The Mechanisms App: Development of a New Learning Tool for Active Learning in Organic Chemistry

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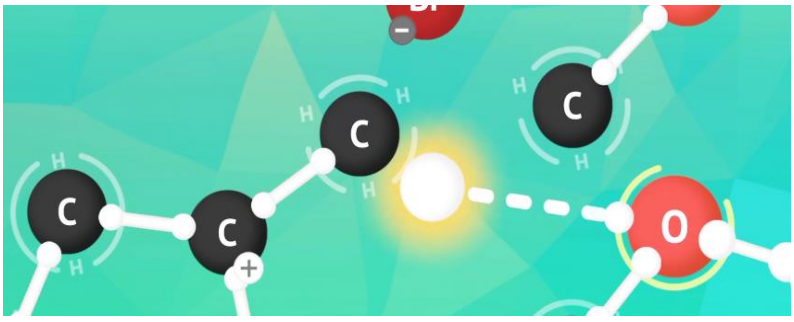
Abstract
Providing formative feedback to each student on mechanism type problems in organic chemistry is challenging, especially in large classes. With the wide availability of touch screen devices, an opportunity for interaction through a game-based learning experience involving the bond-making and breaking arrows of mechanisms was realized by Ms. Winter. From conception to development and early testing, as well as improvements made based on instructor and student feedback, this chapter details the creation of the Mechanisms app. Also included are results of preliminary research studies on the use of Mechanisms by students and instructors, use cases of Mechanisms in active learning activities, and an example of pattern recognition from data collected by the app.



The Mechanisms app started its life in a classroom with two key questions. The author, Julia Winter, had taught organic chemistry at Detroit Country Day School in Beverly Hills, Michigan since 1994. Active learning was the main instructional method. Students would routinely work at the white board or at tables in groups to solve mechanism problems, and with only twelve to fifteen students in each class, it was relatively easy to give students the kind of formative feedback they needed to become proficient at arrow-pushing.

Question 1: Was it possible to use game-based learning and touch-screen apps to scale this kind of interactivity to students in a college setting, where class sizes range from 60-300 students?

Ms. Winter had done some preliminary exploration into game-based learning with Chairs, an app which was developed from a white board game to teach cyclohexane ring flips (*1*). In the Chairs game, the user draