows that item one in modeling activity one did not functioning as intended.

Items four and five in modeling activity one and items two and three in modeling activity five asked students to use the models to show a process and then write the symbolic expression to match that process. These items were not completed as intended. For example, in modeling activity five, students are prompted to models the chemical equation showing the ionization of acetic acid in water and then write the symbolic representation modeled. Out of five groups that competed this section, two groups completely skipped using the models and went right to the symbolic expression, and one group started to build a model and then completed the symbolic expression without completing the model as prompted.

Responses and particle-level images from modeling activity three showed items in this activity were not functioning as intended. The intention of these items was to connect the particle-level processes of a very dilute acid solution (ionization of HCl and the autoprotolysis of water) to the solution's pH. One group did not draw a particle-level image of their model. Review of the video and observation rubric showed this group never used the models for this activity and skipped directly to the calculation questions. All groups were prompted by the facilitator to think about the number of HCl and water models to use to model a dilute acid solution. The item prompt and images from the three groups that completed this item are shown in **figure 7.1.**

Figure 7.1: Modeling activity three item one

1. *Use hydrogen chloride molecules and water molecules to model a dilute HCl solution.*
   Consider a 2.3 x 10^{-9} M hydrochloric acid solution. Use all the water molecules in your kit. Consider the concentration of this HCl solution (2.3 x 10^{-9} M). Discuss with your group and decide how many HCl molecules should be used to model this solution then draw the model in the box below.



The students' particle-level images of their model show one group did not include water and two images show unionized HCl. All groups calculated a basic pH in the follow-up calculation item and only one group indicated the basic pH was not reasonable for an acidic solution writing, "*No, too high, the pH of water is 7 how can it* *go up to basic?*" Students' responses to item four in modeling activity three: *Using your models, discuss any other processes and species that could contribute to the pH of the solution. Write down your answers below*. Showed that three groups did not reply to this follow-up question.

Particle-level images drawn by students for item one in modeling activity three and responses to item four indicate that these items did not function as intended and no group made the connection between the pH calculation for a very dilute acid solution to the process of autoprotolysis. Both items are a validity threat and need to be revised before implementation.

7.4.4.2 Observation rubric data

Data from the observation rubrics included items students skipped and any items participants asked for clarification to complete. For example, two observers noted students asked for clarification of the phrase *'separate species'* for item six in activity one. It was noted for item two in modeling activity five that the group did not build the equation with the models. Other notes from observers included students' unfamiliarity with the term *autoprotolysis*, and clarification for item one in modeling activity one. A total of 12 items were noted by observers. The items noted by observers are listed in **table 7.3**.

Table 7.3: Items noted on observation rubric

Reason item was noted	Item(s)
Needed clarification	1.1, 1.3, 1.5, 1.6, 1.8, 4.3, 5.3, 5.7, 6.1, 6.2
Skipped	1.4, 5.2,

*The first number is the modeling activity followed by the item number (i.e. item 1.8 is item 8 in modeling activity 1).

7.4.4.3 Exit survey data

Exit survey item 1 provided students an opportunity to assess the clarity of the instructions and note questions they found confusing. Exit survey item1 is shown below

Circle how much you agree or disagree with the statement below.

1. *I found the instructions in the activity generally to be clearly worded.*

Strongly agree
Agree
Disagree
Strongly Disagree

Indicate for which questions you found the instructions to be partially or fully unclear.

Two students' responses indicated the table for item one in activity one was unclear. Two students also noted the phrase "*realistic way"* in item eight in activity one was unclear. Other items were noted as unclear by a single student, including the equilibrium table in item seven of modeling activity five and the phrase "*Remain a separate species"* in item 6 of activity one. Item four and 16 in activity one were noted as unclear but no explanation for why the item was unclear was given. Six items were noted by students as unclear (1.1, 1.4, 1.6, 1.8, 1.16, and 5.7). Most students (94%) indicated the learning module was generally clear, with five students (29%) marking *strongly agree* and 11 students (65%) selecting *agree*.

After analysis of item responses, observation rubric data, exit survey data, and review of the videos, 16 out of the 70 items (22.9%) indicated a possible validity threat and needed to be reviewed for revisions. **Table 7.4** shows the identified validity threat, items, and action taken.

Table 7.4: Learning module items indicated for revision

Validity threat	Item(s)*	Action taken
Unclear prompt, asked for clarification or responses did not match intention of item	1.1, 1.4, 1.6, 1.8, 1.16, 4.3, 5.7	Revised wording for clarity
Unclear which modeling pieces were needed or how to use modeling pieces to make their model	1.1, 3.1, 6.1, 6.2	Revised modeling directions for clarity and emphasis of modeling pieces needed
Unfamiliarity of term	1.3 and throughout the learning module	Used term autoionization instead of autoprotolysis throughout learning module
Group skipped modeling of processes to connect with symbolic representation	1.4 & 1.5, 5.2 & 5.3	Revised wording and boxes to draw the particle-level image and then symbolic representation were added.
Item skipped by multiple groups	1.7b, 3.4	Numbered as separate item and revised wording for clarity

*The first number is the modeling activity followed by the item number (i.e. item 1.8 is item 8 in modeling activity 1).

7.4.5 What revisions should be made to the learning module before implementation?

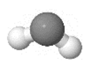
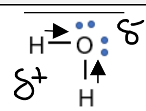
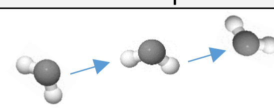
The term autoionization was used throughout the activity instead of autoprotolysis. The term autoprotolysis was unfamiliar to some students and is not used in general chemistry II. However, both terms are used in the analytical chemistry textbook. The term autoprotolysis was left in the introduction to connect the prefix (auto) and root (protolysis) to their meanings and familiarize students with the term. Items four and five in activity one and items two and three in activity five prompted students to build a chemical reaction or process with the models followed by writing the symbolic representation. These items were revised to clearly separate each step, and a box for students to draw the particle-level image of their model was added. This revision emphasized the connection between the models, particle-level drawings, and the symbolic representations.

The table in item one of activity one was revised for clarification and to reduce the time to complete the item. **Figure 7.2** shows the original and revised tables.

Figure 7.2: Modeling activity one item one revisions. Original table (top) and revised table (bottom) (some blank rows have been removed for space)

Use only the water molecules to investigate interactions between the water molecules. Discuss in your group the different species (molecules, particles, or ions) that can result when water molecules interact with each other and the attractive or repulsive forces between species.

1. Draw each species you make with the model in the table below and complete each row. The first row has been completed as an example.

Species (formula + sketch) Include any charge on the species	Draw the Lewis dot structure for the species Show any polarity in the structure with arrows and δ^+ or δ^- symbols	Interactions between species (You may include multiple species here) Use arrows to indicate attraction between species
 H_2O		

Use only the water molecules in your model set to investigate the autoionization of water with your group. Make different species (e.g., molecules, atoms, or ions) using the water molecules.

1. Draw each species you group makes with the water molecules in the table below.

Row #	**Species (formula and sketch)** Draw each species your group made using the water molecules. **Include any charges on species**	**Interactions** Draw images of possible interactions between species your group formed with the models. Use arrows to indicate attraction between molecules or species
1		
2		
3		

Items 11-14 in activity one asked students about water acting as an acid or a base and were repetitive. These items were combined to a single item to reduce the time to complete activity one, which took students an average of 37 minutes. Other items in activity one were revised as outlined in **table 7.4.**

Calculation tables connecting the concentration of H_3O^+ and OH^- with pH were revised to include additional space to show calculations. Repetitive calculation in tables were removed to shorten the time spent on calculations and allow more time to focus on the modeling activities. **Table 7.4** shows examples of revisions

Table 7.4: Revisions to learning module

item	Original item and revision
1.6	Original item: *Is it likely that hydrogen ions (H^+) remain separate species?* Revision: *Discuss all interactions the H^+ ion could have with water molecules during autoionization. What is the product when a proton (H^+ ion) interacts with a water molecule?*
1.16	Original item: *What conditions might influence the autoprotolysis of water? Use the models and think about what happens on the particle-level when, for example, the temperature or pressure changes? Explain.* Revision: *Discuss in your group any conditions that might influence the autoionization of water. What conditions may cause a change in the autoionization of water? Explain your thoughts.*
3.1	Original item: *Consider a 2.3×10^{-9}M hydrochloric acid. Use **all** the water molecules in your kit. Consider the concentration of this HCl solution (2.3×10^{-9}M). Should you use all the HCl molecules?* Revision: *Consider a very low concentration HCl solution (for example 2.3×10^{-9}M). Use **all** the water molecules in your modeling kit to show a **highly diluted HCl solution**.*
3.4	Original item: *Using your models, discuss any other processes and species that could contribute to the pH of the solution* Revision: *Discuss in your group all processes that contribute to the concentration of H_3O^+ in this solution. What other process needs to be considered when calculating the pH of a very dilute acid solution?*
5.7	Revised table to reflect classic ICE table including the initial concentration, the change, and final concentration rows
Directions Modeling activity 6	Original directions: *Compare how the HCl molecules and the CH_3COOH molecules interact with the water molecules. Use the water molecules to try to remove a proton (H^+) form the different acid molecules. Experiment with the distance between the different molecules and discuss any difference in the attraction between modeling pieces.* Revision: *Use the modeling set to compare how a lone pair on an oxygen atom in a water molecule may interact with the proton (H+) from different acid molecules. First, try to remove the proton (H^+) from an HCl molecule using only a water molecule. Have each person in our group try this experiment. Next, have each person try to remove the proton (H^+) from an acetic acid molecule (CH_3COOH) using a water molecule.*

7.5 Conclusions

Results showed 16 out of 70 items may not be function as intended and were a validity threat needing to be revised or removed. Students took longer than expected to compete the entire learning module than intended and some revisions were needed to ensure an appropriate timeline for implementation with analytical chemistry students. The revised learning module is shown in **appendix J**.

The number of modeling pieces provided to each group was in excess of what was used indicating fewer models can be provided to each group for implementation. Using the maximum number of model pieces used by any focus group, 15 water molecules, and 5 of each HCl, NaOH, CH_3COOH and H_2CO_3 would be used for implementation. In addition, labeling each bag of models will help ensure students use the correct models.

7.6 Limitations

Results from a low number of focus groups, with some activities being completed by only three groups, offers insight and guidance for revisions, but may not identify all items to be revised. Some magnets fell out of the modeling pieces and will need to be addressed for any future production of the models.

Chapter 8: Implementation of Learning Module

8.1 Introduction

The learning module uses a modeling-based teaching approach with three-dimensional physical models and aims to support students' connections between particle-level processes and symbolic and mathematical representations in acid-base chemistry. The assessment items measure learning gains in students' understanding of the autoionization of water, acidic strength, pH, and K_a. Implementation of the learning module and pre- and post-assessment with analytical chemistry students seeks to answer these two research questions.

1. Does an acid-base learning module using the novel acid-base models impact students' performance on acid-base content questions using a pre- and post-assessment?
2. Does an acid-base learning module using the acid-base models impact students' understanding of the autoionization of water, acidic strength, pH, and K_a?

The research process described in this chapter is shown in **Figure 8.1**.

Figure 8.1: Research process

8.2 Methods

Data reported for this research was collected under IRB approval #23.008. All students consented to have their data included in this research. The revised learning module and the pre- and-post-assessment was implemented in week six of the fall 2022 semester. Students were recruited by the course instructor. Analytical chemistry students that participated (N=20) received extra credit for completing the learning module and pre- and post-assessment.

Prior to the implementation, five model sets including 15 H_2O molecules, and five of each HCl, NaOH, CH_3COOH, H_2CO_3 molecules were prepared. Each type of model was put into separate bags labeled with the name and chemical formula of the model and the modeling activity or activities that model should be used for. The six modeling activities and the models used for each activity are shown in **table 8.1.**

Table 8.1: Modeling activities and models used

Modeling activity	Models used
1. Autoionization of water	Water
2. Strong acid solution	Water, HCl
3. Dilute strong acid solution	Water, HCl
4. Strong base solution	Water, NaOH
5. Weak acid solution	Water, CH_3COOH
6. Comparison of strong and weak acids	Water, HCl, CH_3COOH, H_2CO_3

The same document was used as the pre-assessment and the post-assessment. For the post-assessment, space on the right side (about 1/3 of the paper) was left blank so that students could write any changes to their responses post-activity. Students completed the research consent form first, then were asked to complete the pre-assessment individually (30-40 min.). Students were then divided into groups of 3 or 4 and completed the learning module using the acid-base models (appr. 90 min), followed by the individual post-assessment using a different colored pen (20-30 min.). Students were allowed to use a calculator throughout this process. The pre- and post-assessment documents and completed learning activities were scanned and saved to a secure USB flash drive stored in a locked cabinet to preserve all data.

The learning module was implemented during a laboratory period with 20 analytical chemistry students that were divided into six groups of 3-4 participants. All 20 participants completed the pre- and post-assessment individually and signed the IRB consent form for their data to be used in this research. The steps for implementation were followed as outlined in the methods. **Table 8.2** shows the number of students in each group and the completion of the learning activities.

Table 8.2: Learning module groups for implementation

Group	Group size	Completed modeling activities					
		1	2	3	4	5	6
1	3	✓	✓	✓	✓	✓	✓
2	4	✓	✓	✓	✓	✓	✓
3	4	✓	✓	✓	✓		50%
4	3	✓	✓	✓	✓	✓	✓
5	3	✓	✓	✓	✓	✓	✓
6	3	✓	✓	✓	✓		✓

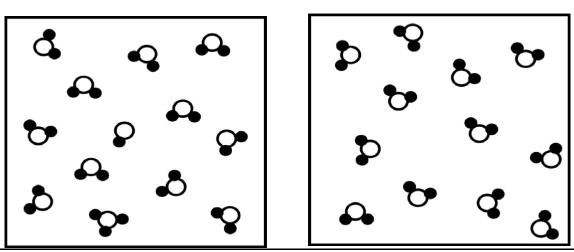
8.2.1 Follow up interviews

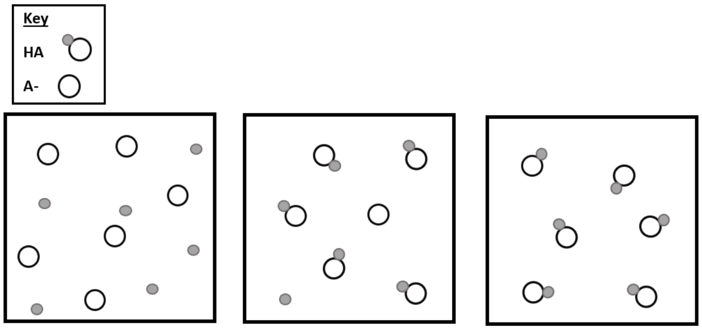
Data reported from student interviews was collected under IRB approval #23.008. All participants consented and agreed to be audio and video recorded. Student interviews were conducted with 19 of the 20 students that completed the pre- and post-assessment. The researcher and principal investigator conducted all interviews. Interviews were one-on-one in a conference room during a laboratory period when students could easily leave for the short interview. Each interview lasted between

9-18 minutes. The camera was focused on the table to capture the students' use of the models and any images drawn.

Individual follow-up student interviews were conducted five weeks after the implementation to clarify student responses and gain insight into students' thinking on why they chose certain responses. Questions selected for the Interviews were directly related to pre- and post-assessment items to investigate responses to items where use of the models was key to correctly answering that item and investigated students' interpretation of particle-level images. An interview protocol was written and revised in group meetings with the researcher and two chemistry education research faculty. The interview protocol included four items that aligned with the four acid-base concept areas being investigated on the pre- and post-assessment. The items are shown in **table 8.3.** The interview protocol is shown in **Appendix K**.

Table 8.3: Interview items, the target of each item, and alignment with the acid-base concepts areas investigated on the pre- and post-assessment

Interview item	Target of item	Concept area alignment
Which image do you think most realistically shows the autoionization of water? 	• Students' understanding of autoionization • Students' interpretation of particle-level images	• Autoionization
In what aqueous systems is the autoionization of water occurring?	• Students' understanding of Autoionization	• Autoionization
Two students calculated the pH of a dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below. A. Student 1, pH = 8.30 B. Student 2, pH = 6.99 Which pH is more reasonable, 8.30 or 6.99?	• Autoionization • pH	• Autoionization • pH

Looking at the three images and the key, can you describe what these three images represent?"  Follow-up: Explain how you think the K_a values for the three acids shown would change.	• Students' understanding of acidic strength • Students' interpretation of particle-level images • Students' connection of acidic strength to K_a	• Acidic strength • K_a

8.3 Scoring of pre- and post-assessment items

The pre- and post-assessment items were scored for correctness to allow for statistical analysis. **Table 8.4** shows the scoring used for each type of assessment item and the number of each type of item.

Table 8.4: Scoring of assessment items

Type of item	Scoring	Explanation	# of items
Multiple-choice and calculation items	Correct (1) Incorrect (0)	Multiple-choice and calculation items	26
two-part items	Both parts correct (1) One part correct (0.5) Both parts Incorrect (0)	Item 9 with two calculations and item 22 multiple-choice selection of strongest and weakest acid	2
Open-response	Correct Partially correct Incorrect	Specific to item: Item 13 scored 1, 0.5, & 0. Item 23 scored 1, 0.5, 0.25, & 0.	2

Multiple-choice items with a place for students to explain their reasoning (items 8, 18, and 21) was used to confirm the student's reasoning matched their response. Reasoning for these items supported the circled response. Open response item 23 asked students to compare structural features that made HF a weak acid and HCl a strong acid even though both molecules contain a hydrogen and halogen. This item was found to show more variability in understanding and was scored on a 1 for correct, and 0.5 or 0.25 for partially correct to differentiate different levels of partial understanding. For example, students that related the difference in acidic strength to bonding without additional details were given a score 0.5. Students that described electronegativity as a factor in acidic strength, but explained electronegative as the reason why HF is weaker were given a score of 0.25. Students showing no understanding were given a score of zero.

8.4 Assessment item categorization

Items were categorized into four acid-base concept areas included in the learning module and the pre- and post-assessment (autoionization, acidic strength, pH, and K_a) to investigate learning gains related to these concepts. Categorization of pre- and post-items was done independently by the researcher and two chemistry education faculty. Items that fit into more than one category were coded for all categories. Items in which the use of the models were considered key to answering the item correctly were coded as being "*in-depth"* instead of a general practice item. Examples of in-depth items are items 5 and 20 and 21 (shown and discussed in detail in the results section), as opposed to item 6 and 7, which are pH calculation items and were considered practice questions. Identification of in-depth items was to help investigate if learning gains may have resulted from the use of the models. Not all items fit into one of the four categories. For example, Item 1 investigates students' understanding of the behavior of water as a solvent, but does not show understanding specific to one of the four categories being investigated. There were discrepancies for 11 items (36.7%) between the three coders. These items were discussed until consensus was reached. The results from categorization of the pre- and post-assessment items are shown in **table 8.5**. Items 14, 15, 16, 17, 18, 19, 20, 21, 26, and 28 are included in more than one category. Items where the use of the models was key to correctly respond to that item, categorized as in-depth, are underlined and bolded.

Table 8.5: Results of pre- and-post-assessment item categorization

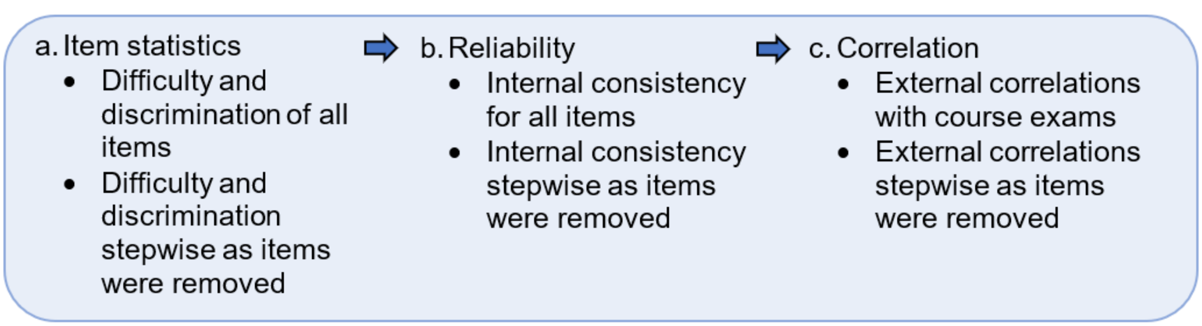
	Autoionization	Acidic strength	pH	K_a
Items	3, 4, **5**, **14***, 18*, **20***, **21***	**14***, **15***, 16*, 17*, 19*, **22**, **23**, **24**, 26*, **30**	6, 7, 8, 9, 10, 15*, 16*, 17*, 18*, 19*, **20***, **21***, 28*	25, 26*, 27, 28*

*Indicates item is included in more than one category.

8.5 Reliability and validity

To identify any assessment items that may be a validly threat and determine what items should be removed before statistical analysis, the pre- and-post items were assessed for validity. Reliability of the assessment was calculated before and after items were removal to support the removal of items. Several steps were taken to determine which items should be removed. This process is shown in **figure 8.2.**

Figure 8.2: Process to determine pre- and post-item removal



The difficulty and discrimination were calculated for each item, once according to student performance on the pre-assessment and again according to the performance on the post assessment. The difficulty index (*p*) is a measure of the percent of students that correctly responded to an item on a 0-1 scale (0-100%), calculated by taking the sum of correct responses (R_c) and dividing it by the total number of attempts (N), $p = \frac{R_c}{N}$. An easy item will have a high difficulty index, and more difficult items have a lower difficulty index.

The discrimination index (D) for each item was calculated using the equation:

$$D = \frac{H_c - L_c}{n}$$

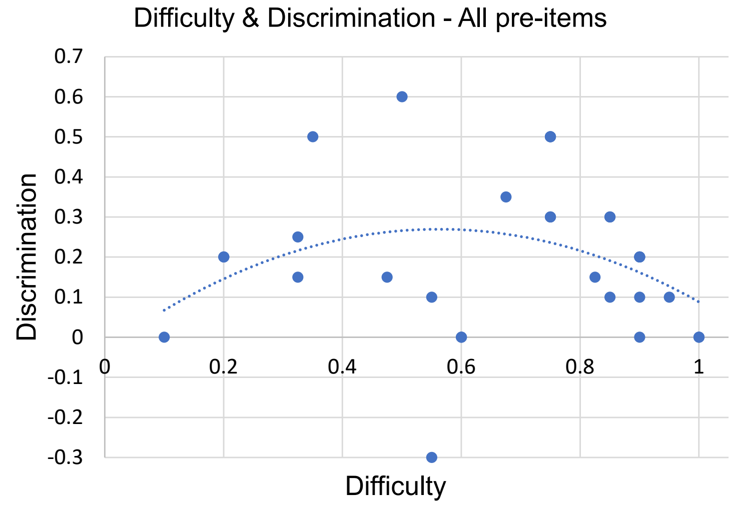
H_c = Number of correct responses in high performing group (highest scoring 50%)
L_c = Number of correct responses in low performing group (lowest scoring 50%)
n = number of participants in group (n=10)

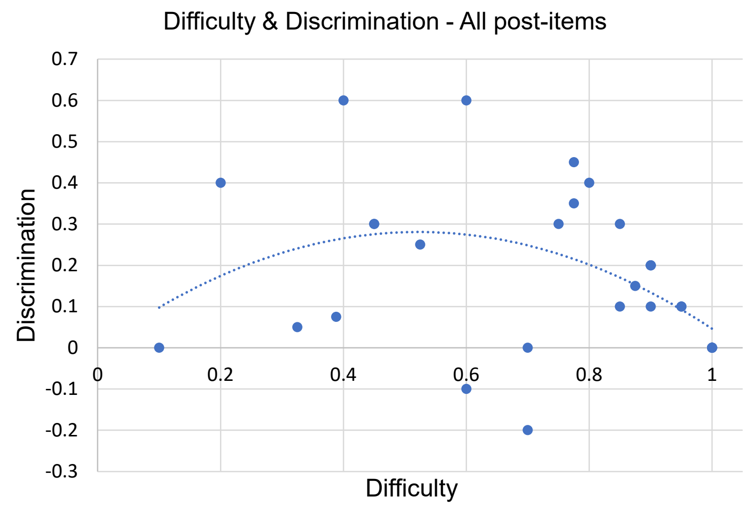
A negative item discrimination indicates that more low performing students answered the item correctly and indicates the item is a validity threat. Scatter plots for the difficulty and discrimination were examined systematically to identify items of concern. A good scatter plot of difficulty vs. discrimination includes no items with a negative discrimination. Due to the low sample size of 20, responses from all students were used to calculate the discrimination of each item. Using a mean of ten responses from each group (high and low performing) to calculate discrimination can be problematic and results from such a small sample size need to be interpreted cautiously. The difficulty and discrimination for all 30 pre- and post-items are shown in **table 8.6**. The scatter plots for these items are shown in **figure 8.3.**

Table 8.6: Difficulty and Discrimination for all 30 pre- and-post items

Item	Difficulty		Discrimination	
	Pre	Post	Pre	Post
1	1	1	0	0
2	0.6	0.6	0	-0.1
3	0.5	0.6	0.6	0.6
4	0.85	0.9	0.3	0.2
5	0.55	0.45	0.1	0.3
6	0.85	0.95	0.3	0.1
7	0.9	0.85	0	0.1
8	0.85	1	0.1	0
9	0.825	0.875	0.15	0.15
10	0.9	0.9	0.1	0.1
11	0.75	0.8	0.3	0.4
12	0.9	0.9	0.2	0.2
13	0.475	0.525	0.15	0.25
14	0.95	1	0.1	0
15	0.675	0.775	0.35	0.35
16	1	1	0	0
17	0.9	0.9	0.2	0.2
18	0.75	1	0.5	0
19	0.75	0.75	0.3	0.3
20	0.2	0.4	0.2	0.6
21	0.55	0.7	-0.3	-0.2
22	0.75	0.775	0.5	0.45
23	0.325	0.388	0.15	0.075
24	0.75	0.85	0.5	0.3
25	0.6	0.7	0	0
26	0.325	0.325	0.25	0.05
27	0.9	0.95	0.2	0.1
28	0.2	0.2	0.2	0.4
29	0.35	0.45	0.5	0.3
30	0.1	0.1	0	0

Figure 8.3: Scatter plots of difficulty vs. discrimination for all items





Items 2 and 21 had a negative discrimination and are threat to the validity. Item 2 was removed, students total scores were recalculated from the remaining items, and discrimination was recalculated. Item 21 still had a negative discrimination. This process was repeated after removing just item 21, and item 2 still showed a negative discrimination. Item 2 and 21 are multiple-choice; however, Item 21 is a multiple-choice follow-up item with item 20. These two items are shown below

20. Two students calculated the pH of dilute HCl solution with a concentration of $4.8x10^{-9}$ M. Their answers are below.
Which pH calculation is correct?

A. Student 1, pH = 8.30
B. Student 2, pH = 6.99

21. Does the autoionization of water needs to be considered when calculating the pH of a dilute acid solution?

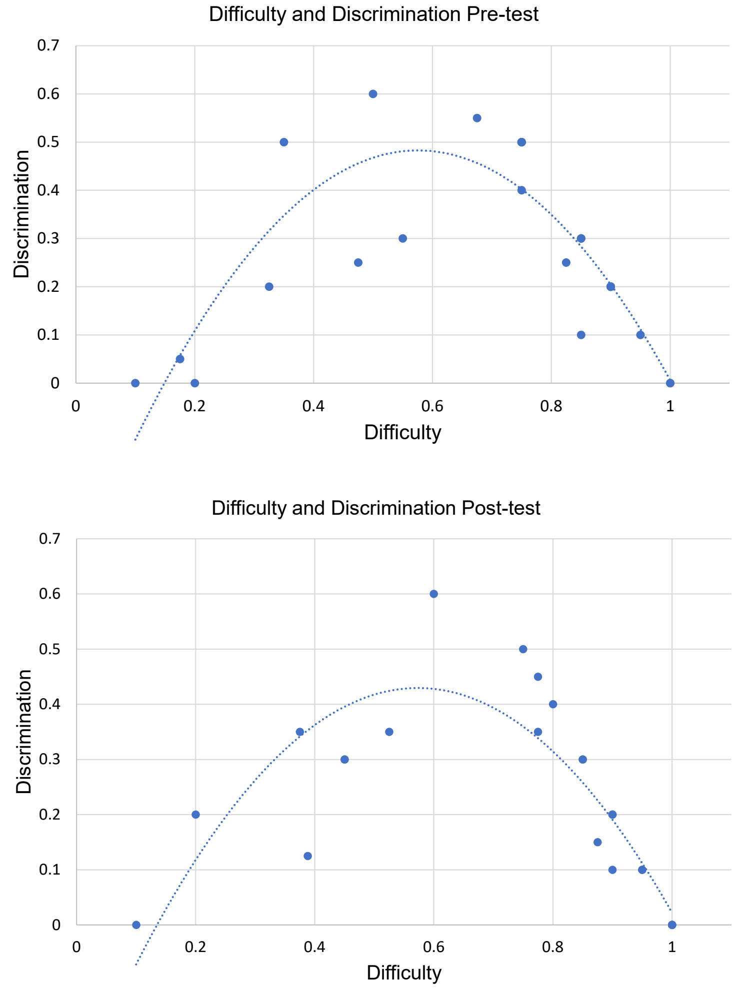
A. Yes
B. No

Item 20 and 21 were originally scored separately as correct or incorrect. Since these two items are related, they were rescored as a two-tiered multiple-choice item (20/21). If a student answered “B” (pH=6.99) for item 20 and “A” for item 21 they were given a score of 1 for correct. If a student answered “B” for both parts they were given a score of 0.5 for partially correct and all other combinations scored zero. Difficulty was calculated for item 20/21 and discrimination for all items was recalculated. Item 2 and 25 still had a negative discrimination. Item 25 was removed and the stepwise process was repeated. Using item 20/21 and removing item 2, item 25 and 26 had a negative discrimination. After removal of items 2, 25, and 26, and using item 20/21, no items had a negative discrimination. **Table 8.7.** shows the difficulty and discrimination for the remaining items after removal of 2, 25, and 26 and **figure 8.4** shows the scatter plots.

Table 8.7: Difficulty & discrimination items 2, 25, 26 removed

Item	Difficulty		Discrimination	
	Pre	Post	Pre	Post
1	1	1	0	0
3	0.5	0.6	0.6	0.6
4	0.85	0.9	0.3	0.2
5	0.55	0.45	0.3	0.3
6	0.85	0.95	0.3	0.1
7	0.9	0.85	0.2	0.3
8	0.85	1	0.1	0
9	0.825	0.875	0.25	0.15
10	0.9	0.9	0.2	0.1
11	0.75	0.8	0.5	0.4
12	0.9	0.9	0.2	0.2
13	0.475	0.525	0.25	0.35
14	0.95	1	0.1	0
15	0.675	0.775	0.55	0.35
16	1	1	0	0
17	0.9	0.9	0.2	0.2
18	0.75	1	0.5	0
19	0.75	0.75	0.5	0.5
20/21	0.175	0.375	0.05	0.35
22	0.75	0.775	0.4	0.45
23	0.325	0.388	0.2	0.125
24	0.75	0.85	0.5	0.3
27	0.9	0.95	0.2	0.1
28	0.2	0.2	0	0.2
29	0.35	0.45	0.5	0.3
30	0.1	0.1	0	0

Figure 8.4: Scatter plots of difficulty vs. discrimination for 26 remaining items



As shown in figure 8.2 (b), the next step was to look at the internal consistency of items as a measure of the instrument's reliability. This was done using Cronbach's alpha for all 30 items and then removing items stepwise. A good internal consistency is generally considered a value of 0.7 or above (Arjoon, et al., 2013; Murphy & Davidshofer, 2014) and shows that participants who respond to one item should respond similarly to other items measuring the same construct. Since all items measure acid base knowledge a good internal consistency supports the reliability of the instrument. Reliability is shown in **Table 8.8**.

Table 8.8: Internal consistency of items

Number of items	Change	Reliability	
		Pre	Post
30	None	0.754	0.698
29	Removal of item 2	0.756	0.720
28	Removal of item 2 with item 20/21	0.804	0.725
27	Removal of item 2 & 25 with item 20/21	0.818	0.748
27	Removal of item 2 & 26 with item 20/21	0.806	0.738
26	Removal of item 2, 25, & 26 with item 20/21	0.822	0.765

The next step as shown in figure 8.2 (c), is to consider the validity of the instrument's scores through external correlations with students' exams scores and total course percent. Students took two mid-term exams and a final course exam. It's expected students' exam and course score will correlate with the pre- and-post-scores because all include knowledge on acid-base chemistry. Both mid-terms were reviewed to evaluate question alignment with the assessment items. Mid-term 1 included pH calculations and charge balance equations that better aligned with the assessment items. Due to the larger number of concepts included in the final exam and course score it was expected these scores would not correlate as strongly. Correlation results are shown in **Table 8.9**.

Table 8.9: External correlations

	Correlation (sig.)					
	Mid-term 1		Final exam		Course total	
	Pre	Post	Pre	post	Pre	Post
All items	.778** (<.001)	.840** (<.001)	.606** (.011)	.620** (.004)	.509* (.005)	.493* (.027)
Removal of items 2, 25, & 26 with item 20/21	.785** (<.001)	.833** (<.001)	.627** (.003)	.661** (.002)	.539* (.014)	.526* (.017)

**Correlation is significant at the 0.01 level (2-tailed).
*Correlation is significant at the 0.05 level (2-tailed).

Results show a high significant correlation between the pre- and post-assessment and mid-term 1 and a moderate significant correlation between the pre- and post-assessment and the final exam and course total. After removal of all items identified as a validity threat, correlations were essentially unchanged. The validity and reliability results support the removal of item 2, 25, 26, and scoring items 20 and 21 as a two-tiered multiple-choice item. The final analysis used 26 pre- and post-items. Due to the removed items, item categorization was adjusted accordingly. **Table 8.10** shows the item groupings after item removal. Items identified as in-depth and more specific to the use of the models are bolded and underlined.

Table 8.10: Results of pre- and-post item categorization

	Autoionization	Acidic strength	pH	K_a
Items	3, 4, **5**, **14**, 18, **20/21**	**14**, **15**, 16, 17, 19, **22**, **23**, **24**, **30**	6, 7, 8, 9, 10, 15, 16, 17, 18, 19, **20/21**, 28	27, 28

As a measure of reliability for the acidic strength and pH concept groupings, the internal consistency was calculated using Cronbach's alpha. Reliability is reported for only these groups because internal consistency cannot be accurately judged using Cronbach's alpha for small samples sizes and number of items. A reliability value equal to or greater than 0.7 indicate good reliability (Bujang et al., 2018). Reliability of the acidic strength and pH concept groupings is shown in **table 8.11.**

Table 8.11: Results of pre- and-post item groupings

	Number of items	Reliability	
		Pre	Post
Acidic strength	9	0.695	0.623
pH	12	0.718	0.516

The results show good or approaching good reliability for items within the acidic strength and pH groupings for the pre-assessment. The decrease in reliability scores on the post-assessment may be due to the difference in learning gains between the high and low performing students. Low performing students are more likely to have larger learning gains compared to high performing students. This is because low performing students answered more items incorrectly and had more opportunity to change an items' responses from incorrect to correct leading to greater variability and lowering the reliability of the post-assessment results.

Test-retest reliability was calculated for the pre-assessment results and post-assessment results for all valid items and each concept grouping. Test-retest reliability measures the consistency of the results when the same items are used with a single population at two different time points. The test-retest reliability is shown in **table 8.12**

Table 8.12: Test-retest reliability

Grouping	Number of items	Test-retest reliability (sig.)
All valid items	26	0.927**(<.001)
Autoionization	6	0.747**(<.001)
In-depth autoionization	3	0.705**(<.001)
Acidic strength	9	0.878**(<.001)
In-depth acidic strength	6	0.845**(<.001)
pH	12	0.717**(<.001)
Ka	2	0.720**(<.001)

**Correlation is significant at the 0.01 level (2-tailed).

The test-retest reliability shows good significant correlation for all groupings. A significant test-retest reliability greater than or equal to 0.7 indicates good test-retest reliability (Bujang et al., 2018; Drost, 2011). The test-retest reliability provides additional evidence of reliability and supports the validity of the assessment.

8.6 Learning gains: statistical difference in means

All statistical analysis was done in IBM SPSS version 28.0.1.1 software. Analysis was done on the results of the pre- and post-assessment and for each grouping using a paired samples t-test for normally distributed data and the Wilcoxon signed-rank test for nonparametric data. The Wilcoxon signed-rank test has been shown to be a powerful and reliable alternative to test nonparametric paired-samples data with 15 or greater pairs (Fritz et al., 2012; Kanyongo et al., 2007; Meek et al., 2007; Orcan, 2020). A paired-samples t-test requires the dependent variable (the difference between the two scores) be normally distributed.

Normality was determined using the guidelines by Orcan (2020) that showed data with skewness and kurtosis values that fell below their standard error multiplied by 1.96 was acceptable for parametric tests, and the parametric test was as reliable or more reliable as the nonparametric alternatives. For data with values that fell outside of this range additional proof of normality was needed, such as normality plots or nonsignificant tests for normality like the Shapiro-Wilk test (Orcan, 2020). Since the paired-samples t-test is known to be a more powerful statistical test than the Wilcoxon signed-rank test, it is preferred when the data is normally distributed (Kanyongo et al., 2007; Meek et al., 2007; Orcan, 2020). The standard error for skewness and kurtosis are based on the sample size. A sample size of 20 has a standard error of 0.512 for skewness and 0.992 for kurtosis. These values multiplied by 1.96 give an acceptable value for skewness less than 1 and an acceptable value for kurtosis less than 1.94. Both values must be below these thresholds to use the parametric test. Normality tests showed data from the pre- and post-assessment, in-depth autoionization group, and acidic strength group was parametric. Data from the autoionization, in-depth acid strength, pH, and K_a groups was not parametric. Results of normality tests are shown in **appendix L.**

The effect size for any significant finding is also reported. The effect size for the paired-samples t-test was measured with Cohen's d. The effect size for the Wilcoxon signed-rank test was measured with r as described by Fritz et al. (2012), and calculated using equation $r = \frac{Z\ score}{Sqrt(n_1 + n_2)}$, where n_1=total number of pre-responses and n_2=total number of post-responses. **Table 8.13** shows accepted interpretations for each effect size.

Table 8.13: Effect size values

Effect size	Cohen's d	r
Large	*Value ≥ 0.8*	*Value ≥ 0.5*
Medium	*Value ≥ 0.5 to < 0.8*	*Value ≥ 0.3 to < 0.5*
Small	*Value ≥ 0.2 to < 0.5*	*Value ≥ 0.1 to < 0.3*

8.6.1 Results

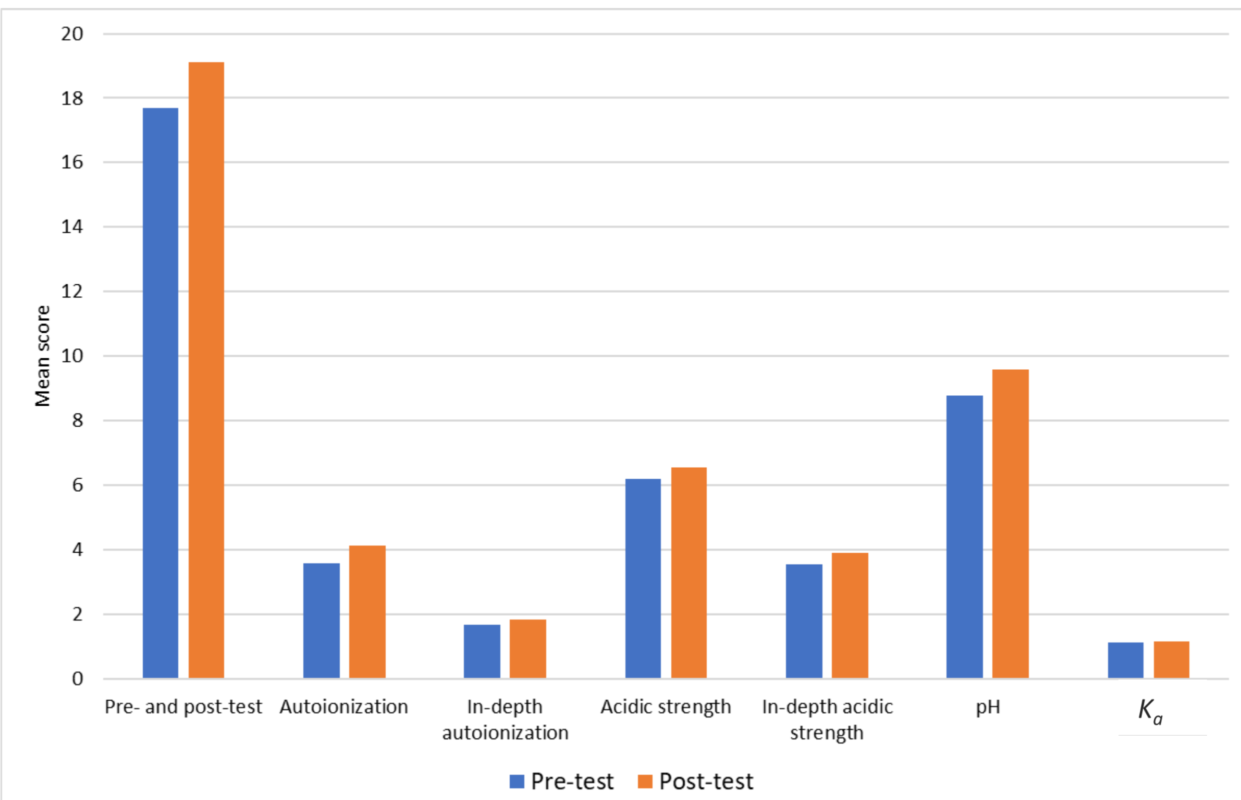
Results showed an increase in the mean of the post-scores compared to the pre-scores for the pre- and post-assessment overall and all concept groupings with four significant results. The results are shown in **table 8.14** and **Figure 8.5**.

Table 8.14: Results of statistical analysis

Grouping	Pre-test	Post-test	Paired differences (post-test - pre-test)				
	Mean (SD)	Mean (SD)	Mean	Std. error mean	t^a/Z^b	Sig (2-tailed)	Effect size
All 26 items	17.72 (4.05)	19.06 (3.32)	1.34	0.35	3.78^a	0.001**	0.85[1]
Autoionization	3.57 (1.18)	4.13 (1.07)	0.55	0.18	2.64^b	0.008**	0.42[2]
In-depth autoionization	1.67 (0.65)	1.83 (0.78)	0.15	0.12	1.19^a	0.249	
Acidic strength	6.20 (1.62)	6.54 (1.37)	0.34	0.17	1.94^a	0.068	
In-depth acidic strength	3.55 (1.17)	3.89 (0.96)	0.34	0.14	2.18^b	0.029*	0.34[2]
pH	8.77 (2.06)	9.57 (1.45)	0.80	0.32	2.52^b	0.012*	0.40[2]
K_a	1.10 (0.55)	1.15 (0.49)	0.05	0.09	0.58^b	0.564	

**Significant at the *p*<.01
*Significant at the *p*<.05
[1]Cohen's d
[2]r Calculated using $r=Z/Sqrt(n_1+n_2)$ (Fritz et al., 2012)

Figure 8.5: Pre- and post-results



Results from the dependent-samples t-test showed a statistically significant increase on the post-scores (M=19.06, SD=3.32) compared to the pre-scores (M=17.72, SD=4.05), t(19)=3.78, *p*=0.001 (two-tailed) with a large effect size. Results from the Wilcoxon signed-rank test showed a statistically significant increase on the post-test scores for the autoionization, in-depth acidic strength, and pH groupings all with a medium effect size.

To investigate the difference between low and high performing students, students were divided into a low performing (N=10) or high performing (N=10) group according to their mid-term 1 score. Mid-term 1 aligned most closely to the pre- and post-assessment items and had the strongest and most significant correlation to students' pre- and post-scores (table 8.7). Nonparametric paired-samples tests used on sample sizes as small as 10 have been shown to be unreliable. However, no dramatic differences were found in error rates of symmetric data even with a sample size as small as 5 and a paired samples t-test was still reliable (Kanyongo et al., 2007; Meek et al., 2007). To avoid false interpretations of results from nonparametric data, only parametric data was analyzed using a paired-samples t-test. The pre- and post-test results for both the high and low performing groups showed normality with skewness and kurtosis values in the acceptable range, nonsignificant Kolmogorov-Smirnov and Shapiro-Wilk tests for normality, and normality plots. Results of normality tests is shown in **appendix L.** Data from the low (N=10) and high (N=10) performing students for all concept groupings was not parametric, and statistical analysis would not be reliable. Results of the low and high groups on the pre- and post-assessment is shown in **table 8.15.**

Table 8.15: Results of the low vs high performing students

26 valid items	Pre-test	Post-test	Paired differences (post-test - pre-test)				
	Mean (SD)	Mean (SD)	Mean	Std. error mean	t	Sig (2-tailed)	Effect size
High performing	20.38 (2.00)	21.43 (1.44)	1.05	0.36	2.91	0.017*	0.92[1]
Low performing	15.07 (3.88)	16.70 (2.97)	1.63	0.62	2.64	0.027*	0.83[1]

*Significant at the p<.05
[1]Cohen's d

Results from the dependent-samples t-test show a statistically significant increase on the post-scores for both the high performing and low performing groups with a large effect size. High performing students pre-test (M=20.38, SD=2.00) compared to the post-test (M=21.43, SD=1.44), t(9)=2.91, p=0.017 showed high performing students increased their post-test score an average of 1. For students in the low performing group, scores on the pre-test (M=15.017, SD=3.88) compared to the post-test (M=16.70, SD=2.97), t(9)=2.64, p=0.027 showed low performing students increased their post-assessment score an average of 1.6 points.

8.7 Learning module item categorization

Learning module items identified as in-depth and aligned with one of the four concept groups of the pre- and post-assessment items, were categorized to support findings of students learning gains from the use of the models. Calculation and general practice items in the learning module were not included in the categorization to focus specifically on effects from the use of models. Coding was done independently by the same three raters and any discrepancies were discussed until consensus was reached. Results are shown in **table 8.16**.

Table 8.16: Results of learning module item categorization

	Autoionization	Acidic strength	pH	K_a
Items	3a, 3b, 4, 5, 6, 7, 8, 14, 23b, 28, 29, 30, 31, 32	17, 18, 19, 20, 22, 23d, 28, 41, 42, 43, 54, 55, 59, 60	3c, 29, 30, 31, 32	17, 20, 21, 22, 23d, 28, 41, 42, 44

All learning module items were coded for engagement based on completion of that item, a completed response was coded as a 1 and no response was given a zero. Results showed all six groups were engaged with all items except for items 38, 39, and 40 that were skipped by one group and items in modeling activity 5 and 6 that were not completed due to time.

Correctness coding was done for 62 items on the learning module. Each question with multiple parts (i.e. 23a, b, & c) were coded individually for correctness. Seven items were identified as “brainstorming” questions and were only coded for engagement (items 2, 15, 16, 56, 57, 58, and 61). Calculation and most open response items were coded with a 1 for correct or a zero for incorrect. More difficult open-response items and particle-level images were coded based on the variety of responses for that item. These items were coded independent by two raters and any discrepancies were discussed until consensus was reached. The results of the correctness coding of the learning module items are to support the results of the pre- and post-analysis and help determine if learning gains are due to the use of the models or additional practice in the learning module. The results show the percent of correct response from each group for all items in each modeling activity and the percent of in-depth items scored as correct in each concept area. Results are shown in **table 8.17**.

Table 8.17: Results from modeling activities and in-depth item categorization

Modeling activity	Percent Correct by Group						
	1	2	3	4	5	6	Avg. %
1: Autoionization	93.3	83.3	93.3	86.7	90.0	86.7	88.9
2: Strong acid soln.	98.9	67.8	98.3	85.6	71.1	78.3	83.3
3: Dilute strong acid	37.1	54.3	77.1	74.3	52.9	72.9	61.4
4: Strong base	88.9	88.9	66.7	100	100	88.9	88.9
5: Weak acid soln.	57.7	93.6	0	100	83.3	0	83.7*
6: Acidic strength	56.3	68.8	50.0	56.3	37.5	75.0	57.3
Average %	72.0	76.1	77.1*	83.8	72.5	80.4*	
In-depth items that align with pre- and post-items for concept groupings							
Autoionization	77.6	69.4	84.7	80.1	65.3	76.0	75.5
Acidic strength	82.7	57.7	77.5	86.3	71.4	67.5	73.9
pH	40.0	50.0	80.0	70.0	60.0	80.0	63.3
K_a	90.5	61.9	93.8	83.3	78.6	68.8	79.5
Average %	72.7	59.8	84.0	79.9	68.8	73.1	73.1

*Average calculated using the scores from completed modeling activities

The number of low and high performing students in each group was considered to investigate if the difference between group scores may be due to groups composed of all high or all low performing students. All groups showed a relatively even distribution of high and low performing students, with each group including at least one high performing and one low performing student. **Table 8.18** shows the number of participants in each group according to performance.

Table 8.18: Learning module group participants' performance

Group	High performing group	Low performing group
1	1	2
2	3	1
3	2	2
4	2	1
5	1	2
6	1	2

8.8 Coding of interview responses

Follow-up interviews investigated students' understanding of the autoionization of water, acidic strength and related K_a values, pH, students' interpretation of particle-level images, and students' personal evaluation of the impact of the model use on their learning.

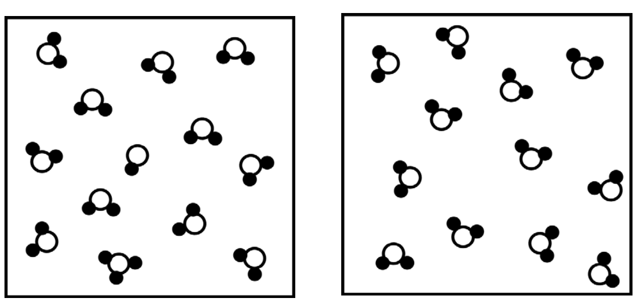
Interviews responses were coded for correctness based on the students' initial response and explanation, and correctness after follow-up questions and/or model use if their response changed. Coding was done by the researcher and any responses that were unclear were noted and discussed with the principal investigator to determine the final coding. Coding of interview responses was to provide evidence to support student learning and provide clarity of students' responses.

8.8.1 Results of interview items

The first interview question focused on students' understanding of autoionization and interpretation of particle-level images. **Figure 8.6** shows the first interview question.

Figure 8.6: Interview question one

Which image do you think most realistically shows the autoionization of water?



Results show 16 of the 19 students (84%) were coded as correct, with 15 correct students selecting the left image. All students coded as correct were able to explain their response using sound reasoning to support their choice. All three students coded as incorrect are students in the low performing group. Example responses shown for students A, B & C were coded as correct and student D's response was coded as incorrect.

Student A*: "*[pointing at left image] *I think this one because it actually has an OH and H_3O molecules and I don't see any in here* [pointing at right image]*."*
Interviewer*: "Would you consider this image* [pointing at right image] *to be incorrect?"*
Student A*: "No, because the OH and H_3O exist in such minuscule amounts that it could be represented as this."*

Student B*: "Probably this one* [pointing at right image] *because it's super super dilute, because it's a really small amount that ionizes. I guess it depends on the sample you collect, both are, I guess, viable realistically. I guess this one* [point at right image]*"*
Interviewer: "Would you consider this image [pointing at left image] *to be incorrect?"*
Student B: "No, because both are viable."

Student C: "[pointing at left image] *I'd say this one on the left because it shows hydronium, hydroxide, and water."*
Interviewer: *"Would you consider this image [pointing at image on right] to be incorrect?"*
Student C: "Um, if you are asking the specific autoionization of water I probably would just because as water autoionizes it's not all H_2O.

Student D: "[pointing at right image] *The right one because every oxygen has two hydrogens."*
Interviewer: *"Would you consider this image* [pointing at left image] *to be incorrect?"*
Student D: *"It's the wrong answer because this oxygen has only one hydrogen, which is OH and you can't have this in the water."*
Interviewer: "*Is there any time you see an OH in the autoionization of water?"*
Student D: *"Only like the equation in class, it's the OH + H will equal H_2O."*

Interview question two probed deeper into student's understanding of the autoionization of water by asking, "*In what aqueous systems is the autoionization of water occurring?*" 15 out of 19 students (79%) were coded as correct for identifying that it occurs in all aqueous systems. Again, all high performing students were coded as correct with all four incorrect responses from students in the low performing group. An example of a correct response (student E) and an incorrect response (student F) are shown below.

Student E: "*In all systems where there's like water present there would be autoionization. It's just like in situations where it's a solution we don't care about it as much because there's other things in higher concentrations, but anywhere water is present autoionization is there.*"

Student F: "*In what aqueous system, I'm not sure.*"
Interviewer: "*What is an aqueous system?*"
Student F: "*A liquid.*"
Interviewer: "*What do you mean by liquid? Are there any models you would use specifically to make an aqueous system?*"
Student F: "*Probably not. Molecules are close together, I guess, that's one way to put it.*"
Interviewer: "*If you were to define aqueous, how would you define that?*"
Student F: *"A large amount of molecules really close together."*

Interview question 3 was very similar to the pre- and post-item 20 shown below.

20. Two students calculated the pH of a dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below.
Which pH calculation is correct?

C. Student 1, pH = 8.30

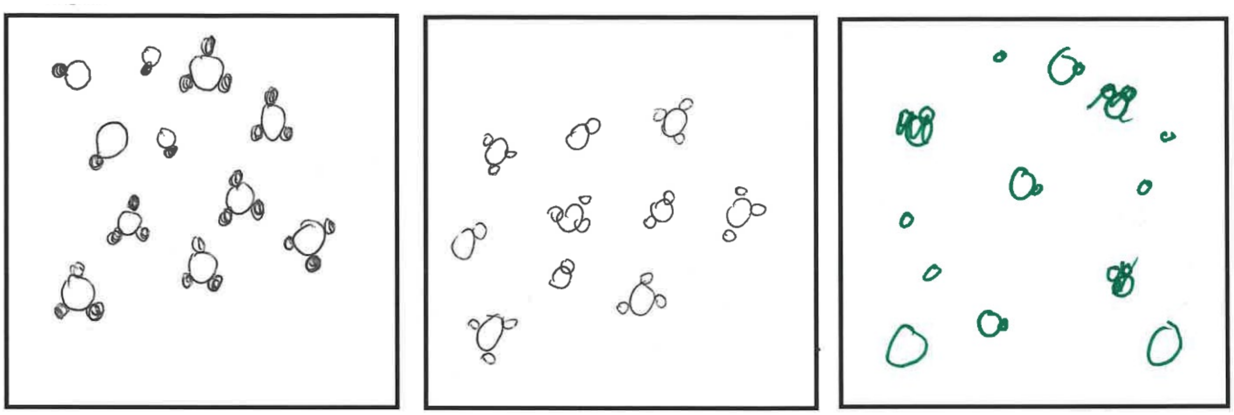
D. Student 2, pH = 6.99

During the interview students were shown question 20 (above) while the interviewer read it out loud, but the words "*which pH calculation is correct*" were replaces with "*Which pH is more reasonable, 8.30 or 6.99?*" No calculator was present and no student requested a calculator during the interview. Sixteen out of 19 students (84%) answered the correct acidic pH of 6.99 as their first response. The three students that answered pH=8.30 all expressed in their reasoning they were comparing the amount of HCl, 4.8×10^{-9} M, to 1.0×10^{-7}. For this item, two of the three students that answered incorrectly are in the high performing group. One of the students in the high performing group explains his thinking when selecting the basic pH.

Student G: "*I would say A [pH=8.30] since pH is based on the -log of the concentration of protons, and since the concentration here is less than 10^{-7}, which is neutral, it would be basic and 8.3 is the only basic pH here*".

The students that chose the pH=8.30 were asked to draw a diagram and use the models to show a neutral solution of water showing only the ions and no water molecules. All three students drew and used the models to show an equal amount of hydroxide and hydronium or H^+ ions in a neutral solution of water. After showing the ions in a neutral solution of water, they were asked if any additional ions should be added to the solution from the addition of the HCl (referring back to the question). All three students correctly used the HCl models to show additional H_3O^+ or H^+ ions would be in their solution after the addition of HCl and added these additional ions to their particle-level images. One student also added the Cl^- ions to their image. The images from these students are shown in **figure 8.7.**

Figure 8.7: Student images for modeling follow-up to interview item three



After this modeling activity and drawing the corresponding particle-level image, all three students decided to change their answer to pH=6.99 as more reasonable. Student G explained their thoughts during and after the modeling activity.

Interviewer: "*Now you are adding the hydrochloric acid. What would that look like in the diagram and with the models?"*

Student G: *"You would add more since HCl is a strong acid and it would dissociate fully* so *there would be no just HCl*, *this is an H and a Cl like that* [pulling apart 2 HCl molecule models]. [Adding ions to the particle-level image] *These are chlorines this time and then more H's."*

Interviewer: "*What is the pH of pure water?"*

Student G: "7"

Interviewer: "Which one of the pH's you looked at is more reasonable?"

Student G: *"It should go down to 6.99."*

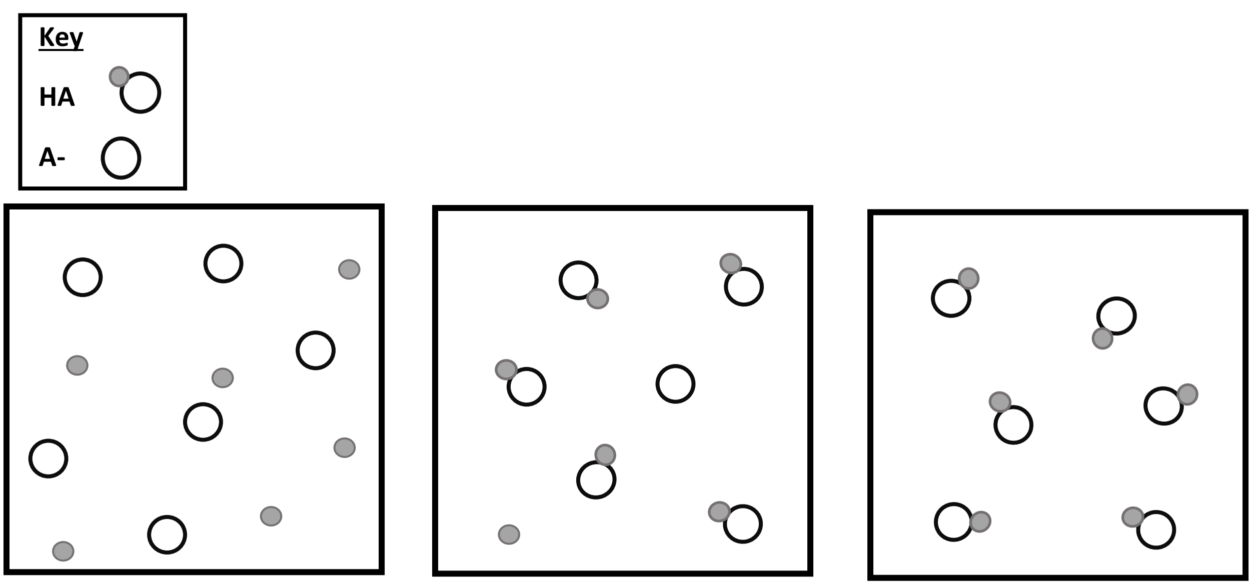
Interviewer: *"Which is different from the reasoning before?"*

Student G: *"Yeah, I guess I did it wrong the first time. I over thought the first time."*

Interview question number four investigated students understanding of particle level images of acid ionization. Interview question four is shown in **figure 8.8.**

Figure 8.8: Interview question four

Interviewer: "*Looking at the three images and the key, can you describe what these three images represent?"*



The first response from six students identified the images as a process or described the ionization in each picture without relating it to strength. When asked the follow-up question, "*If all three images show a different acid, can you explain the difference between the acids shown in each image?*" All six students were able to correctly identify the relative strength of the acids shown in each image. Fifteen out of 19 students (79%) correctly identified the difference between the images as a strong acid on the left, a weak acid in the middle, and a very weak or undissociated acid on the right (including the six students that needed the follow-up question to describe the difference in acidic strength). Some examples of correct responses are shown below.

Student H: "[pointing at left image] *This one represents a complete reaction so they all separate and go from HA to A and H+*, [pointing at middle image] *this one is not a complete reaction,* [pointing at right image] *and this one is a reaction that doesn't occur.*

Interviewer: "*If these are three images of different acids, what is the difference between the acids?"*

Student H: [pointing at left image] *The one is a strong acid as it completely dissociated,* [pointing at middle image] *this one would be a weak one because it didn't,* [pointing at right image] *this one, I don't know exactly, the reaction might not occur it didn't dissociate at all.*

Student I: "[pointing at left image] *This looks like a strong acid since it's completely dissociated,* [pointing at middle image] *this looks like a weak acid since it's partially dissociated,* [pointing at right image]: *and this could be an extremely weak acid.*"

Out of the four students coded as incorrect, three students were in the low performing group. One student identified the middle image as neutral with the image on the left as basic because, "*it has all base molecules,*" and the image on the right as acidic because, "*it has all acid molecules.*" The other three incorrect students used similar reasoning and identified the strongest acid as either basic, because it contained basic molecules, or neutral because there was an equal amount of base and H^+. All incorrect students identified the image representing the weakest acid as the strongest acid because it had all acid molecules.

When students were asked to relate the K_a values to the images, three students that correctly identified the relative strength of the acids reversed the order of the K_a values assigning the largest K_a value to the weakest acid. Three of the incorrect students identified the K_a correctly for how they assigned the relative strength of each image, identifying the largest K_a for the image they identified as the strongest acid and the smallest K_a to the image they identified as a base. One student was not asked this follow-up item.

When students were asked, "*In what ways do the models help you understand acid and base concepts?*" Only one student expressed that the models were confusing for them and explained:

"*The models were pretty confusing for me, especially during the activity. It's a good visual, but they are a little confusing, they take some getting used to. Which molecule is which and what way to connect them properly, and once you have bigger structure, like, what did I just create? I have no idea what it is.*"

The remaining 95% of students had positive comments about the models, often expressing that they were hands on learners or visual learners and the models helped them understand. Some examples of student response are shown below.

Student 1: "*They have the positive and negative charges which makes it a little bit easier to actually see it since obviously we can't physically see atoms it makes it easier to see it on a larger scale to be able to visualize."*

Student 2: *"I think the ability to be able to kind of take them apart and visualize the concepts. Just how like the models can bring what you are thinking in your mind to life.*"

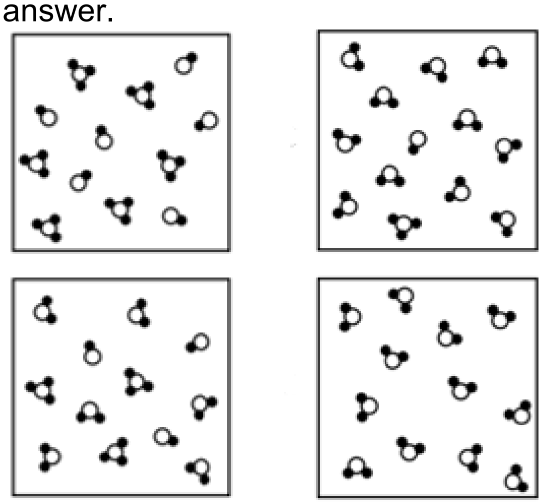
Student 3: "*These are more fun, they're more tangible than just numbers on a page or even writing on a whiteboard or chalkboard. That's honestly my answer, and I've gone through a bunch of chemistry courses, and these things are ridiculously helpful for* *people who are more hands on. So being able to play with these, pull them apart, see how they do or don't interact for that matter, how these can and cannot add to each other is extremely important in trying to understand something I think a lot of people struggle with.*"

Student 4: "*One important thing is to understand autoionization of water, it shows that really well. And then it also shows how acid protonate and how bases will accept it, like the Bronsted-Lowry concept pretty well. And I think, just like for most people, they can be visual learners, so I think models can be pretty beneficial to help someone understand, like bridge the gap between the confusion, I guess, between the two. I guess that's my stance on that."*

Assessment item five was analyzed case wise to make connections between interview responses related to the autoionization of water the pre- and post-results. Assessment item five used the same two images investigated in the interviews with two additional images shown in **figure 8.9.**

Figure 8.9: Pre- and post-assessment item five

Which image most realistically shows the autoionization of water? **Circle** your answer.



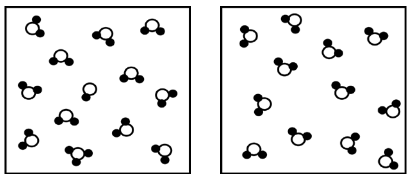
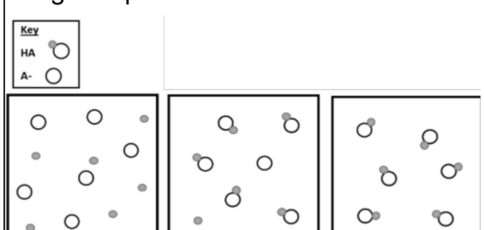
The image with all water molecules and the image with a single OH^- and H_3O^+ were both scored as correct on the pre- and post-assessment. Three students changed their response on the post-assessment. These students were in the lower performing group according to their mid-term 1 exam and all changed their response to the images with half ions and half water molecules in their post-assessment. Two originally responded with the image of all water molecules and one with the image of all ions.

Results to assessment item 20/21 were investigated case wise to connect interview responses for the pH of a very dilute HCl solution to the pre- and post-assessment results. Six students changed their pre-assessment response to item 20/21 from an incorrect response to a correct response on the post-assessment. Two of these students were in the low performing group and 4 students were in the high performing group. During the interview only 3 students answered the incorrect basic pH, two in the high performing group and 1 in the low performing group. All three of these students showed an improvement in their understanding after completing the modeling activity in the interview.

Responses to learning module items 29-32 in modeling activity three were analyzed for evidence of learning. Item 29 had students calculate the pH of a solution containing 2.3×10^{-9} M HCl. Results showed all groups incorrectly answered the same basic pH. Item 30 asked if the pH calculated in item 29 was reasonable. Five out of six groups answered “no” to item 30. In item 31 all six groups indicated that the autoionization of water should be considered when calculating the pH of a very dilute acid solution. In item 32 (calculate the pH of a 5.8×10^{-9} M HCl solution) three groups included the autoionization of water in their calculation to get an acidic pH, while three groups still calculated a basic pH using just the concentration of HCl.

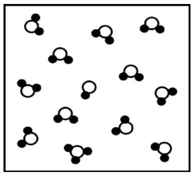
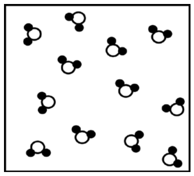
Students’ responses as they progressed through the interview items provided additional evidence of students’ understanding. The responses to the interview items from two students in the high performing group is shown in **table 8.19.**

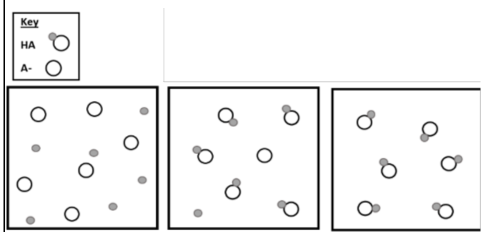
Table 8.19: Example of high performing students' interview responses

Interview item	Response	
	Student 1	Student 2
Which image do you think most realistically shows the autoionization of water? 	Student: *This one on the left because it shows hydronium, hydroxide, and water.* Interviewer: *If a student selected this image* [right image] *would you consider that incorrect?* Student: *If you are asking the specific autoionization of water, I probably would, just because as water autoionizes it isn't just H_2O.*	Student: *I would say this one* [left image] *because you can see one hydronium and one hydroxide in very small proportion compared to water which shows the K_w value.* Interviewer: *"Would you consider the other image* [left image] *to be incorrect?* Student: *Well, I think the picture is not showing autoionization.*
In what aqueous systems is the autoionization of water occurring?	Student: *The autoionization of water occurs in any aqueous system. It's always relevant if anything is in aqueous solution. It's always part of that system.*	Student: *I would say all of them.* Interviewer: *What do mean by all of them?* Student: *Any aqueous systems the autoionization of water is occurring no matter what else. Although other interactions might be happening water is still interacting with itself.*
Two students calculated the pH of a dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below. A. Student 1, pH = 8.30 B. Student 2, pH = 6.99 Which pH is more reasonable, 8.30 or 6.99?	Student: *Right off the bat since it's an acid logically you'd think it would be under 7. So, I'd say student 2 would be correct because 8.30 is above 7 meaning it'd be basic.* Interviewer: *What's the relationship to a pH of 7?* Student: *It'd be neutral. Anything under 7 would be acidic and over would be basic.*	Student: *Without any calculations, I would say answer B would make more sense because it's an acid and you expect a pH lower than 7.* [After modeling the dilute solution] Interviewer: *Did the modeling support your answer?* Student: *I think so, with the models I was able to make more hydronium and a higher concentration of hydronium will bring the pH down.*
Looking at the three images and the key, can you describe what these three images represent?"  Follow-up: Explain how you think the K_a values for the three acids shown would change.	Student: [Points to first image] *It looks like it completely dissociated so I'd say that's a pretty strong acid. This one [middle image] only dissociated one so it's pretty weak, and this one* [last image] *didn't dissociated at all showing different strength of a weak acid. This one would be the weakest* [pointing to last image]. Follow-up response: *The biggest Ka value would be for this one* [first image] *cause it's strong. I'd say the middle K_a, like 10^{-3}, would be this image* [middle image]. *It's not a strong acid but it's definitely stronger than the last one so I'd give the smallest K_a value to this guy* [last image] *because it doesn't dissociate very much compared to the one in the middle.*	Student: [Points to first image] *This is a strong acid*. [middle image] *This is weak acid. And, I'm not sure* [pointing to last image], *umm. . .* Interviewer: *What are you thinking about this image?* Student: *It's not dissociating at all.* Interviewer: *Any idea what the value of the K_a is for each of those images, approximately?* Student: *This would be a Ka bigger than one* [first image], *this is lower than one* [middle image], *and this maybe, is like, very very low* [last image].

Ten of the 19 students that were interviewed were in the high performing group. The responses from the two students shown in table 8.16 are representative of the responses from students in the high performing group and provide evidence of these students' understanding of the autoionization of water, pH, and relationship between acidic strength and K_a values. It also shows these students were able to correctly interpret the particle-level images of the autoionization of water and the ionization of weak acids. This is representative of the responses from students in the high performing group. Only two high performing students did not initially answer all items correctly. Those two students responded incorrectly to interview item three initially by selecting the basic pH, but changed their response after completing the modeling activity (as discussed in the results to interview item three). One student in the high performing group that initially answered item three incorrectly also answered item four incorrectly by describing the acidic strength represented in the images in the opposite order. This student did not change their response after follow up items and was the only high performing student to incorrectly respond to item four compared to three students in the low performing group that incorrectly responded to item four. This indicates that more low performing students struggled to correctly interpret particle-level images compared to high performing students. It also suggests that some high performing students may need additional instruction to correctly interpret particle-level representations. To compare example responses from students in the low performing group, the progression of the interview responses from two student in the low performing group is shown in **table 8.20.**

Table 8.20: Example of low performing students' interview responses

Interview item	Response	
	Student 1	Student 2
Which image do you think most realistically shows the autoionization of water?  	Student: *This first one* [left image] *because the autoionization of water is two H_2O going to H_3O^+ and OH^-.* Interviewer: *If a student selected this image* [right image] *would you consider that incorrect?* Student: *Yes, because it shows water but it doesn't show the autoionization of water.*	Student: *This one* [left image] *because there's H3O+ and OH- and other H2O molecules. This one just has H2O molecules* Interviewer: *"Would you consider the other image* [left image] *to be incorrect?* Student: *I guess, because it doesn't actually show the autoionization at all. It just shows H2O molecules*
In what aqueous systems is the autoionization of water occurring?	Student: *The autoionization of water is occurring in, like, acids and base to form H_3O^+ and OH^-.* Interviewer: *Does the autoionization only occur in acid and base solutions?* Student: *No* Interviewer: *Can you think of other aqueous systems?* Student: *Not of the top of my head.* Interviewer: *What does aqueous mean?* Student: *It means it contains water.* Interviewer: *Are there any aqueous systems that you think it would not be occurring in?* Student: *No*	Student: *Oh, like all the experiments we do. All the time. Water is always involved so, autoionization happens anytime water is included. In all of our titration systems.* Interviewer: *Are there any aqueous systems where it would not be occurring?* Student: *It's not going to happen unless water is present.* Interviewer: *Does water have to be present to have an aqueous system?* Student: *Yeah* Interview: *In an aqueous system is autoionization occurring?* Student: *Yes, for anytime there is water.*
Two students calculated the pH of a dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below. A. Student 1, pH = 8.30 B. Student 2, pH = 6.99 Which pH is more reasonable, 8.30 or 6.99?	Student: *6.99* Interviewer: *Why did you chose that answer* Student: *Because hydrochloric acid is a strong acid and the 8.30 is basic.*	Student: *6.99* Interviewer: *Can you explain why?* Student: *Because HCl is a really strong acid so there's no way it should be above 7.* Interviewer: *What is the pH of a neutral solution?* Student: *7* Interviewer: *How does pH change when you add an acid?* Student: *The pH is going to be reduced.*

Looking at the three images and the key, can you describe what these three images represent?"  Follow-up: Explain how you think the K_a values for the three acids shown would change.	Student: *The first image represents where there is mainly A^- and hydrogens and the next one* [middle image*] is mainly HA with only one hydrogen and A^- and the last one is all HA molecules.* Interviewer: *If each image is a different acid. Can you tell me the difference between the acids?* Student: *They would have different pH's* Interviewer: *What cause the pH difference?* Student: *The pH would change because the pH measures free hydrogens are in a solution.* Interviewer: *How would the pH change for each acid?* Student*: I'd say more acidic* [first image], *less acidic* [middle image], *and even less acidic* [last image] Interviewer: *Can you describe it in terms of acid strength?* Student: *It would be a strong acid* [first image] *to a weak acid* [last image] Response to follow-up: *Higher K_a* [last image] *and lowest K_a* [first image].	Student: [First image] *This is a neutral solution because it's an A^- molecule and an H^+. This one* [middle image] *has mainly acid parts so this solution is probably more acidic. And this one is fully acidic* [pointing to last image], it'*s like very acidic.* Interviewer: *Can you explain what makes this one* [last image] *the most acidic?* Student: *It's the most acidic because it doesn't have any lone base molecules and HA stands for acid.* Interviewer: *When you said this one is neutral* [first image] *can you explain?* Student: *These ones are base ions, the A-, and these ones are H^+ ions so there's six hydrogen ions and six base ions.* Interviewer: *If these images are showing three different acids, which of the three acids is the strongest? I'm just clarifying.* Student: *This one, yeah* [points at last image] *No base molecules*. Interviewer*: If I give you the HCl and acetic acid models so you have some different acids. Can you place the model on an image that best represent it?* Student: Places 3 unionized HCl on last image (student identified HCl as a really strong acid in question three) and one ionized and one unionized acetic acid model on the middle image. Response to follow-up: *Higher K_a is more acidic. This would have a high K_a* [last image] *and it would decrease* [points at middle image and then first image].

Three of the nine students in the low performing group answered all interview items correctly. All students that incorrectly connected K_a to acidic strength were in the low performing group. Results show more low performing students incorrectly interpreted particle-level images compared to high performing students even after completing the learning module and supports the need for more instructional support.

8.9 Conclusions

The results from the the pre- and post-assessment show significant positive learning gains in acid-base chemistry after completing the learning module. These results and analysis of the interview items supports the effectiveness of modeling-based teaching with physical three-dimensional acid-base models. The conclusions for each research question is discussed below.

1. Does an acid-base learning module using the novel acid-base models impact students' performance on acid-base content questions using a pre- and post-assessment?

Statistical analysis showed that students' scores on the post-test had a statically significant increase with a large effect size with an average gain of 1.3 points. This shows that the learning module positively impacted students' performance on acid-base questions. There was also a statistically significant increase in post-scores for both the high and low performing students with large effect sizes. The results from low and high performing groups are based on a small sample size, but still suggest the learning module had a positive impact on students in both groups. The low performing students showed an average gain of 1.63 points compared to an average gain of 1 point for the high performing students. These larger gain for students in the low performing group could be the result of the additional practice in the learning module. Analysis of the interview responses suggest that although low performing students, on average, had learning gains after completing the learning module, these students may still struggle to understand concepts in acid-base chemistry and may need additional instructional support to interpret particle-level images.

2. Does an acid-base learning module using the acid-base models impact students' understanding of the autoionization of water, acidic strength, pH, and K_a?

Statistical analysis for acid-base concept groups showed that students' scores on autoionization items significantly increased on the post-test compared to the pre-test. This group included six items that were considered both general practice and in-depth. Analysis of the four pre- and post-assessment items identified as "in-depth", in which the use of the models, and connections to the particle-level process of autoionization, was key to answering the item correctly, showed the mean of the post-scores increased, but not significantly. These results indicate the average gain in post-scores for autoionization items is due to additional practice items and the impact of the models. A future implementation with a control group completing the learning module without the models and treatment group completing the learning module with the models could help determine the impact from model use.

Interview responses explaining how the models helped students learn acid and base concepts suggests that the models did help students learn autoionization. Data from interview item three, asking students to pick the more reasonable pH of a very dilute HCl solution, showed the use of the models helped students in the high and low performing group and provided evidence that the models improved students processing when responding to this item. This modeling activity was not part of the learning module and suggests that this activity may be a good addition to help students connect the pH of a dilute acid solution to the particle-level process that influence pH.

Results from pre- and post-item five showed students in the lower performing group were able to connect the modeling to particle-level images of autoionization and changed their post-response more often than students in the high performing group. All three students in the low performing group that changed their response recognized that OH^- and H_3O^+ ions from autoionization could be present along with water molecules after the modeling activity, but did not fully connect the K_w value to the concentration of each species shown in the images. This suggests that lower performing students may need more modeling-based activities to support their learning and make connections between particle-level images and the K_w expression.

The model-based acidic strength grouping showed a statistically significant increase on post-scores with an average gain of 0.34 points. There were six items in the model-based acidic strength group. The results of all nine items in the acid strength group (practice and in-depth items) showed the same average gain (0.34 points) on post-scores but was not statistically significant. This supports that the significant gains in post-scores on the acid strength items was due to the use of the models and not simply additional practice. Scores from in-depth items related to acidic strength in the modeling activities ranged from 57.7-86.3% correctness with 100% engagement. This large range of scores may help explain why the average gain, although significant, was only 0.34 points for acidic strength items on the post-assessment. The two groups that did not complete modeling activity five (weak acid solution) may have impacted the average gain seen in post-scores and help explain why the average gain was small.

The significant increase in scores on the post-assessment for in-depth acidic strength items is supported by students' ability to interpret the particle-level images for acidic strength used in the interviews. Seventy nine percent of students in the interview were correctly able to identify the relative strength of all three acids. Out of the four students that did not correctly interpret the particle-level images, three were in the low performing group and one in the high performing group. This suggests that low performing students may benefit more from additional instruction connecting the ionization of acids to acidic strength and interpreting particle-level images. However, there is no indication that there is any negative impact on any students and all students may benefit. An additional modeling activity focused on different amounts of ionization of weak acids with connections to particle-level images may better support students' understanding of acidic strength.

The pre- and post-assessment items categorized as pH showed a statistically significant increase in post scores with an average gain of 0.80 points. This group included 12 pH items with only one item (20/21) identified as an in-depth item. Analysis from pre- and post-assessment item 20/21 and the interviews data for the same question, showed the use of the models helped both low and high performing students make connections to the ions in solution and the pH calculation.

There were five learning module items identified as in-depth pH items. The group scores on these items ranged from 40-80% with 100% engagement. A closer look at these five items showed the two lowest scoring items were in modeling activity three (very dilute HCl solution). All students incorrectly answered the first pH calculation by responding with a basic pH. However, the follow up items in modeling activity three showed student were engaged and the items successfully helped all groups consider the autoionization of water as a process that can influence pH. Three groups (50%) were able to connect the process of autoionization to a follow-up pH calculation and correctly calculate the pH of a very dilute strong acid.

8.10 limitations

One limitation for this study was analysis from a smaller than expected number of students in Analytical Chemistry. Another limitation is that not all concepts included in the learning module were included in the pre- and post-assessment items. The learning module included a modeling activity of a strong base solution (activity four) but no items on the assessment measured learning gains related to students' understanding of strong base solutions. Another limitation is from the two groups not completing all modeling activities. Some groups took longer and were not able to finish all the items in modeling activities five and six. Since these modeling activities included concepts related to autoionization and acidic strength smaller gains may have been seen from this analysis than if all participants had completed these modeling activities.

8.11 Implications for teaching and future implementation

The acid-base models are useful for students and could be implemented with students in introductory chemistry, general chemistry, or high school chemistry courses to better prepare them for an analytical chemistry course. The results of this research support the effectiveness of modeling-based teaching using three-dimensional acid-base models and accompanying learning module to supports students' understanding of the particle-level processes in aqueous acids and concepts related to the autoionization of water, pH, and acidic strength.

An additional modeling activity for a dilute strong acid solution connecting the process of autoionization to pH calculations may be necessary to support students' understanding of different processes that can influence the pH of an acid solution. Adding an activity prompting student to build models showing different amounts of acid ionization and drawing corresponding particle-level images may better support students' understanding of acid-base strength and connections between the particle-level processes and images representing weak acid ionization.

Results from future implementations may be clearer if learning activity four (strong base solution) is taken out of the learning module to allow students to focus on the concepts covered in the pre- and post-assessment items. The removal of modeling activity four would also allow more time for students to complete the learning module as a single laboratory activity. The concepts related to strong bases covered in modeling activity four could be saved for a different learning activity for a future study using the models.

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Appendices

Appendix A: Laboratory and quiz schedule for fall 2018 and spring 2019 semesters. Quiz given during second lab session of the week listed is noted with a "Yes".

Week	Lab	Fall 2018	Quiz F2018	Lab	Spring 2019	Quiz S2019
1		Lab safety and check in			Lab safety and check in	
2	1	Acid-Base Titrimetry: Determination of Acetic Acid in Commercial Vinegar	No	1	Acid-Base titrimetry: Determination of Acetic Acid in Commercial Vinegar	No
3	2	Ion-Exchange/ Acid-Base Titrimetry: Determination of Calcium in Dietary Supplement tablets	No	2	Ion-Exchange/ Acid-Base Titrimetry: Determination of Calcium in Dietary Supplement tablets	Yes
4	3	Complexation Titrimetry: Determination of Calcium in Dietary Supplement tablets	No	3	Complexation Titrimetry: Determination of Calcium in Dietary Supplement tablets	Yes
5		Improvement lab/Exam review			Improvement lab/Exam review	
6	4	Precipitation Gravimetry: Determination of Chloride in water by Fajan's Method	Yes	4	Precipitation Gravimetry: Determination of Chloride in water by Fajan's Method	Yes
7	5	Acid-Base Titrimetry: Determination of Carbonate in Soda Ash	Yes	5	Acid-Base Titrimetry: Determination of Carbonate in Soda Ash	Yes
8	6	Redox Titrimetry: Determination of Sodium Hypochlorite in Laundry Bleach	Yes	6	Redox Titrimetry: Determination of Sodium Hypochlorite in Laundry Bleach	Yes
9		Improvement lab/Exam review			Spring Break	
10	7	UV-visible Spectrophotometry: Determination of Phosphate Commercial Detergent	Yes	7	Spectrophotometric Determination of the pKa of an Acid-Base Indicator	Yes

11	8	Complexation Titrimetry: Formula of a Complex Ion by the Mole Ratio Method	Yes		Improvement lab/Exam review	
12		Thanksgiving break		8	UV-visible Spectrophotometry: Determination of Phosphate Commercial Detergent	Yes
13	9	Fluorescence Spectroscopy: Determination of Quinine in Tonic Water	Yes	9	Complexation Titrimetry: Formula of a Complex Ion by the Mole Ratio Method	Yes
14		Improvement lab		10	Fluorescence Spectroscopy: Determination of Quinine in Tonic Water	Yes
15		Exam review/lab check out	Yes		Improvement lab	
16		(no week 16 in fall 2018 semester)			Exam review/lab check out	Yes

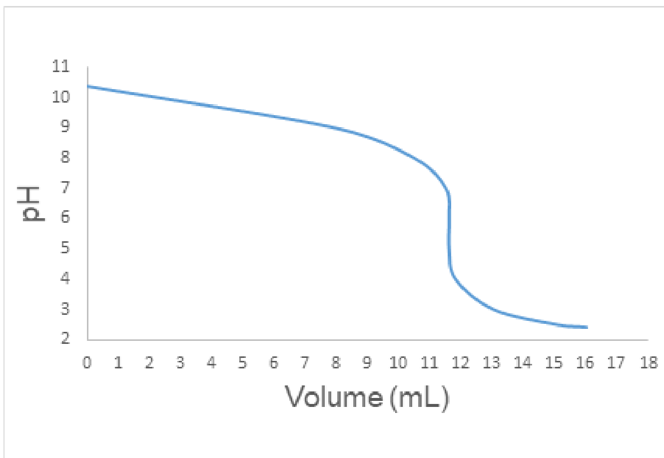
Appendix B: Subset of fall 2018 and spring 2019 acid-base questions analyzed

1. Why was it important to control the pH in this experiment?

2. What is pH?

3. What is a conjugate acid-base pair? Please explain with as much detail as possible using an example.

4. Draw an arrow pointing to the equivalence point on the titration curve below.



   a) A good indicator to mark the end point of this titration would change colors at approximately what pH?

   b) The titrant in an experiment producing this titration curve is a ___________

      a) Strong acidb) strong base c) weak acid d) weak base

5. Clearly identify all the conjugate acid-base pairs in the reaction below. **Label each species in the conjugate acid-base pair as the <u>acid</u> or the <u>base</u>.**

   i. $PO_4^{3-} + H_2O \rightleftharpoons HPO_4^{2-} + OH^-$

   Conjugate acid-base pair 1:

   Conjugate acid-base pair 2:

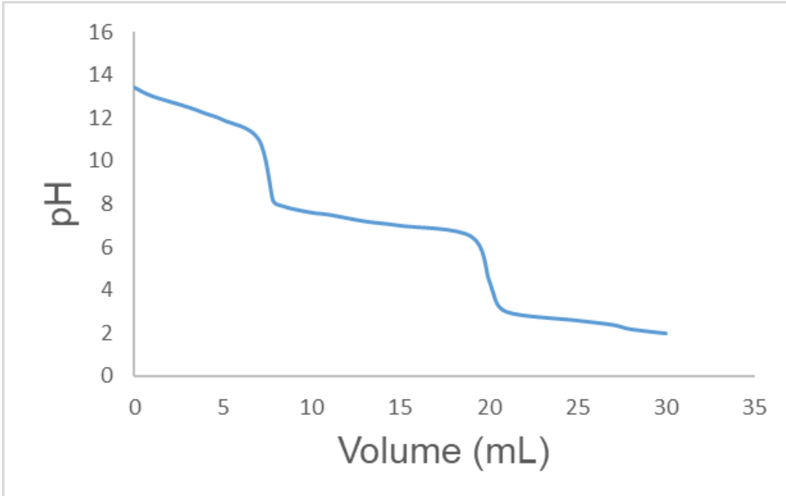
   ii. $H_2CO_2 + CN^- \rightleftharpoons HCN + HCO_2^-$

   Conjugate acid-base pair 1:

   Conjugate acid-base pair 2:

Use the titration curve below to answer questions 6-8

6. Draw an **arrow(s)** pointing to the equivalence point(s) on the titration curve below.



7. The titrant in this experiment is a ___________________

    a) strong base b) weak base c) strong acid d) weak acid

8. A possible analyte for the titration curve above is ___________________

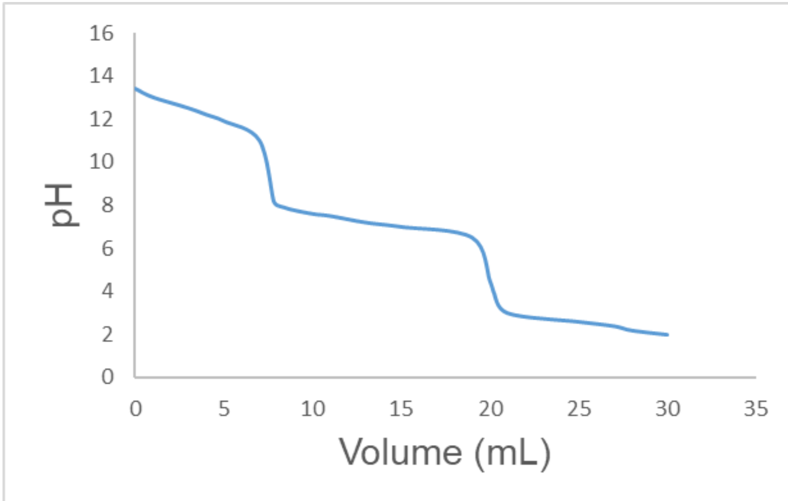
Circle all that apply

NH_4^+ PO_4^{3-} CO_3^{2-} SO_4^{2-} NO_3^-

9. Complete the table below by circling the correct pH in each box in column 2. Then explain how you made your choice in column 3.

Titration type	pH at the equivalence point	Explain your choice. (Excess of what species leads to this pH?)
strong acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak base – strong acid	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	

10. Draw an **arrow(s)** pointing to the equivalence point(s) on the titration curve below.



11. The titrant in this experiment is a ___________________

b) strong base b) weak base c) strong acid d) weak acid

12. A possible analyte for the titration curve above is ___________________

Circle all that apply

NH_4^+ PO_4^{3-} CO_3^{2-} SO_4^{2-} NO_3^-

Correctly complete each statement below by circling the correct **bolded and underlined** word in each question below.

13. A strong acid/weak base titration will have a pH **greater / less** than 7 at the equivalence point?

14. A weak acid/strong base titration will have a pH **greater / less** than 7 at the equivalence point?

Appendix C: Coding of acid-base Items from fall 2018 and spring 2019

Item 1) Why was it important to control the pH in this experiment?	
Code	Description
acidic/basic	Describes acidic, basic, acidity or basicity in response
deprotonate	Describes deprotonation in response. May or may not be directly linked to indicator – must express loss of proton.
ionization/ dissociation	Describes or uses ionization or dissociation in response, but does not specify the species ionizing (proton)
end point/ equivalence point	Describes end point or equivalence point in response.
indicator function	Describes indicator will only function in specific pH or describes indicator as pH dependent or pH sensitive.
ion interactions	Describes general ion interactions in response
Level of understanding	Description
Sound understanding	Connects specific pH (high or basic) to deprotonation of indicator and function of indicator.
Correct with partial understanding	Expresses understanding that indicator functions in a specific pH, but does not connect to deprotonation of indicator or pH
Incorrect with partial understanding	Refer to interactions between ions being affected by pH, but gives no clear connection between basic pH and specific species/ions, or indicator function
No understanding	Describes the pH as indicating if the solution is acid or basic, but does not connect to any species or the indicator function. Response is illogical or does not apply to question
Item 2) What is pH?	
Code	Description
Mathematical definition	pH=-log[H+] or pH equals the negative log of the hydrogen/H+ concentration
Range or scale definition	Describes a logarithmic scale, pH scale, or pH range (low/high pH is acid/basic).
General definition	Describes general measurement of acidity, basicity, or H+, but does not include enough details to fit into the concentration or scale definition
Concentration definition	Describes measure of concentration of H+, proton, hydronium or hydrogen ions
Power of hydrogen	Uses the specific phrase “power of hydrogen” in response.
Level of understanding	Description
Sound understanding	Correctly defines pH using at least two concept codes other than “power of hydrogen”.

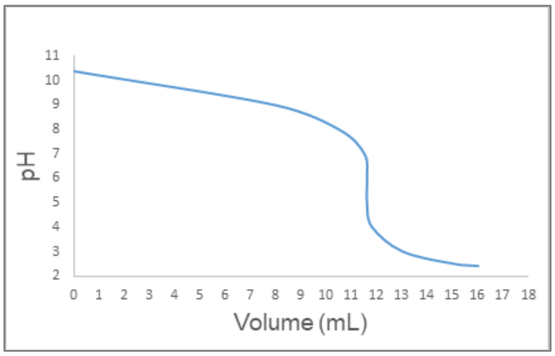
Correct with partial understanding	Correctly uses just one concept code to define pH (excluding "power of hydrogen")
Incorrect with partial understanding	Incorrectly describes a concept code (i.e. a high pH is acidic or pH ranges from 1-7) to explain pH
No understanding	Does not describe pH, answer is illogical or does not apply to question, or only uses phrase "power of hydrogen"

Item 3) What is a conjugate acid-base pair. Please explain with as much detail as possible using an example.

Code	Description
Acid reacts with base	Explicitly describes the acid and base reacting together. Not coded for using the word react, reacts, reaction if used more generally (i.e. "*In a reaction when the acid loses its H….*")
Autoprotolysis	Specifically uses the term autoprotolysis in response
Buffer	Uses the term buffer in response, relates questions to buffers
Neutralization	Uses a neutralization reaction as the example and/or describes a neutralization reaction in response. Any neutralization example where water and a salt are formed.
Proton/H+ relationship	Describes relationship between movement of H+, proton, or hydrogen atom and conjugate pair, or shown in example by labeling each species
Reverse or opposite reaction	Describes conjugate pair by using the terms "reverse" or "opposite" reaction.
Strength relationship	Expresses the acid or base must be a weak species
Strong acid/base	Uses a strong acid and/or strong base in the example but does not show neutralization. Must shows correct movement of the proton between pair
Generic example	Uses generic species in their example, such as HA, BOH, AB + CD, etc. instead of real compounds
Correct example	Includes a correct example. This can be in the form of a single pair (i.e. H_2O/OH^-) or in an equation. Must show correct movement of proton
Incorrect example	Example does not correctly show the movement of the proton between pairs (i.e. HCl and NaCl)
No example	No example provided
Level of understanding	**Description**
Sound understanding	Gives a correct example with a clear definition that describes or shows the movement or loss/gain of proton between pair.

Correct with partial understanding	Response includes only a correct example with species labeled but not a correct definition, or correct definition (describes the proton/H+ relationship) but does not provide an example
Incorrect with partial understanding	Response included relevant concepts used incorrectly or unclearly with no example or an incorrect example (i.e. $HCl + NaOH \rightarrow H_2O + NaCl$).
No understanding	Irrelevant or incorrect information given without an example or with an incorrect example (i.e. describes neutralization reaction and shows neutralization reaction as example), or incorrect example with no explanation

Item 4) Draw an arrow pointing to the equivalence point on the titration curve below.



a) A good indicator to mark the end point of this titration would change colors at approximately what pH?

b) The titrant in an experiment producing this titration curve is a ___________

a) Strong acid b) strong base c) weak acid d) weak base

Code: part 1	Identification of Eq. point with arrow	Correctness Code
Equivalence point	Arrow pointing to the vertical section of graph	Correct
Top of curve	Above the vertical section of graph	Incorrect
Bottom of curve	Below the vertical section of graph	Incorrect
Code: part a)	Numeric open-response	Code
Correct pH	pH between 5-6	Correct
Basic pH	pH greater than or equal to 11 (no responses between >7 to <11)	Incorrect
Neutral pH	pH = 7	Incorrect
pH below 5	pH below 5	Incorrect
pH matches marked eq. point	If numeric pH given corresponded to location arrow was drawn.	
Code: part b)	Multiple-choice response	
Correct	Choice a circled	
incorrect	Choice b, c, or d circled	

Item 5) Clearly identify all the conjugate acid-base pairs in the reactions below. **Label each species in the conjugate acid-base pair as the <u>acid</u> or the <u>base</u>.**

i) $PO_4^{3-} + H_2O \leftrightarrow HPO_4^{2-} + OH^-$

Conjugate acid-base pair 1:

Conjugate acid-base pair 2:

ii) $H_2CO_2 + CN^- \leftrightarrow HCN + HCO_2^-$

Conjugate acid-base pair 1:

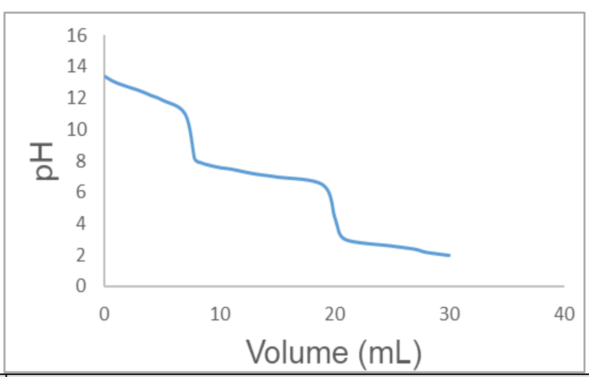
Conjugate acid-base pair 2:

Code	Description
Correct pairs & identification	Shows all correct pairs and correct identification
Missing identification	Correct pairs shown but response does not include all identification of which species is the acid or the base
No clear pair	Does not clearly identify the acid-base conjugate pair or includes a single species as a pair
Reversed acid/base identification	Correct pairs shown but the base is identified as an acid and the acid is identified as the base

Level of understanding	Description
Sound understanding	Coded with correct pairs and identification
Correct with partial understanding	Coded with missing identification
Incorrect with partial understanding	Coded with no clear pair or reversed acid/base identification
No understanding	Response does not answer question or shows a single species for all pairs – no pairs shown

Use the titration curve below to answer questions 6-8

Item 6) Draw an **arrow(s)** pointing to the equivalence point(s) on the titration curve below.



Code	Description	Correctness code
Equivalence point	Arrows point to the vertical sections of graph	Correct
Top of curve	Above the vertical sections of graph	Incorrect
Bottom of curve	Below the vertical sections of graph	Incorrect

Item 7) The titrant in this experiment is a ___________________

c) strong base b) weak base c) strong acid d) weak acid

Code	Description
Correct	Circled option c
Incorrect	Circled option a, b, or d

Item 8) A possible analyte for the titration curve above is ___________________

Circle all that apply

NH_4^+ PO_4^{3-} CO_3^{2-} SO_4^{2-} NO_3^-

Code	Description
Sound understanding	Response included both dibasic compounds CO_3^{2-} & SO_4^{2-}
Correct with partial understanding	Responses with: 1) CO_3^{2-}, SO_4^{2-} and PO_4^{3-} 2) CO_3^{2-} and PO_4^{3-} 3) SO_4^{2-} and PO_4^{3-} 4) CO_3^{2-} 5) SO_4^{2-} (Titration curves of tribasic compounds like phosphate may look dibasic as all equivalence points may not be clearly visible).
Incorrect with partial understanding	Response is only PO_4^{3-} or NO_3^- or response includes any anion and NO_3^-
No understanding	Response includes NH_4^+ alone or in any combination

Item 9) Complete the table below by circling the correct pH in each box in column 2. Then explain how you made your choice in column 3.

Titration type	**pH at the equivalence point**	**Explain your choice. (Excess of what species leads to this pH?)**
strong acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak base – strong acid	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	

Code: column 2	Description
Correct	Circled correct pH in all three boxes
Incorrect	Circled incorrect pH (10 response were coded as incorrect with 9/10 students circling the correct pH for the strong acid-strong base titration but reversed the pH for the weak-strong titrations. The remaining response circled the same pH multiple times)

Code: column 3	Description
Amount of Ionization of acid or base	Response uses the term ionization, dissociation, dissociate, dissociates, or dissociated in explanation

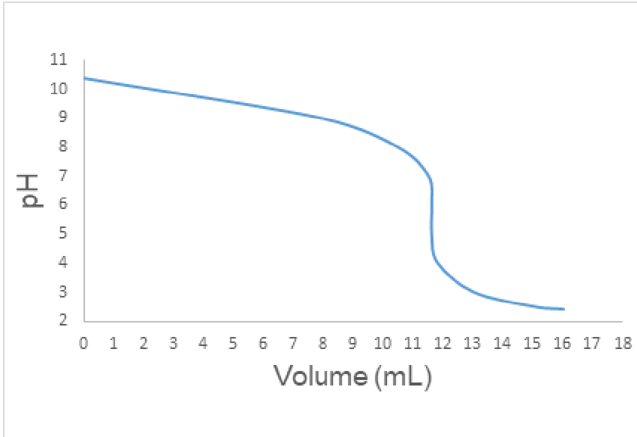
Excess species to match pH	Explanation is the species H_2O, OH-, H+ associated with the pH of that species (ie. pH is greater than 7 excess species is OH-, pH is less than 7 excess species is H+).
[H+]=[OH-]	Describes the hydrogen ion and hydroxide ion are in equal concentration or shows symbolically [H+]=[OH-] (Only occurred in strong acid-strong-base titration explanations)
Autoprotolysis	Uses the term autoprotolysis in explanation
Forms water	Response state strong acids and bases form water Or shows equation: $H^+ + OH^- \rightarrow H_2O$ (Only occurred in strong acid-strong-base titration explanations)
Neutralization	Use the term neutralize, neutralizes, or neutral to explain pH. (Only occurred in strong acid-strong-base titration explanations)
No excess species	Response states no species is in excess (Only occurred in strong acid-strong-base titration explanations).
Unclear reasoning	The reasoning does not fit into any other concept code and explanation is unclear
Conjugate of weak acid or base	Response includes the term “conjugate” to explain pH trend in strong/weak titration. (Only occurred in weak-strong titration explanations)
Excess strong species	States the strong species is in excess. (Only occurred in weak-strong titration explanations)
Excess weak species	States the weak species is in excess. (Only occurred in weak-strong titration explanations)
Strong species dominates	Response describes the strong acid or strong base as dominating the solution. Does not specify what will be in excess, but indicates strong species is responsible for pH. (Include terms dominates, contributes more, overpowers, takes over, and more influence. (Only occurred in weak-strong titration explanations)
Item 10) Identical to item 6	
Item 11) Identical to item 7	
Item 12) Identical to item 8	
Item 13 and 14	Correctly complete each statement below by circling the correct **bolded and underlined** word in each question below. 13. A strong acid/weak base titration will have a pH **greater / less** than 7 at the equivalence point? 14. A weak acid/strong base titration will have a pH **greater / less** than 7 at the equivalence point?

Code	Description
Correct (item 13)	Circled less
Incorrect (item 13)	Circled greater
Correct (item 14)	Circled greater
Incorrect (item 14)	Circled less

Appendix D: Results of qualitative coding of acid-base quiz item responses

Item 1) (N=54) Why was it important to control the pH in this experiment?		
Code	# of responses	Percent
acidic/basic	6	11.1
deprotonate	4	7.4
ionization/ dissociation	9	16.7
end point/ equivalence point	12	22.2
indicator function	18	33.3
ion interactions	18	33.3
Sound understanding	12	22.2
Correct with partial understanding	15	27.8
Incorrect with partial understanding	15	27.8
No understanding	12	22.2
Item 2) (N=58) What is pH?		
Mathematical definition	22	37.9
Range or scale definition	24	41.4
General definition	21	36.2
Concentration definition	29	50.0
Power of hydrogen	3	5.2
Sound understanding	27	46.6
Correct with partial understanding	26	44.8
Incorrect with partial understanding	3	5.2
No understanding	2	3.4
Item 3) (N=58) What is a conjugate acid-base pair. Please explain with as much detail as possible using an example.		
Acid reacts with base	5	8.6
Autoprotolysis	2	3.4
Buffer	2	3.4
Neutralization	11	19.0
Proton/H+ relationship	23	39.7
Reverse or opposite reaction	4	6.9
Strength relationship	6	10.3
Strong acid/base	7	12.0
Generic example	8	13.8
Correct example	26	44.8
Incorrect example	18	31.0
No example	14	24.1
Sound understanding	14	24.1
Correct with partial understanding	14	24.1
Incorrect with partial understanding	17	29.3
No understanding	13	22.4

Item 4) Draw an arrow pointing to the equivalence point on the titration curve below.



c) A good indicator to mark the end point of this titration would change colors at approximately what pH?

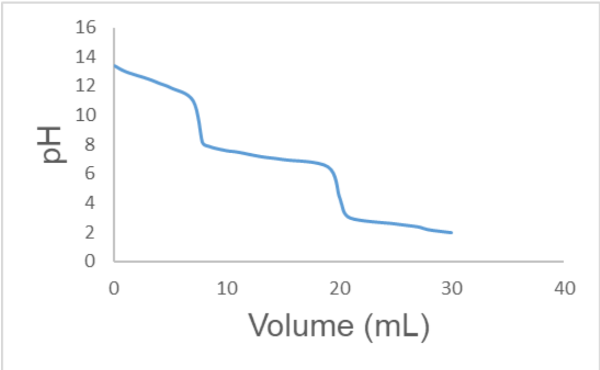
d) The titrant in an experiment producing this titration curve is a ___________

a) Strong acid b) strong base c) weak acid d) weak base

Code: Part 1 (N=56)	# of responses	percent
Equivalence point	40	71.4
Top of curve	15	26.8
Bottom of curve	1	1.8
Correct	40	71.4
Incorrect	16	28.6
Part 2 (a) (N=58)	# of responses	percent
Correct pH	29	50.0
Basic pH	8	13.8
Neutral pH	14	24.1
pH below 5	7	12.1
pH matches marked eq. point	36	64.3
Correct	29	50.0
Incorrect	29	50.0
Part 3 (b) (N=57)	# of responses	Percent
Correct	34	59.6
incorrect	23	40.4

Item 5) (N=55) Clearly identify all the conjugate acid-base pairs in the reactions below. **Label each species in the conjugate acid-base pair as the <u>acid</u> or the <u>base</u>.** i)$PO_4^{3-} + H_2O \leftrightarrow HPO_4^{2-} + OH^-$ Conjugate acid-base pair 1: Conjugate acid-base pair 1: ii)$H_2CO_2 + CN^- \leftrightarrow HCN + HCO_2^-$ Conjugate acid-base pair 1: Conjugate acid-base pair 1:		
Code	# of responses	Percent
Correct pairs and identification	33	60.1
Missing identification	16	29.1
No clear pair	2	3.6
Reversed acid/base identification	3	5.58
Sound understanding	33	60.0
Correct with partial understanding	16	29.1
Incorrect with partial understanding	5	9.1
No understanding	1	1.8

Item 6 (N=54) and item 10 (N=48)
Draw an **arrow(s)** pointing to the equivalence point(s) on the titration curve below.



Code	# of responses		Percent	
	Item 6	Item 10	Item 6	Item 10
Equivalence point	45	42	83.3	87.5
Top of curve	5	6	9.3	12.5
Bottom of curve	4	0	7.4	0.0
Correct	45	42	83.3	87.5
Incorrect	9	6	16.7	12.5

Item 7 (N=55) and item 11 (N=54)
The titrant in this experiment is a ________________

d) strong base b) weak base c) strong acid d) weak acid

Code	Number of responses		Percent	
	Item 7	Item 11	Item 7	Item 11
Correct	29	35	52.7	64.8
Incorrect	26	19	47.3	35.2

Item 8 (N=55) and item 12 (N=54)
A possible analyte for the titration curve above is ________________

Circle all that apply

NH_4^+ PO_4^{3-} CO_3^{2-} SO_4^{2-} NO_3^-

Code	Number of responses		Percent	
	Item 8	Item 12	Item 8	Item 12
Sound understanding	16	19	29.1	35.2
Correct with partial understanding	12	8	21.8	14.8
Incorrect with partial understanding	14	14	25.5	25.9
No understanding	13	13	23.6	24.1

Item 9 Complete the table below by circling the correct pH in each box in column 2. Then explain how you made your choice in column 3.

Titration type	**pH at the equivalence point**	**Explain your choice. (Excess of what species leads to this pH?)**
strong acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak acid – strong base	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	
weak base – strong acid	pH < 7 (less than 7) pH = 7 pH > 7 (greater than 7)	

Code: column 2 (N=58)	# of responses	Percent
Correct	48	82.8
Incorrect	10	17.2
Code: column 3 (N=57)	# of responses	Percent
Amount of ionization of acid or base	22	38.6
Excess species to match pH	7	12.3

[H+]=[OH-]	9	15.8
Autoprotolysis	2	3.5
Forms water	11	19.3
Neutralization	15	26.3
No excess species	7	12.3
Unclear reasoning	9	15.8
Conjugate of weak acid or base	3	5.3
Excess strong species	21	36.8
Excess weak species	3	5.3
Strong species dominates	12	21.1

Item 13 and 14 (N=54)
Correctly complete each statement below by circling the correct **bolded and underlined** word in each question below.

13. A strong acid/weak base titration will have a pH **greater / less** than 7 at the equivalence point?

14. A weak acid/strong base titration will have a pH **greater / less** than 7 at the equivalence point?

Code	Number of responses			percent		
	Item 13	Item 14	Item 13 & 14	Item 13	Item 14	Item 13 & 14
Correct	47	48	47	87.0	88.9	87.0
Incorrect	7	6	6	13.0	11.1	11.1

Appendix E: Qualtrics assessment items spring 2022 semester

1. Describe how water behaves as a solvent when the solute hydrogen chloride (HCl) is added to the water to make a solution. Explain how the particles interact with each other.

2. What intermolecular forces exist between water molecules?
   Select all that apply.

   ☐ Covalent bonding

   ☐ Dispersion forces (also known as London forces)

   ☐ Dipole-dipole forces

   ☐ Hydrogen bonding

   ☐ Ionic bonding

3. What is the equilibrium expression for the autoprotolysis of water (defined as K_w)?

   ○ $K_w = [OH^-]$

   ○ $K_w = [H_3O^+]$

   ○ $K_w = [H_2O]$

   ○ $K_w = [H_3O^+][OH^-]$

   ○ $K_w = \frac{[H_3O^+][OH^-]}{[H_2O]}$

4. What does the equilibrium expression for water, $K_w = [H_3O^+][OH^-]$, mean in your own words?

5. Which equation most accurately shows the autoprotolysis of water?
   Consider the reaction arrow when making your choice.

   ○ $H_2O + H_2O \rightleftharpoons H_3O+ + OH-$

   ○ $H_2O + H_2O \longrightarrow H_3O+ + OH-$

6. Which equation most accurately shows the autoprotolysis of water?

○ $H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$

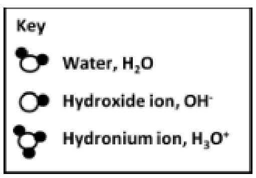
○ $H_2O \rightleftharpoons H^+ + OH^-$

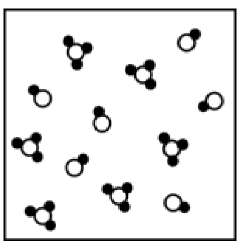
7. What are the H_3O^+ and OH^- concentrations in pure water at 25 °C with a pH=7? Please write a numeric answer for each species.

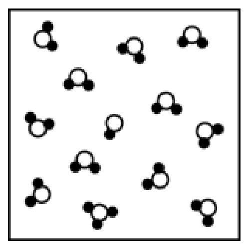
$[H_3O^+]$ =

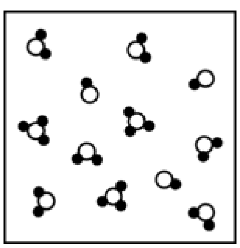
$[OH^-]$ =

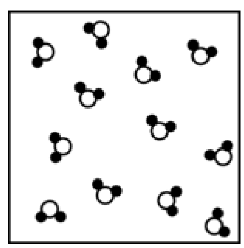
8. Which image most realistically shows the autoprotolysis of water?



○ 

○ 

○ 

○ 

9. Calculate the pH of water when the $[H_3O^+] = 1.0 \times 10^{-9}$ M.
($K_w = 1.0 \times 10^{-14}$)
Enter the pH value in the box below.

10. What is the pH of water when the $[H_3O+] = 1.6 \times 10^{-6}$ M?
   ($K_w = 1.0 \times 10^{-14}$)

   - ○ 0.8
   - ○ 5.8
   - ○ 6.3
   - ○ 8.2

11. Calculate the pH of water when the $[OH-] = 1.7 \times 10^{-6}$ M.
   ($Kw = 1.0 \times 10^{-14}$)
   Enter the pH value in the box below.

   [ ]

12. Are the equations **pH = -log [H+]** and **pH = -log [H3O+]** equivalent? Why or why not? Select your response and explain your reasoning in the box.

   - ○ Yes

     [ ]

   - ○ No

     [ ]

13. Calculate the concentration of H_3O^+ in water when the $[OH^-] = 2.90 \times 10^{-7}$ M.
   ($K_w = 1.0 \times 10^{-14}$) Enter the concentration (in M) in the box below.

   [ ]

14. Select **all** statements that are correct about pH?

☐ pH= -log [H+]

☐ pH is the measure of hydronium ions (H3O+) in solution

☐ pH is the measure of how neutral a solution is

☐ pH is the power of hydrogen

☐ pH measures the acidity of a solution ranging from a pH=1 (most acidic) and pH =7 (most basic)

☐ pH is a logarithmic scale of the hydronium ion concentration in solution

15. Consider the following reactions

$HCl(aq) + H_2O(l) \longrightarrow H_3O^+(aq) + Cl^-(aq)$

$HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$

Do these equations represent different reactions?

○ Yes

○ No

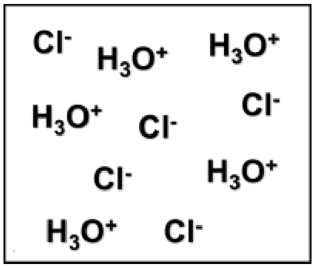
16. Which equation is a more realistic representation of HCl solution?

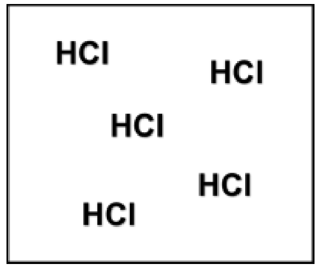
○ $HCl(aq) + H_2O(l) \longrightarrow H_3O+(aq) + Cl^-(aq)$

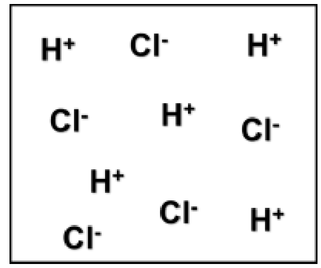
○ $HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$

17. In acid-base chemistry, the H+ ion is also referred to as a proton. Explain why these terms are equivalent.

18. When hydrogen chloride, HCl, ionizes in aqueous solution, which image below is the most realistic representation of the particles in solution? (H_2O molecules have been omitted for clarity.)







○ ○ ○

19. What does it mean when we describe an acid as strong?
Select the statement that you agree with most.

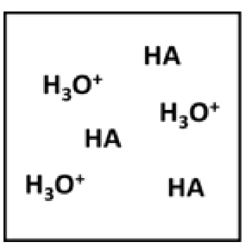
○ A strong acid contains more hydrogen atoms in its structure than a weak acid

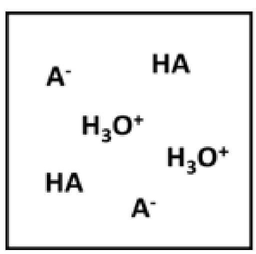
○ A strong acid is an acid with high concentration in solution.

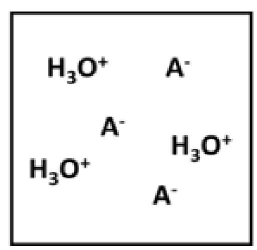
○ A strong acid will ionize into H+ and anion completely in aqueous solution.

○ A strong acid reacts with any base in solution to yield a solution with pH = 7

20. Generally, the reaction of a strong acid in aqueous solution can be shown as:
$HA(aq) + H_2O(l) \rightarrow H_3O+(aq) + A^-(aq)$
Which particle image below best represents a strong acid in aqueous solution? (Water molecules have been omitted for clarity.)







○ ○ ○

21. What is the pH of 0.050 M solution of HCl?

- ○ pH = 3.00
- ○ pH = 1.30
- ○ pH = -3.00
- ○ pH = -1.30

22. Calculate the pH of a 0.15 M solution of nitric acid (HNO3). Enter the pH in the box below.

Does the autoprotolysis of water need to be considered when calculating the pH above? Explain why or why not.

23. What is the pH of a solution containing 5.5 x 10-4 moles of HBr dissolved in 500 mL of water?

- ○ pH = 2.96
- ○ pH = 3.26
- ○ pH = 6.81
- ○ pH = 7.51

24. Two students calculated the pH of dilute solution of HCl with a concentration of 4.8×10^{-9} M.

Their answers are in the table below.

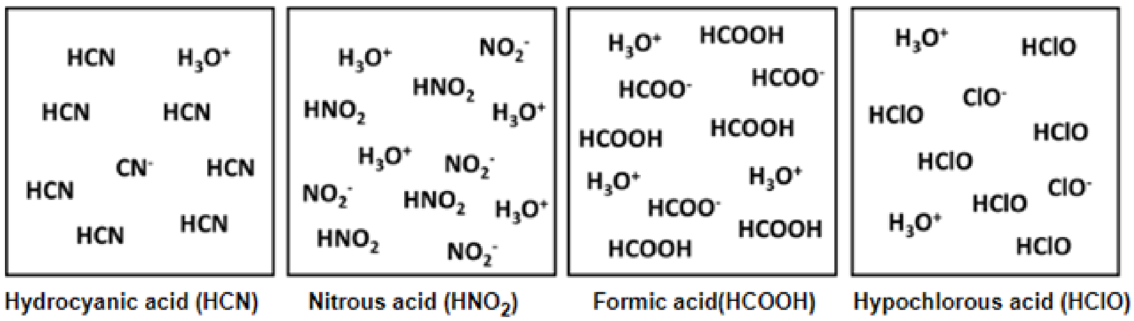
Student 1	pH = 8.30
Student 2	pH = 6.95

Which pH calculation is correct?

- ○ Student 1
- ○ Student 2

Does the autoprotolysis of water need to be considered when calculating the pH of a dilute acid solution? Explain why or why not.

25. The same concentration of four different acids (HCN, HNO_2, HCOOH, HClO) are shown below in aqueous solution. Based on these particle images, which acid is the strongest and which acid is the weakest? (H_2O molecules has been omitted for clarity)



Select the **strongest acid** based on the images above.

- ○ Hydrocyanic acid (HCN)
- ○ Nitrous acid (HNO_2)
- ○ Formic acid (HCOOH)
- ○ Hypochlorous acid (HClO)
- ○ Cannot be determined because they are all weak acids

Select the **weakest acid** based on the images above.

- ○ Hydrocyanic acid (HCN)
- ○ Nitrous acid (HNO_2)
- ○ Formic acid (HCOOH)
- ○ Hypochlorous acid (HClO)
- ○ Cannot be determined because they are all weak acids

26. HF and HCl are both binary acids, both containing hydrogen and a halogen atom. Despite these similarities, HF is considered a weak acid because it only ionizes partially in solution, while HCl is a strong acid that completely ionizes in water.

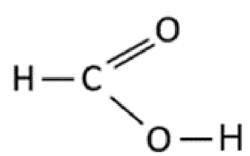
Based on the structures of HF and HCl, explain why HF is a weak acid and HCl is a strong acid. Please do not explain what it means to ionize partially or completely. Instead, explain **WHY** both acids behave differently.

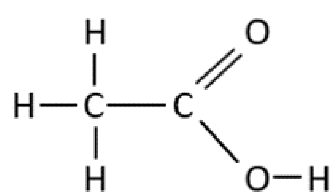
Which acid, HF or HCl, must have a stronger hydrogen-halogen bond?

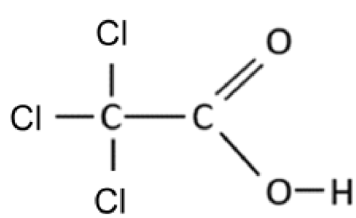
○ HF (the weak acid)

○ HCl (the strong acid)

27. Compare the structures of the three acidic molecules shown below. Rate the molecules from most acidic (1) to least acidic (3).







28. **Describe** what the acid ionization constant, K_a, value means. Do not give an equation or mathematical expression.

29. **Describe** what the base hydrolysis constant, K_b, value means. Do not write an equation or mathematical expression.

30. How are K_a and K_b related for a conjugate acid-base pair? Please explain in words and/or use a mathematical expression.

31. Select the correct statement about the acid ionization constant, Ka.

   - ○ Strong acids have a Ka > 1, weak acids have a Ka = 1
   - ○ Strong acids have a Ka = 1, weak acids have a Ka < 1
   - ○ Strong acids have a Ka < 1, weak acids have a Ka > 1
   - ○ Strong acids have a Ka > 1, weak acids have a Ka < 1

32. What does the term ***percent ionization*** (also called fraction of dissociation) mean in the context of acids and bases?
   Explain with as much detail as you can using examples and/or equations.

33. Select the statement that is **incorrect** about the fraction of dissociation.

   - ○ The fraction of dissociation multiplied by 100% is the percent an acid or base dissociates in solution
   - ○ The fraction of dissociation for a strong acid or strong base is very close to 1
   - ○ The fraction of dissociation is greater than 1 for any strong acid or strong base
   - ○ The fraction of dissociation of a weak acid is equal to the concentration of the conjugate base

34. What is the relationship between the pH and the pOH?

- ○ pH = pOH
- ○ pH = -pOH
- ○ pH + pOH = 7
- ○ pH + pOH = 14

35. Select the correct Ka expression for acetic acid (CH_3COOH).

- ○ $K_a = \dfrac{[H^+][CH_3COO^-]}{[CH_3COOH]}$
- ○ $K_a = \dfrac{[H^+][CH_3COOH]}{[CH_3COO^-]}$
- ○ $K_a = \dfrac{[H_2O][CH_3COO^-]}{[CH_3COOH]}$
- ○ $K_a = \dfrac{[CH_3COOH]}{[H^+][CH_3COO^-]}$

36. What is the pH of a 0.25 M solution of formic acid (HCOOH), Ka = 1.80 x 10-4?

- ○ pH = 0.60
- ○ pH = 2.17
- ○ pH = 3.74
- ○ pH = 4.35

What is the percent ionization for formic acid in this solution?

- ○ 2.68%
- ○ 41.7%
- ○ 16.3%
- ○ 100%

Appendix F: Final pre- and post-assessment items

1. Select the statement that best describes how water behaves as a solvent when the solute hydrogen chloride (HCl) is added to water to create a solution.

    A. Water is a polar solvent that attracts the hydrogen ion from hydrogen chloride (HCl) molecules to form an aqueous solution of H^+ and Cl^- particles.
    B. Water is a polar solvent that attracts the hydrogen ion from hydrogen chloride (HCl) molecules to form an aqueous solution of H_2 and Cl^- particles.
    C. Water is a polar solvent that dissolves the hydrogen chloride (HCl) molecules because water is in greater quantity that HCl
    D. Water is a polar solvent that attracts the hydrogen ion from hydrogen chloride (HCl) molecules to form an aqueous solution of H_3O^+ and Cl^- particles.

2. Which forces exist <u>between</u> water molecules?

Select all that apply.

A. Covalent bonding
B. Dispersion forces (aka London Dispersion forces)
C. Dipole-dipole forces
D. Hydrogen bonding
E. Ionic bonding

3. Write the equilibrium expression for the autoionization of water (defined as K_w)?

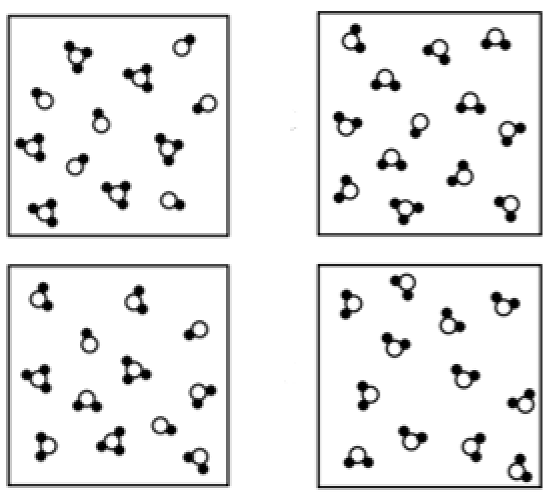
K_w =

4. Which equation most accurately shows the autoionization of water? Consider the reaction arrow when making your choice.

A. $H_2O + H_2O \leftrightharpoons H_3O^+ + OH^-$
B. $H_2O + H_2O \rightarrow H_3O^+ + OH^-$
C. $H_2O \leftrightharpoons H^+ + OH^-$
D. $H_2O \rightarrow H^+ + OH^-$

5. Which image most realistically shows the autoionization of water?

Circle your answer.



6. Calculate the pH of water when the $[H_3O^+] = 1.0 \times 10^{-9}$ M. ($K_w = 1.0 \times 10^{-14}$).

7. Calculate the pH of water when the $[OH^-] = 1.7 \times 10^{-6}$ M. ($K_w = 1.0 \times 10^{-14}$).

8. Are the equations **pH = -log $[H^+]$** and **pH = -log $[H_3O^+]$** equivalent? Select your response and add your reasoning underneath.

   A. Yes

   B. No

   Reasoning:

9. Calculate the H_3O^+ concentration and the pH for an aqueous solution with an $[OH^-] = 2.90 \times 10^{-7}$ M. ($K_w = 1.0 \times 10^{-14}$).

Calculation of $[H_3O^+]$:

Calculation of pH:

10. Select **all** statements that are correct about pH?

A. pH= -log $[H^+]$
B. pH is the measure of hydronium ions (H_3O^+) in solution
C. pH measures the acidity of a solution ranging from a pH=1 (most acidic) and pH =7 (most basic)
D. pH is a logarithmic scale of the hydronium ion concentration in solution

11. Do the equations below represent different processes?

$HCl(aq) + H_2O(l) \longrightarrow H_3O^+(aq) + Cl^-(aq)$

$HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$

A. Yes
B. No

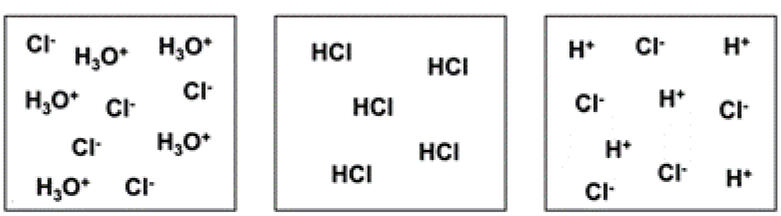
12. Which equation represents an aqueous HCl solution more realistically?

A. $HCl(aq) + H_2O(l) \longrightarrow H_3O^+(aq) + Cl^-(aq)$

B. $HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$

13. Explain why an H^+ ion can also be referred to as a proton.

14. When hydrogen chloride, HCl, ionizes in aqueous solution, which image below is the most realistic representation of the particles in solution? (H_2O molecules have been omitted for clarity.)



A. B. C.

15. Select the statements that are true for a strong acid.

    A. A strong acid contains more hydrogen atoms in its structure than a weak acid
    B. A strong acid is an acid with high concentration in solution.
    C. A strong acid will ionize into H+ and anion completely in aqueous solution.
    D. A strong acid reacts with any base in solution to yield a solution with pH = 7

16. What is the pH of 0.050 M solution of HCl?

    A. pH = 3.00
    B. pH = 1.30
    C. pH = -3.00
    D. pH = -1.30

17. Calculate the pH of a 0.15 M solution of nitric acid (HNO_3).

18. Does the autoionization of water need to be considered when calculating the pH in question 17?

    A. Yes
    B. No

    Reasoning:

19. What is the pH of a solution containing 5.5×10^{-4} moles of HBr dissolved in 500 mL of water?

A. pH = 2.96
B. pH = 3.26
C. pH = 6.81
D. pH = 7.51

20. Two students calculated the pH of dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below.

Which pH calculation is correct?

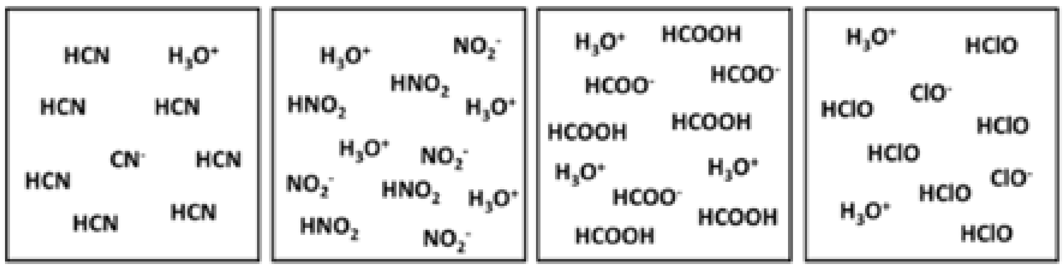
A. Student 1, pH = 8.30
B. Student 2, pH = 6.99

21. Does the autoionization of water needs to be considered when calculating the pH of a dilute acid solution?

A. Yes
B. No

Reasoning:

22. The same concentration of four different acids (HCN, HNO_2, HCOOH, HClO) are shown in the images below. Judging by the images, which acid is the strongest and which acid is the weakest? (H_2O molecules have been omitted for clarity)



Hydrocyanic acid (HCN) | Nitrous acid (HNO_2) | Formic acid(HCOOH) | Hypochlorous acid (HClO)

Select the **strongest acid** based on the images above.

A. Hydrocyanic acid (HCN)
B. Nitrous acid (HNO_2)
C. Formic acid (HCOOH)
D. Hypochlorous acid (HClO)
E. Cannot be determined because they are all weak acids

Select the **weakest acid** based on the images above.

A. Hydrocyanic acid (HCN)
B. Nitrous acid (HNO_2)
C. Formic acid (HCOOH)
D. Hypochlorous acid (HClO)
E. Cannot be determined because they are all weak acids

23. HF and HCl are both binary acids, both containing hydrogen and a halogen atom. Despite these similarities, HF is considered a weak acid because it only ionizes partially in solution, while HCl is a strong acid that completely ionizes in water.

Based on the structures of HF and HCl, explain why HF is a weak acid and HCl is a strong acid.

Please do not explain what it means to ionize partially or completely. Instead, explain **WHY** both acids behave differently.

24. Which acid, HF or HCl, must have a stronger hydrogen-halogen bond?

A. HF (the weak acid)

B. HCl (the strong acid)

25. Select the correct statement about the acid ionization constant, K_a.

A. Strong acids have a $K_a > 1$, weak acids have a $K_a = 1$
B. Strong acids have a $K_a = 1$, weak acids have a $K_a < 1$
C. Strong acids have a $K_a < 1$, weak acids have a $K_a > 1$
D. Strong acids have a $K_a > 1$, weak acids have a $K_a < 1$

26. Select **all** statements that are incorrect about the fraction of dissociation.

A. The fraction of dissociation multiplied by 100% is the percent an acid or base dissociates in solution
B. The fraction of dissociation for a strong acid or strong base is very close to 1
C. The fraction of dissociation is greater than 1 for any strong acid or strong base
D. The fraction of dissociation of a weak acid is equal to the concentration of the conjugate base

27. Select the correct K_a expression for acetic acid (CH_3COOH).

A. $K_a = \frac{[H^+][CH_3COO^-]}{[CH_3COOH]}$

B. $K_a = \frac{[H^+][CH_3COOH]}{[CH_3COO^-]}$

C. $K_a = \frac{[H_2O][CH_3COO^-]}{[CH_3COOH]}$

D. $K_a = \frac{[CH_3COOH]}{[H^+][CH_3COO^-]}$

28. What is the pH of a 0.25 M solution of formic acid (HCOOH), $K_a = 1.80 \times 10^{-4}$?

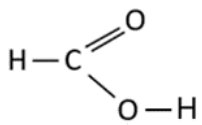
A. pH = 0.60
B. pH = 2.17
C. pH = 3.74
D. pH = 4.35

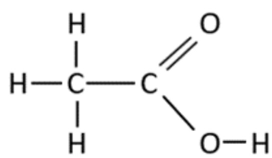
29. What is the percent ionization for formic acid in this solution?

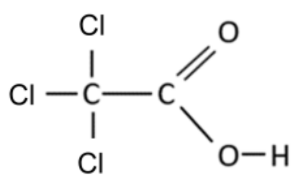
A. 2.68%
B. 41.7%
C. 16.3%
D. 100%

30. Compare the structures of the three acids below.

Circle the parts of each molecule (not the entire molecule!) that contribute to the acidity of the molecule and rate the acids from most acidic (1) to least acidic (3).







Appendix G: Spring 2022 draft of Autoprotolysis, Strength, & pH learning module used in focus groups during the summer 2022 semester.

Autoprotolysis (autoionization) of water and strength of acids and bases

Material: Acid-base model set

FOCUS 1: Autoprotolysis (autoionization) of water

Introduction

Almost 150 years ago, the German Physicist Friedrich Kohlrausch (1840-1910) discovered that water conducts electricity to a small extent even though it had been thoroughly purified.

This phenomenon is based on the autoprotolysis of water.

The term "autoprotolysis" is a combination of the Greek Prefix "auto" and "protolysis".

1. Discuss and fill your definition of the terms in the table below.

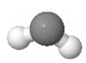
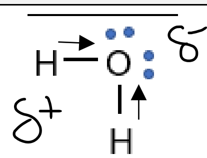
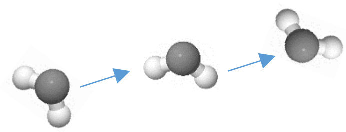
Term	Meaning
auto-	
protolysis	
autoprotolysis	

2. Which molecules from the model kit do you need to model **autoprotolysis**?

Modeling activity 1

Use only the water molecules to investigate interactions between the water molecules. Discuss in your group the different species (molecules, particles, or ions) that can result when water molecules interact with each other and the attractive or repulsive forces between species.

2. Draw each species you make with the model in the table below and complete each row. The first row has been completed as an example.

Species (formula + sketch) Include any charge on the species	**Draw the Lewis dot structure for the species Show any polarity in the structure with arrows and δ⁺ or δ⁻ symbols**	**Interactions between species (You may include multiple species here) Use arrows to indicate attraction between species**
 H_2O		

3. Consider all the species you included in the table. Do you think some species are more reasonable than others in water? Explain why or why not?

4. What species is likely most abundant in the autoprotolysis of water? Explain.

5. Use the models to show the process of **autoprotolysis of water**. Consider the true species that are present and the most appropriate reaction arrow. Should you start with one or two water molecules on the reactant side? Explain.

6. Write the ***symbolic representation*** (chemical equation) for the process you modeled in #4.

7. Is it likely that hydrogen ions (H^+) remain separate species? Explain.

Review: The equilibrium constant, K, for the autoprotolysis of water is expressed as:

$K_w = [H_3O^+]\cdot[OH^-]$

According to the rules for writing equilibrium constants, the concentration of water is not included. For pure water at 25°C the concentration of each ion in the equilibrium expression is 1.0×10^{-7} M.

8. Use the equilibrium expression above to calculate the K_w of water at 25°C.

Thinking critically! Is K_W dimensionless or should it have a unit?

In acid-base chemistry the autoprotolysis of water, also called the self-ionization or autoionization of water, is fundamental in understanding the interactions of acids and bases in aqueous solution.

Review: *The equation to calculate the pH of a solution is commonly written as* ***pH = -log[H⁺]****.*

9. Reviewing the modeling activity on the previous page, discuss the equation ***pH = -log[H⁺]***.
   Can you think of a way to express the pH equation in a more "realistic way"?

10. Calculate the pH of pure water at 25°C based on the K_w (calculated in #7). Show your work.

11. Complete the table using the value for the K_w of water at 25°C. The first row has been completed as an example.

$[H_3O^+]$ (M)	**$[OH^-]$ (M)**	**pH**
1.0×10^{-7}	1.0×10^{-7}	7.00
	1.0×10^{-6}	
1.0×10^{-9}		
		10.00
2.3×10^{-6}		

12. Discuss in your group if water should be classified as an acid or a base. Did your group determine that water acts as an acid or a base? Explain.

13. If your group determined water can act as an acid, use the model to show how water molecules act as an acid. How many water molecules did you use to show water acting as an acid?

14. If your group determined water can act as a base, use the model to show how water molecules act as a base. How many water molecules did you use to show water acting as a base?

15. Give the ***symbolic representation*** (chemical equation) for water acting as an acid and the ***symbolic representation*** for water acting as a base.

    Acid:

    Base:

Are these equations different? Why or why not?

16. Discuss in your group when the autoprotolysis of water occurs. Explain your thoughts.

17. What conditions might influence the autoprotolysis of water? Use the models and think about what happens on the particle level when, for example, the temperature or pressure changes? Explain.

18. In pure water, only about two out of a billion water molecules are ionized at 25°C. Discuss in your group any conditions under which the autoprotolysis of water can still influence the pH of an acidic or basic solution? Explain.

Thinking critically! In autoprotolysis can water act as only and acid or only a base ?

FOCUS 2: Acidic Strength

Modeling activity 2

Use the hydrogen chloride (HCl) molecules and water molecules to investigate pH and acidic strength.

1. Using all the water molecules and all the hydrogen chloride molecules model an aqueous solution of HCl. Consider the acid ionization constant, K_a, for HCl, K_a=1.3x10^6. (K_a is also known as the acid ionization constant)
   Draw your group's model of aqueous HCl into the box below.

2. Write the chemical equation for the ionization of HCl in water based on your model. Consider the most appropriate reaction arrow for the equation.

3. Does your model of aqueous HCl match the reaction arrow you chose for the chemical equation? If not, discuss and make any changes needed with your model to show the strength of HCl in aqueous solution.

4. Does HCl have a large or small K_a? Does your model and chemical equation reflect the K_a value for HCl as given above? Explain.

5. A hydrochloric acid solution is made by dissolving 0.015 moles of HCl in 1.0 L of water at 25°C.
   a. What is the concentration of H_3O^+ ions in the solution from the HCl?

   b. Do you need to consider the H_3O^+ ions produced from autoprotolysis (or autoionization) of water in this solution? Why or why not?

   c. What is the pH of this solution? Show your work.

   d. Write a fraction to show the concentration of ionized HCl molecules compared to the initial concentration of the hydrogen chloride molecules. This is the fraction of ionization (also known as the fraction of dissociation).

   e. What percent of the HCl molecules are ionized?

   f. Write the K_a expression for this HCl solution.

   g. Is it necessary to write a K_a expression for a strong acid solution like $HCl_{(aq)}$? Explain.

6. Each row in the table below shows the initial concentration of HCl, equilibrium concentration of H_3O^+, and the pH of the solution. Fill the missing values for each row to complete the table.

[HCl] M	**[H_3O^+] M**	**pH**
1.0		
		1.00
0.010		
	1.0×10^{-3}	
	0.31	
		1.51

7. As the pH changes by a value of 1 how much does the concentration of H_3O^+ change? Give an example from the table above.

8. Consider the pH values from the table above. What concentration of HCl would result in a pH less than zero? Show the pH calculation for this concentration.

Modeling activity 3

Use hydrogen chloride molecules and water molecules to model a **dilute** HCl solution.

1. Consider a 2.3×10^{-9} M hydrochloric acid solution. Use **all** the water molecules in your kit.
   Consider the concentration of this HCl solution (2.3×10^{-9} M)
   Should you use all the HCl molecules?

   Discuss with your group and decide how many HCl molecules should be used to model this solution then draw the model in the box below.

2. Calculate the pH of a solution containing 2.3×10^{-9} M HCl. Show your work.

3. Is the pH you calculated above reasonable? Explain.

4. Using your models, discuss any other processes and species that could contribute to the pH of the solution. Write down your answer below.

5. Calculate the pH of a aqueous solution containing 2.3×10^{-9} M HCl. Be sure to include all H_3O^+ producing processes in your calculation. Show all your work.

Modeling activity 4

Use the sodium hydroxide (NaOH) models and water molecules to model a NaOH solution.

1. Consider the base ionization constant, K_b (also known as the base hydrolysis constant) for NaOH, $K_b=10^{20}$. Does your model accurately reflect how sodium hydroxide ionizes in water? Sketch your model of aqueous sodium hydroxide in the box below.

2. Write the chemical equation for the ionization of NaOH in water. Consider the most appropriate reaction arrow for this chemical equation.

3. Discuss different ways the model can be used to show different concentrations of sodium hydroxide solution. Explain any changes made to your model to show a different concentration of aqueous sodium hydroxide.

4. Consider a 0.50 M sodium hydroxide solution.
   a. What is the concentration of hydroxide (OH^-) in this solution?

   b. What information is needed to calculate the pH of this solution? Please explain.

To calculate the pH of basic solutions, remember that the **K_w = 1.0 x 10^{-14} = $[H_3O^+][OH^-]$**. This equation can be helpful to calculate the concentration of H_30^+ from the concentration of a strong base.

5. Use the information above to complete table below for a strong base solution.

[NaOH] (M)	**$[H_3O^+]$ (M)**	**$[OH^-]$. (M)**	**pH**	**pOH**
0.010				
1.0 x 10^{-5}				
			11.00	
	1.0 x 10^{-8}			
				2.10
7.1 x 10^{-4}				

6. Write an equation for the relationship between pH and pOH.

7. Calculate the pH of a NaOH solution made from dissolving 75mg of NaOH in 500mL of water. Show your work. (Periodic table provided)

8. Did you need to consider the autoprotolysis of water in your calculation above? Explain.

Modeling activity 5

Acetic acid, CH_3COOH, is a weak acid found in vinegar and other foods. The acid ionization constant for acetic acid, K_a, is 1.75×10^{-5}.

1. Use the acetic acid molecules and water molecules to model aqueous acetic acid and discuss how to model the strength of acetic acid in water.
   Draw your model of aqueous acetic acid in the box below.

2. Use the modeling pieces to show the chemical equation for the ionization of acetic acid in water. Select the correct reaction arrow for this equation.

3. Write the equation you modeled in #2 using chemical symbols for reactant(s) and product(s).

4. Write the K_a expression for acetic acid.

5. Did you omit water in the K_a expression above? Explain why or why not.

6. The pK_a is equal to the negative logarithm of the K_a – analogous to the $pH = -\log [H_3O^+]$.
   Calculate the pK_a for acetic acid ($K_a = 1.75 \times 10^{-5}$). Show your work.

Consider a solution containing 0.15 mol of acetic acid in 1.00 L of water. Recall that the K_a of acetic acid is 1.75×10^{-5}. Every acetic acid molecule that dissociates will form a H_3O^+ molecule and a CH_3COO^- molecule, but many of the acetic acid molecules will not dissociate and will not contribute to the amount of H_3O^+ present in the solution.

7. Complete the table below for 0.15 M solution of acetic acid in water. Use the variable *X* to indicate changes in concentration.

	$CH_3COOH_{(aq)}$ +	$H_20_{(l)}$ ←→	$CH_3COO^-_{(aq)}$ +	$H_3O^+_{(aq)}$
Initial concentration	0.15	solvent		
Final concentration		solvent		

8. Consider the K_a expression for acetic acid that you wrote on the last page. What is the K_a expression for 0.15 M acetic acid (use the values from the table above)?

9. Calculate the pH of 0.15 M acetic acid using the quadratic equation: $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ Show your work.

10. Which answer calculated from the quadratic equation must be rejected? Explain?

11. What is the percent of ionization for acetic acid in this solution?

12. Calculate the pH of pH of 0.15 M acetic acid, now assuming that the value of X is much smaller than 0.15 M and the value of X can be omitted from the denominator of the K_a expression.

How does this change the values in your table? Show the values in the table below.

	$CH_3COOH_{(aq)}$ +	$H_20_{(l)}$ ←→	$CH_3COO^-_{(aq)}$ +	$H_3O^+_{(aq)}$
Initial concentration	0.15	solvent		
Final concentration		solvent		

Show your calculation of pH:

13. Compare your results for #9 and #12? Was the assumption made in #12 reasonable? Explain.

Modeling activity 6

Compare how the HCl molecules and the CH_3COOH molecules interact with the water molecules. Use the water molecules to try to remove the proton (H^+) from the different acid molecules. Experiment with the distance between the different molecules and discuss any differences in the attraction between modeling pieces.

1. Explain any difference you notice between how the hydrogen chloride molecules interact with the water compared to how the acetic acid and water molecules interact.

2. How do your observations relate to the relative strength of both acids that you discussed in previous modeling activities?

3. Compare the structure of these two acids. What difference in the structure of hydrogen chloride molecules compared to the acetic acid might account for their difference in strength?

4. Now compare the structures of the acetic acid molecules and the carbonic acid molecules. Do you think acetic acid or carbonic acid is a stronger acid? Explain.

5. What trend on the periodic table might explain your answer for the last question?

Appendix H: Observation rubric for focus groups

Focus Group Observation Rubric

Modeling activity one: Autoprotolysis and Strength.

Note the time the group starts the activity and each time the group transitions to the next page of the activity in the box provided on each page. While observing make a ✓ for each criterion that occurs for each question. Use the note section to write additional details about observations.

Observer ________________________________**Date** __________________

Introduction: Page 1

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
1. Discuss and fill your definition of the term: auto	Asked for clarification		
	Discussed as a group		
	Skipped question		
Discuss and fill your definition of the term: protolysis	Asked for clarification		
	Discussed as a group		
	Skipped question		
Discuss and fill your definition of the term: Autoprotolysis	Asked for clarification		
	Discussed as a group		
	Skipped question		
2. Which molecules from the model kit do you need to model **autoprotolysis**?	Asked for clarification		
	Discussed as a group		
	Interacting with modeling pieces		
	Used the magnetic properties to investigate model		

Modeling activity 1: Page 2

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
1. Draw each species you make with the model in the table below and complete each row. The first row has been completed as an example.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. Consider all the species you included in the table. Do you think some species are more reasonable than others in water? Explain why or why not?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. What species is likely most abundant in the autoprotolysis of water? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 3

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
4. Use the models to show the process of **autoprotolysis of water**. Consider the true species that are present and the most appropriate reaction arrow. Should you start with one or two water molecules? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
5. Write the ***symbolic representation*** (chemical equation) for the process you modeled in #4.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
6. Is it likely that hydrogen ions (H^+) remain separate species? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
7. Use the equilibrium expression above to calculate the K_w of water at 25°C. **Thinking critically! Is K_W dimensionless or should it have a unit?**	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
8. Reviewing the modeling activity on the previous page, discuss the equation ***pH = -log[H⁺]***. Can you think of a way to express the pH equation in a more "realistic way"?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 4

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
9. Calculate the pH of pure water at 25°C based on the K_w (calculated in #7). Show your work.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
10. Complete the table using the value for the K_w of water at 25°C.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
11. Discuss in your group if water should be classified as an acid or a base. Did your group determine that water acts as an acid or a base? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
12. If your group determined water can act as an acid, use the model to show how water molecules act as an acid. How many water molecules did you use to show water acting as an acid?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
13. If your group determined water can act as a base, use the model to show how water molecules act as a base. How many water molecules did you use to show water acting as a base?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 5

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
14. Give the ***symbolic representation*** (chemical equation) for water acting as an acid and the ***symbolic representation*** for water acting as a base. Are these equations different? Why or why not?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
15. Discuss in your group when the autoprotolysis of water occurs. Explain your thoughts.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
16. What conditions might influence the autoprotolysis of water? Use the models and think about what happens on the particle level when, for example, the temperature or pressure changes.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
17. In pure water, only two out of a billion water molecules are ionized at 25°. Can you think of any conditions under which the autoprotolysis of water can still influence the pH of an acidic or basic solution?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
Thinking critically! In autoprotolysis can water act as only and acid or only a base ?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Modeling activity 2: Page 6

Question	Criteria	✓ if observed	Notes
Start time:			
1. Using all the water molecules and all the hydrogen chloride molecules model an aqueous solution of HCl. Consider the acid ionization constant, K_a, for HCl, K_a=1.3x10^6. Draw your model into the box below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. Write the chemical equation for the ionization of HCl in water based on your model. Consider the most appropriate reaction arrow for the equation.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. Does your model of aqueous HCl match the reaction arrow you chose for the chemical equation? If not, discuss and make any changes needed with your model to show the strength of HCl in aqueous solution.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Does HCl have a large or small K_a? Does your model and chemical equation reflect the K_a value for HCl as given above? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 7

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
5. A hydrochloric acid solution is made by dissolving 0.015 moles of HCl in 1.0 L of water at 25°C. a) What is the conc of H_3O^+ ions in the solution from the HCl?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
b) Do you need to consider the H_3O^+ ions produced from autoprotolysis (or autoionization) of water in this solution? Why or why not?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
c) What is the pH of this solution? Show your work	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
d) Write a fraction to show the concentration of ionized HCl molecules compared to the initial concentration of the hydrogen chloride molecules.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
e) What percent of the HCl molecules are ionized?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
f) Write the K_a expression for this HCl solution?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
g) Is it necessary to write a K_a expression for a strong acid solution like $HCl_{(aq)}$? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 8

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
5. Each row in the table below shows the initial concentration of HCl, equilibrium concentration of H_3O^+, and the pH of the solution. Fill the missing values for each row to complete the table.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
6. As the pH changes by a value of 1 how much does the concentration of H_3O^+ change? Give an example from the table above.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
7. Consider the pH values from the table above. What concentration of HCl would result in a pH less than zero? Show the pH calculation for this concentration.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Modeling activity 3: Page 9

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
1. Discuss with your group and decide how many HCl molecules should be used to model this solution then draw the model in the box below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. Calculate the pH of a solution containing 2.3 x 10^{-9} M HCl. Show your work.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. Is the pH you calculated above reasonable? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Using your models, discuss any other processes and species that could contribute to the pH of the solution. Write down your findings below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
5. Calculate the pH of a solution containing 2.3 x 10^{-9} M HCl. Be sure to include all H_3O^+ producing processes in your calculation. Show all your work.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Modeling activity 4: Page 10

Start time:

Question	**Criteria**	**✓ if observed**	**Notes**
1. Consider the base ionization constant, K_b for NaOH, $K_b=10^{20}$. Does your model accurately reflect how sodium hydroxide ionizes in water? Sketch your model of aqueous NaOH in the box below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. Write the chemical equation for the ionization of NaOH in water. Consider the most appropriate reaction arrow for this chemical equation.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. Discuss different ways the model can be used to show different concentrations of sodium hydroxide solution. Explain any changes made to your model to show a different concentration of aq. sodium hydroxide.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Consider a 0.50 M sodium hydroxide solution. a. What is the concentration of hydroxide (OH^-) in this solution?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Consider a 0.50 M sodium hydroxide solution. b. What information is needed to calculate the pH of this solution? Please explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 11

<table>
<tr><td>Start time:</td><td></td><td></td><td></td></tr>
<tr><td>Question</td><td>Criteria</td><td>✓ if observed</td><td>Notes</td></tr>
<tr><td rowspan="4">5. Use the information above to complete table below for a strong base solution.</td><td>Asked for clarification</td><td></td><td rowspan="4"></td></tr>
<tr><td>Discussed as a group</td><td></td></tr>
<tr><td>Skipped question</td><td></td></tr>
<tr><td>Interacting with modeling pieces</td><td></td></tr>
<tr><td rowspan="4">6. Write an equation for the relationship between pH and pOH.</td><td>Asked for clarification</td><td></td><td rowspan="4"></td></tr>
<tr><td>Discussed as a group</td><td></td></tr>
<tr><td>Skipped question</td><td></td></tr>
<tr><td>Interacting with modeling pieces</td><td></td></tr>
<tr><td rowspan="4">7. Calculate the pH of a NaOH solution made from dissolving 75mg of NaOH in 500mL of water. Show your work.</td><td>Asked for clarification</td><td></td><td rowspan="4"></td></tr>
<tr><td>Discussed as a group</td><td></td></tr>
<tr><td>Skipped question</td><td></td></tr>
<tr><td>Interacting with modeling pieces</td><td></td></tr>
<tr><td rowspan="4">8. Did you need to consider the autoprotolysis of water in your calculation above? Explain.</td><td>Asked for clarification</td><td></td><td rowspan="4"></td></tr>
<tr><td>Discussed as a group</td><td></td></tr>
<tr><td>Skipped question</td><td></td></tr>
<tr><td>Interacting with modeling pieces</td><td></td></tr>
</table>

Modeling activity 5: Page 12

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
1. Use the acetic acid molecules and water molecules to model aqueous acetic acid and discuss how to model the strength of acetic acid in water. Draw your model in the box below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. Use the modeling pieces to show the chemical equation for the ionization of acetic acid in water. Select the correct reaction arrow for this equation.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. Write the equation you modeled in #2 using chemical symbols for reactant(s) and product(s).	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Write the K_a expression for acetic acid.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
5. Did you omit water in the K_a expression above? Explain why or why not.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
6. The pK_a is equal to the negative logarithm of the K_a – analogous to the pH = -log $[H_3O^+]$. Calculate the pK_a for acetic acid (K_a = 1.75 x 10^{-5}). Show your work.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 13

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
7. Complete the table below for 0.15 M solution of acetic acid in water. Use the variable *X* to indicate changes in concentration.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
8. Consider the K_a expression for acetic acid that you wrote on the last page. What is the K_a expression for 0.15 M acetic acid (use the values from the table above)?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
9. Calculate the pH of 0.15 M acetic acid using the quadratic equation: $x = \frac{-b\pm\sqrt{b^2-4ac}}{2a}$ Show your work	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
10. Which answer calculated from the quadratic equation must be rejected? Explain?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
11. What is the percent of ionization for acetic acid in this solution?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Page 14

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
12. Calculate the pH of pH of 0.15 M acetic acid, now assuming that the value of X is much smaller than 0.15 M and the value of X can be omitted from the denominator of the K_a expression. How does this change the values in your table? Show the values in the table below.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
12. Show your calculation of pH:	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
13. Compare your results for #9 and #12? Was the assumption made in #12 reasonable? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Modeling activity 6: Page 15

Start time:			
Question	**Criteria**	**✓ if observed**	**Notes**
1. Explain any difference you notice between how the hydrogen chloride molecules interact with the water compared to how the acetic acid and water molecules interact.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
2. How do your observations relate to the relative strength of both acids that you discussed in previous modeling activities?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
3. Compare the structure of these two acids. What difference in the structure of hydrogen chloride molecules compared to the acetic acid might account for their difference in strength?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
4. Now compare the structures of the acetic acid molecules and the carbonic acid molecules. Do you think acetic acid or carbonic acid is a stronger acid? Explain.	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		
5. What trend on the periodic table might explain your answer for the last question?	Asked for clarification		
	Discussed as a group		
	Skipped question		
	Interacting with modeling pieces		

Appendix I:Focus group exit survey

Focus Group Exit Survey

Circle how much you agree or disagree with each statement below.

1.	I found the instructions in the activity generally to be clearly worded.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Indicate for which questions you found the instructions to be partially or fully unclear.
2.	The modeling activities helped me to connect particle-level interactions and phenomena to symbolic representations and/or mathematical expressions and calculations.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Indicate for which questions you think the models helped make important connections and solve problems.
3.	The modeling activity gave me a deeper understanding of interactions between water molecules in autoprotolysis.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Please explain what new information you have learned.

4.	The modeling activity gave me a deeper understanding of acid and base strength.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Please explain what new information you have learned.
5.	It helped me to complete the activity as a group.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Please explain your answer.
6.	I could have completed the activity easily on my own.	**Strongly agree** **Agree** **Disagree** **Strongly disagree**	Please explain your answer.

7. What, in your opinion, is the reason the models include magnets?

8. Did you experience any issues while using the modeling pieces? Please explain.

9. For the learning of which other chemistry concepts could the models be used? Please give your suggestions.

Do you have additional comments?

Appendix J: Implemented Autoionization of water and the strength of acids and bases learning module

Names:____

____

Autoionization of water and the strength of acids and bases

Material: Acid-base model set

FOCUS 1: Autoionization of water

Introduction

Almost 150 years ago, the German Physicist Friedrich Kohlrausch (1840-1910) discovered that water conducts electricity to a small extent due to the presence of ions in water even though it had been thoroughly purified.

This phenomenon is based on the autoionization of water, also referred to as **<u>autoprotolysis</u>**. The term "autoprotolysis" is a combination of the Greek prefix "auto" and "protolysis".

2. Consider the term **<u>autoprotolysis</u>**. Discuss the meaning of each term in the table below and fill in your group's definition.

Term	**Meaning**
auto-	
protolysis	
autoprotolysis	

To investigate the phenomenon of autoprotolysis or the autoionization of water use only the water molecules in your model set.

Modeling activity 1

Use only the water molecules in your model set to investigate the autoionization of water with your group. Make different species (e.g., molecules, atoms, or ions) using the water molecules.

3. Draw each species you group makes with the water molecules in the table below.

Row #	**Species (formula and sketch)** Draw each species your group made using the water molecules. **Include any charges on species**	**Interactions** Draw images of possible interactions between species your group formed with the models. Use arrows to indicate attraction between molecules or species
1		
2		
3		
4		
5		
6		
7		
8		

4. Consider all the species your group made. Write the row number(s) to answer each question below.
    a. What species do you think are present in water due to the autoionization of water?
    b. What species do you think are unreasonable in the autoionization of water?
    c. Which species influences the pH of water?

5. What species is most abundant in the autoionization of water? **Explain.**

6. Show the process of the **autoionization of water** (like showing a chemical reaction) using just a few of the water molecules. Consider the most realistic species from your table on page 2. **Draw your model for the autoionization of water in the box below**.

7. Write the ***symbolic representation*** (chemical equation) for this process. Consider the true species present and the most appropriate reaction arrow for this equation.

8. Considering your group's model for the autoionization of water (drawn in the box above), is water classified as an acid or a base? Explain your answer.

9. Discuss all interactions the H^+ ion could have with water molecules during autoionization. What is the product when a proton (H^+ ion) interacts with a water molecule?

Review: The equilibrium constant, *K*, for the autoionization of water is expressed as: $K_w = [H_3O^+][OH^-]$

According to the rules for writing equilibrium constants, the concentration of water is not included. For pure water at 25°C the concentration of each ion in the equilibrium expression is 1.0×10^{-7} M.

10. Use the equilibrium expression above to calculate the K_w of water at 25°C. **Show your work.**

11. What is the **unit** for K_w?

In acid-base chemistry the autoionization of water is fundamental in understanding interactions of acids and bases in aqueous solution. Now consider the pH equation for aqueous solutions.

Review: *The equation to calculate the pH of a solution is commonly written as* ***pH = -log[H⁺].***

Consider the two equations (a & b): a. ***pH = -log[H^+]***

b. ***pH = -log[H_3O^+]***

12. Are these equations the same equation (symbolically equivalent)? Explain your answer.

13. Which equation (a or b) describes the protons (H+) in solution in the most realistic way?

14. Complete the table using the value for the K_w of water at 25°C (calculated in question 9). **Show your work.**

[H_3O^+] (M)	**[OH^-] (M)**	**pH**	**Calculation**
1.0×10^{-7}		7.00	
	1.0×10^{-6}		
		10.00	
2.3×10^{-6}			
	4.5×10^{-8}		

15. Discuss in your group when the autoionization of water occurs. Explain your thoughts.

16. Discuss in your group any conditions that might influence the autoionization of water. What conditions may cause a change in the autoionization of water? Explain your thoughts.

17. Discuss in your group any conditions under which the autoionization of water can still influence the pH of an acidic or basic solution? Explain your thoughts.

FOCUS 2: Acidic Strength

Modeling activity 2

Use the hydrogen chloride (HCl) molecules and water molecules to investigate pH and acidic strength.

18. Use the models to **model aqueous HCl**. Consider the acid ionization constant, K_a, for HCl, K_a=1.3x10^6. (K_a is also known as the acid dissociation constant)
Draw your group's model of aqueous HCl into the box below.

19. Write the chemical equation for the ionization of HCl in water based on your model. Consider the **most appropriate reaction arrow** for the equation and the most realistic species present.

20. Discuss in your group what the reaction arrow you chose (in the box above) indicates about the amount of ionized HCl in solution? Explain your answer.

21. Does HCl have a large or small K_a? Does your model and chemical equation reflect the K_a value for HCl as given above? Explain your answer.

22. Write the K_a expression for this HCl solution

23. Is it necessary to write a K_a expression for a strong acid solution like $HCl_{(aq)}$? Explain.

24. A hydrochloric acid solution has been prepared by dissolving 0.015 moles of HCl in 1.0 L of water at 25°C.

a. What is the concentration of H_3O^+ ions in the solution from the HCl? **Show your work.**

b. Do you need to consider the H_3O^+ ions produced from the autoionization of water to calculate the pH of this solution? Why or why not?

c. What is the pH of this solution? **Show your work.**

d. Write a fraction to show the concentration of ionized HCl molecules compared to the initial concentration of the hydrogen chloride molecules. This is the fraction of ionization (also known as the fraction of dissociation).

e. What percent of the HCl molecules are ionized? **Show your work.**

25. Each row in the table below shows the initial concentration of HCl, equilibrium concentration of H_3O^+, and the pH of the solution. Fill the missing values for each row to complete the table.
Show your work in the last column.

[HCl] M	$[H_3O^+]$ M	pH	Calculation
1.0			
		1.00	
	1.0×10^{-3}		
2.5			
	0.31		
		1.51	

26. As the pH changes by a value of 1 how much does the concentration of H_3O^+ change? Give an example from the table above.

27. Consider the pH values from the table above. Can an aqueous solution of HCl result in a pH less than zero?

28. Discuss in your group if a negative pH value indicates a solution with a very high H_3O^+ concentration or a very low H_3O^+ concentration? Explain your answer.

Modeling activity 3

Use hydrogen chloride molecules and water molecules to model a **dilute** HCl solution.

29. Consider a very low concentration HCl solution (for example 2.3×10^{-9} M). Use **all** the water molecules in your modeling kit to show a **highly diluted HCl solution**.

    Discuss with your group how many HCl molecules should be used to model this solution then draw the model in the box below.

30. Calculate the pH of a solution containing 2.3×10^{-9} M HCl. **Show your work**.

31. Is the pH you calculated above reasonable? Explain your answer.

32. Discuss in your group all processes that contribute to the concentration of H_3O^+ in this solution. What other process needs to be considered when calculating the pH of a very dilute acid solution?

33. Calculate the pH of a 5.8×10^{-9} M HCl solution. Be sure to include all H_3O^+ producing processes in your calculation. **Show all your work**.

Modeling activity 4

Use the sodium hydroxide (NaOH) models and water molecules to model a basic solution.

34. Consider the base ionization constant, K_b (also known as the base hydrolysis constant) for NaOH, K_b=1 x 10^{20}. Discuss if your model accurately reflects how sodium hydroxide ionizes in water. Draw your model of aqueous sodium hydroxide in the box below.

35. Write the chemical equation for the ionization of NaOH in water. Consider the most appropriate reaction arrow for this equation.

36. Consider a 0.50 M calcium hydroxide ($Ca(OH)_2$) solution.
    a. What is the concentration of hydroxide (OH^-) in this solution from the calcium hydroxide? **Show your work.**

    b. What information is needed to calculate the pH of this solution? Please explain.

    c. Calculate the pH of a 0.50 M calcium hydroxide ($Ca(OH)_2$) solution. **Show your work.**

To calculate the pH of basic solutions, remember that the $\mathbf{K_w = 1.0 \times 10^{-14} = [H_3O^+][OH^-]}$. This equation can be helpful to calculate the concentration of H_30^+ from the concentration of hydroxide (OH^-).

37. Complete the table below for a strong base solution. **Show all your work**

[NaOH] (M)	**$[H_3O^+]$ (M)**	**$[OH^-]$. (M)**	**pH**	**pOH**	**Calculations**
		0.010			
			11.00		
				2.10	
7.1×10^{-4}					

38. Write an equation for the relationship between pH and pOH.

39. Calculate the concentration of hydronium (H_3O^+) in a NaOH solution made by dissolving 0.075g of NaOH (40.00g/mol) in 500 mL of water. **Show your work.**

40. Calculate the pH of the NaOH solution in question 38. **Show your work.**

41. Did you need to consider the autoionization of water in your calculation above? Explain.

Modeling activity 5

Acetic acid, CH_3COOH, is a weak acid with the acid ionization constant, $K_a = 1.75 \times 10^{-5}$.

42. Use the acetic acid molecules and water molecules to **model aqueous acetic acid**. Consider the strength of acetic acid and the behavior of the proton (H+) in solution. Discuss if your model shows the most realistic species in aqueous acetic acid. **Draw your group's model of aqueous acetic acid in the box below.**

43. In the box, draw and label all species present at equilibrium in aqueous acetic acid.

44. Write the ***symbolic representation*** (chemical equation) for an aqueous solution of acetic acid. Consider the most appropriate reaction arrow for this equation.

45. Write the K_a expression for acetic acid.

46. Calculate the pK_a for acetic acid ($K_a = 1.75 \times 10^{-5}$). **Show your work**.

Consider a solution containing 0.15 mol of acetic acid in 1.00 L of water (K_a = 1.75 x 10^{-5}).

47. Complete the table below for 0.15 M solution of acetic acid in water. Use the variable *X* to indicate changes in concentration.

	$CH_3COOH_{(aq)}$ +	$H_20_{(l)}$ ←→	$CH_3COO^-_{(aq)}$ +	$H_3O^+_{(aq)}$
Initial concentration	0.15	solvent		
Change				
Final concentration				

48. Consider the K_a expression for acetic acid that you wrote on the last page. What is the K_a expression for 0.15 M acetic acid (use the values from the table above)?

49. Calculate the pH of 0.15 M acetic acid using the quadratic equation: $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ **Show all your work.**

50. Circle the correct answer form the quadratic equation.

51. What is the percent of ionization for acetic acid in this solution? **Show your work.**

52. Calculate the pH of 0.15 M acetic acid assuming that the value of X is much smaller than 0.15 M and can be omitted from the denominator of the K_a expression. (X<<0.15)

How does this change the values in your table? Fill in the values in the table below.

	$CH_3COOH_{(aq)}$ +	$H_20_{(l)}$ ←→	$CH_3COO^-_{(aq)}$ +	$H_3O^+_{(aq)}$
Initial concentration	0.15	solvent		
Change				
Final concentration				

Show your calculation for pH using the small X approximation (X<<0.15): **Show all work**

53. Compare your results for the pH of a 0.15 M acetic acid using the quadratic equation and using the small X approximation (X<<0.15). Is it necessary to use the quadratic to calculate this pH? **Explain your answer.**

54. Discuss in your group under what conditions it is necessary to use the quadratic equation to find the concentration of X before calculating the pH? **Explain your answer**.

Modeling Activity 6

Use the modeling set to compare how a lone pair on an oxygen atom in a water molecule may interact with the proton (H^+) from different acid molecules.

First, **try to remove the proton (H^+) from an HCl molecule using only a water molecule**. Have each person in your group try this experiment. Next, have each person in your group **try to remove the proton (H^+) from an acetic acid molecule (CH_3COOH) using a water molecule.**

55. Discuss in your group any differences you notice between how each acid interacted with the water molecules. What differences did your group notice? **Explain your answer**.

56. Discuss how your observations relate to the strength of each acid. **Explain your thoughts**.

57. Discuss and compare the structure of these two acids in your group. What difference in the structure of hydrogen chloride compared to acetic acid might account for their difference in acidic strength?

Next, using the model set, **compare the structures of the acetic acid molecules (CH_3COOH) and the carbonic acid molecules (H_2CO_3)**.

The strength of the magnets in the weak acid models is the same. However, the actual strength of acetic acid and carbonic acid is not the same. (This is a limitation of the model set.)

58. Discuss in your group if acetic acid or carbonic acid is stronger. What acid did your group determine was stronger? **Explain your answer.**

59. What trend(s) on the periodic table help explain your group's answer for the last question?

60. Examine an acetic acid molecule from the model set and compare the hydrogens in acetic acid. Discuss in your group why only some of the protons can be removed. What does this indicate about the different hydrogens in acetic acid? **Explain your answer**.

61. Now consider the carbonic acid molecules. Can all the protons be removed from carbonic acid? Discuss this in your group. What does this indicate about the hydrogens in carbonic acid. **Explain your answer**.

62. What additional information can be used to determine the relative strength of weak acids? **Explain your thoughts.**

Appendix K: Interview protocol

Opening

Hello. I have some follow up questions from the modeling activity in early October. I would really like you to explain your thinking when answering these questions and include all details you think of.

For example:

I may write down some notes and ask some follow up questions, but that does not mean that your answer is right or wrong, they are just to help me remember and understand your thoughts. Any details you can share are helpful, even if you are not sure they are correct. Dr. Aldstadt does not get a report from this interview.

Question 1

Showing two image **Page 3**, have models of water molecules on table, encourage to use them. Ask:

Which image do you think most realistically shows the autoionization of water? Please explain why.

Is the other image incorrect? Can you explain why/why not?

Question 2

Keep water molecules on the table with blank paper and a pen for student if they want to write/draw and ask:

In what aqueous systems is the autoionization of water occurring? Explain your thinking.

Possible follow up questions:

Can you explain what you meant by . . . (repeat phrase/words used by student)

If no response: ***Which aqueous systems do you know?***

If no response: ***Can you describe an aqueous system?***

If they say a system: ***Is the autoionization of water happening in that system?***

If student's response is that it only occurs in pure water:

Why doesn't the autoionization occur in other systems?

Question 3

Follow up for pH question for very dilute acidic solution. Have HCL and water models on table.

Show question on **page 4** to student. Ask:

Which pH is more reasonable, 8.30 or 6.99?

If response is 6.99: ***Please explain your reasoning.***

If response is 8.30 – give students **page 5** with K_w expression and empty box:

Use the box to diagram a neutral solution of water showing only the ions and no water molecules.

If you add this concentration, 4.8 x 10 –9 M (refer to concentration in the question), ***how does that change your diagram? Are there any additional ions when we add the acid?***

If no response: ***In what range do you expect the pH of an acid to be?***

Question 4

Question is targeting particle-level understanding and connection to K_a.

Have models of HCl, acetic acid, and water molecules out for students.

In what ways do the models help you understand acid/base concepts?

Show student **page 6** with three particle-level images.

Looking at the three images and the key, can you describe what these three images represent.

If student doesn't recognize images as acids: ***If all three images show a different acid can you explain the difference between the acids shown in each image?***

Explain how you think the K_a ***values for the three acids shown would change.***

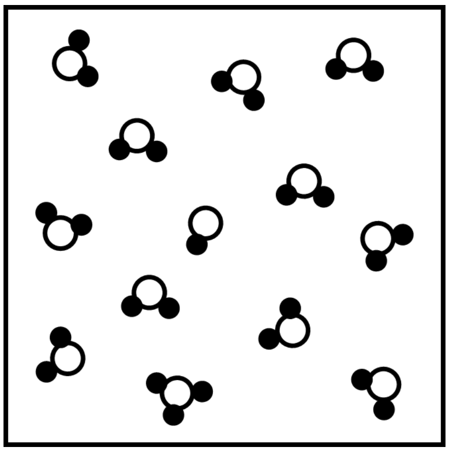
If needed, show students the three K_a values on **page 7**.

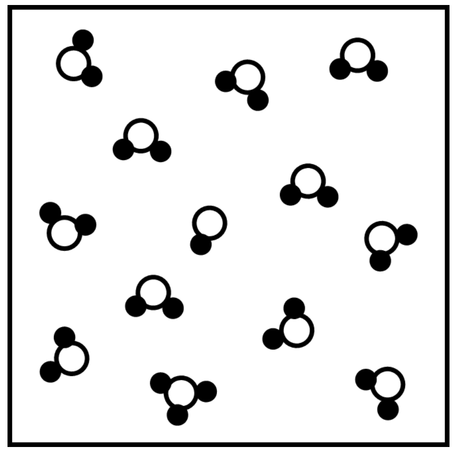
What Ka value you would give to each image? Can you give each image one of these Ka values (pointing to ka values on page 7).

(Page 3)

Question 1

Which image do you think most realistically shows the autoionization of water?





(Page 4)

Question 3

Two students calculated the pH of a dilute HCl solution with a concentration of 4.8×10^{-9} M. Their answers are below.

C. Student 1, pH = 8.30

D. Student 2, pH = 6.99

Which pH is more reasonable, 8.30 or 6.99?

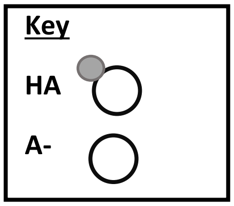
(page 5)

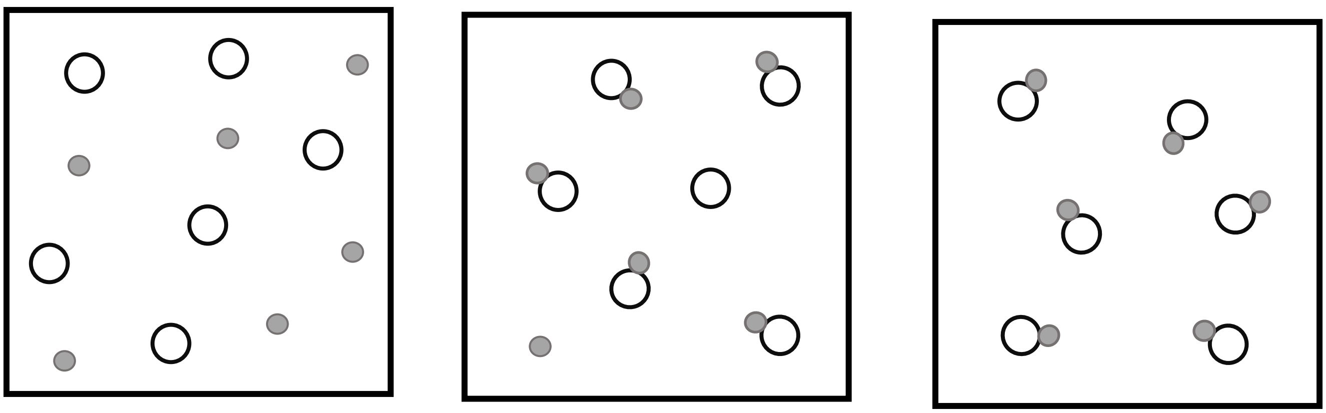
Question 3

$K_w = [H_3O^+][OH^-]$

(Page 6)

Question 4





(Page 7)

Question 4

$K_a = 6.30 \times 10^{-6}$

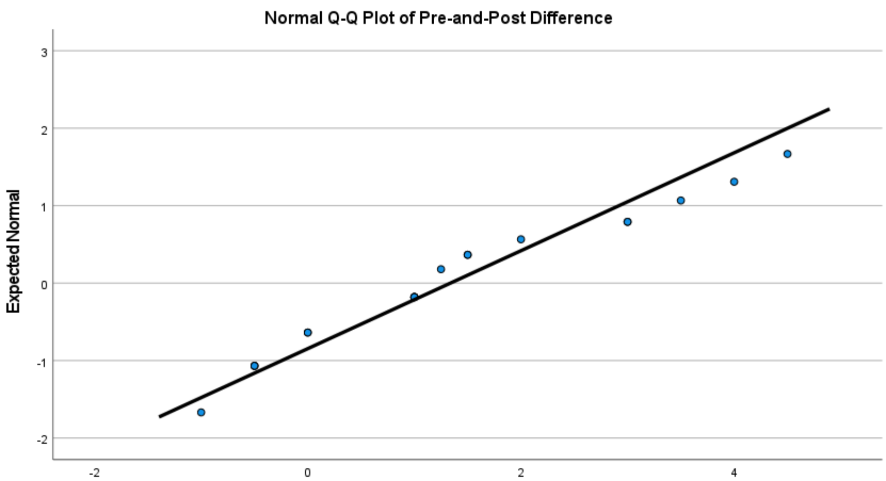
$K_a = 5.80 \times 10^{-3}$

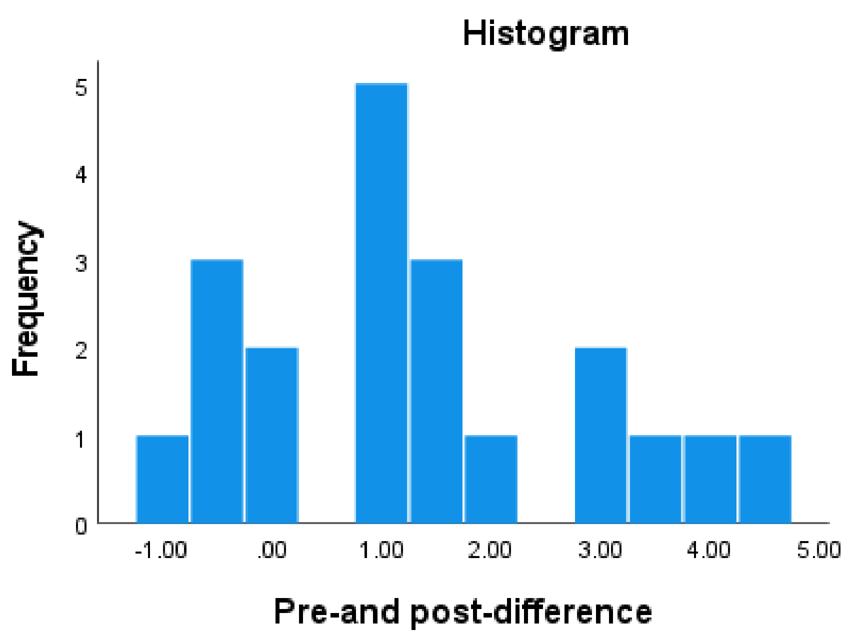
$K_a = 1.30 \times 10^{6}$

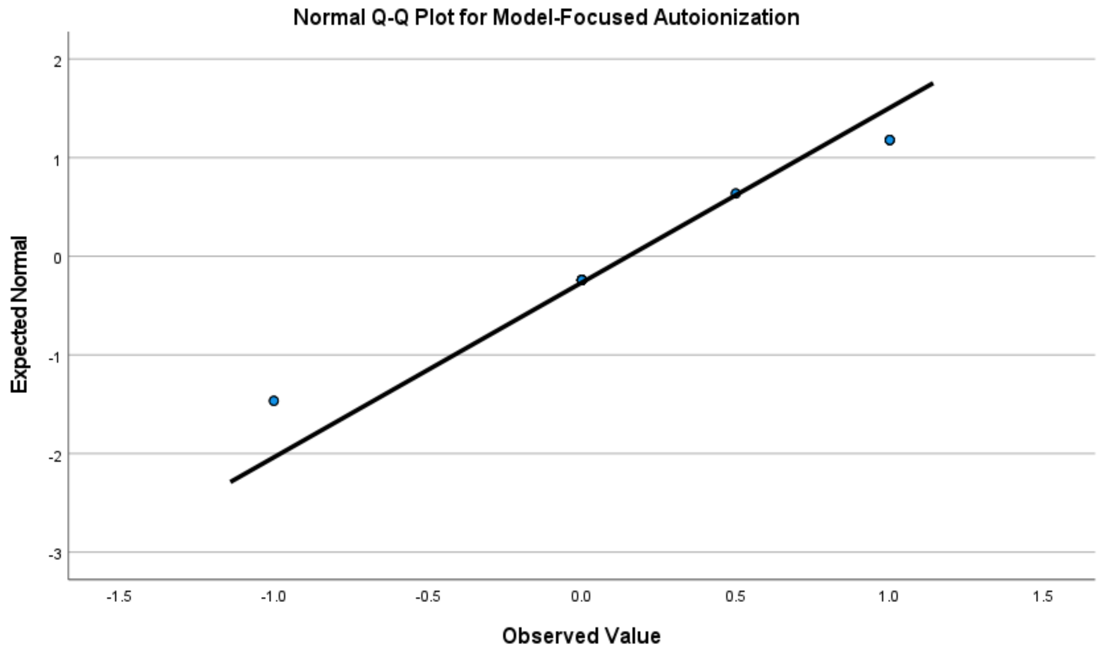
Appendix L: Normality test results for all paired (N=20)

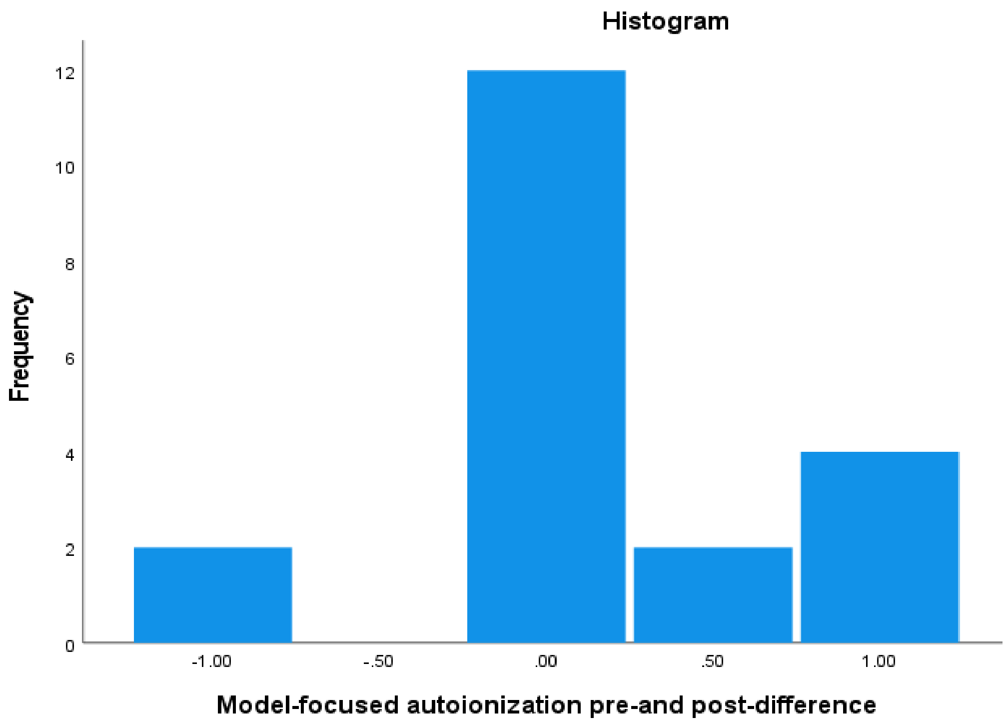
Grouping	Skewness*	Kurtosis*	Normality assumption satisfied
All items	0.50	0.56	Yes
Autoionization	1.14	3.67	No
Model-focused autoionization	0.18	0.47	Yes
Acidic strength	0.98	0.64	Yes
Model-focused acidic strength	1.40	1.37	No
pH	1.97	5.24	No
Ka	0.53	4.99	No

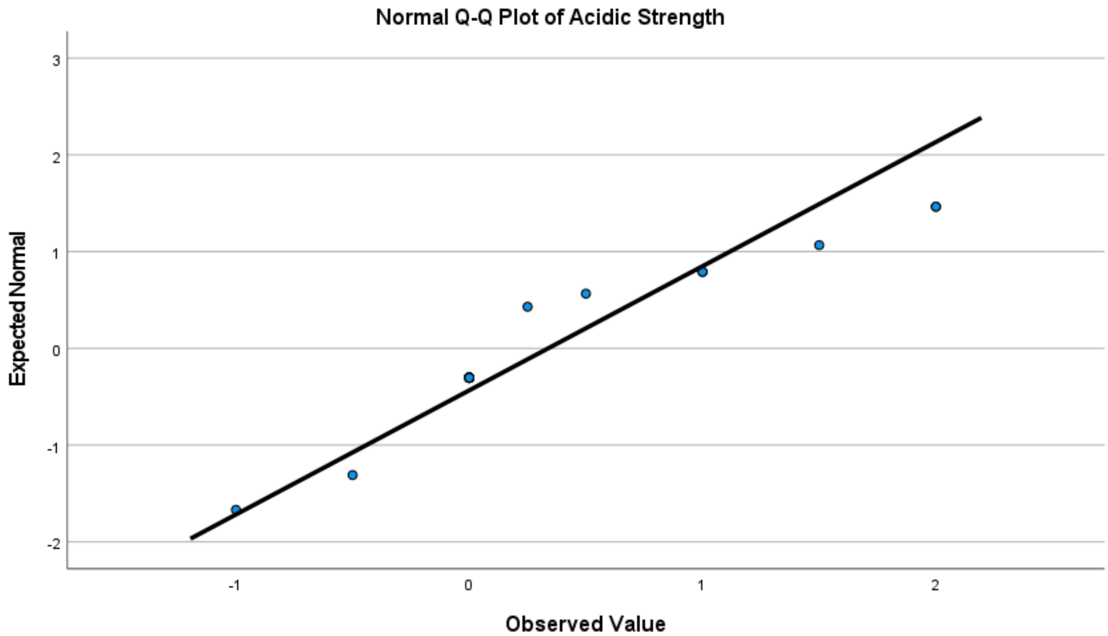
*Acceptable values for skewness are below 1 and acceptable values for kurtosis are below 1.94. Both values must fall below these thresholds to satisfy the normality assumption for a paired-samples T-test.

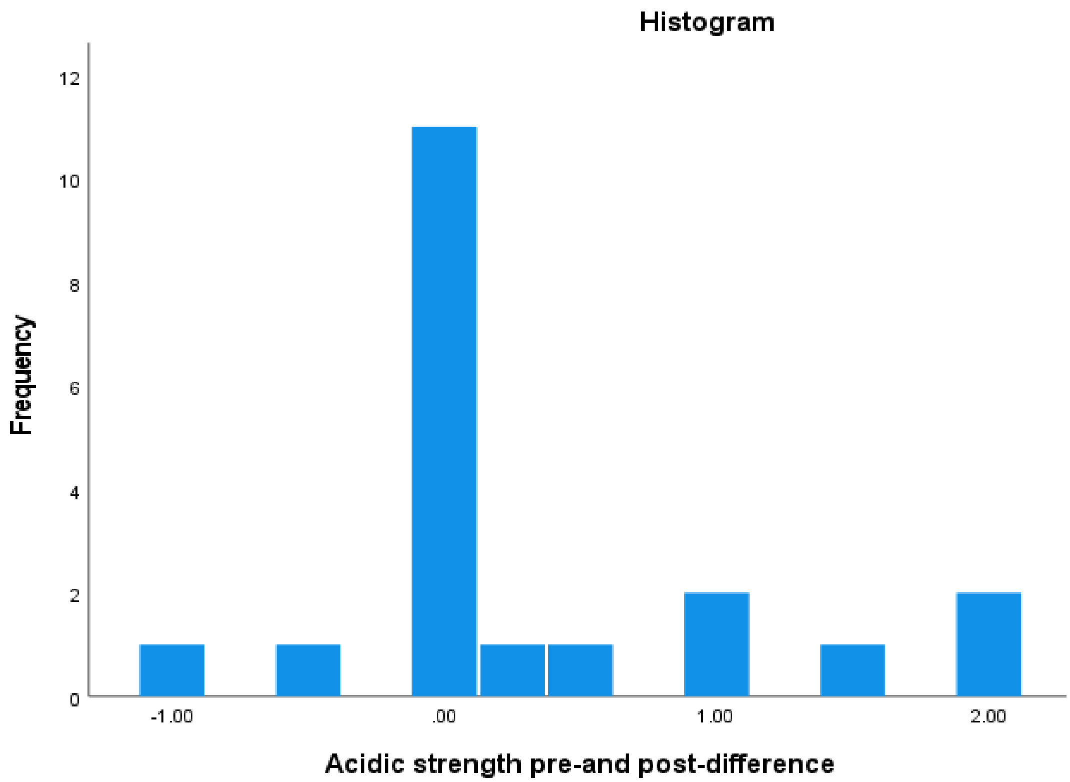





Normal Q-Q Plot for Model-Focused Autoionization
Expected Normal
Observed Value
2
1
0
-1
-2
-3
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5


Histogram
Frequency
12
10
8
6
4
2
0
-1.00
-.50
.00
.50
1.00
Model-focused autoionization pre-and post-difference

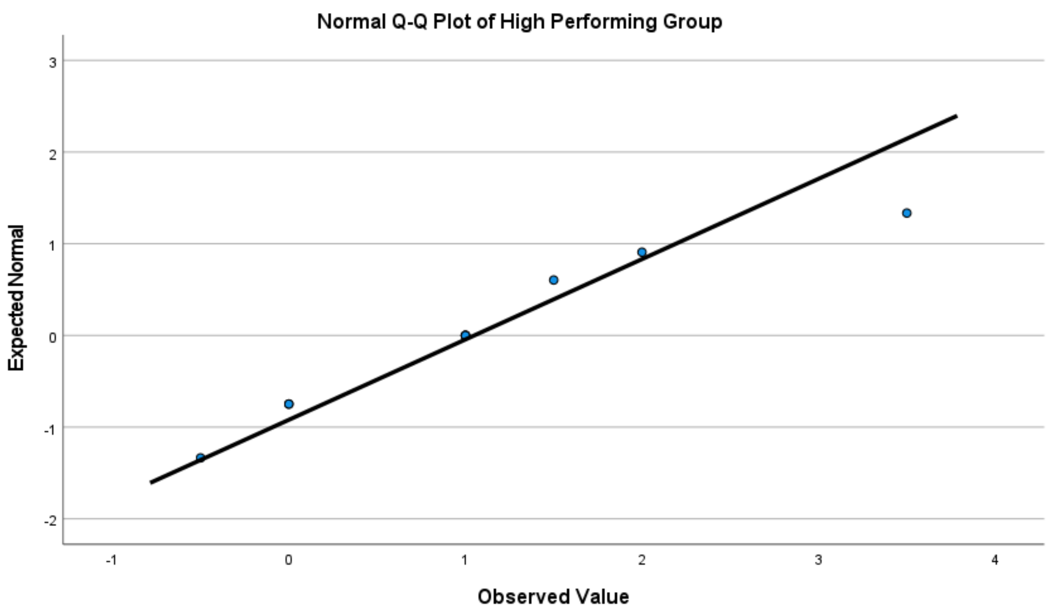

Normal Q-Q Plot of Acidic Strength
Expected Normal
3
2
1
0
-1
-2
-1
0
1
2
Observed Value

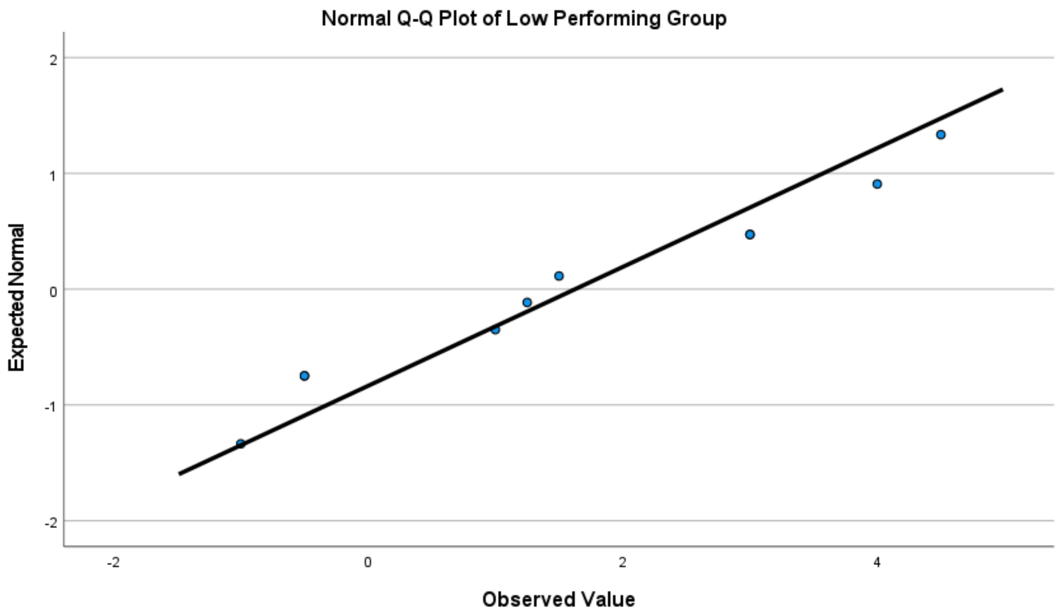

Histogram
Frequency
12
10
8
6
4
2
0
-1.00
.00
1.00
2.00
Acidic strength pre-and post-difference

Results for normality tests on pre- and post-assessment results for each group of students

Group	Skewness*	Kurtosis*	Significance** Kolmogorov-Smirnov	Significance** Shapiro-Wilk
High performing	0.89	1.46	0.20	0.31
Low performing	0.09	1.37	0.20	0.47

*Acceptable values for skewness are below 1.3 and acceptable values for kurtosis are below 2.6. Both values must fall below these thresholds to satisfy the normality assumption for a paired-samples T-test.
**Significance (p<0.05) indicates the data is significantly different from a normal distribution.




Normal Q-Q Plot of Low Performing Group
Expected Normal
Observed Value
2
1
0
-1
-2
-2
0
2
4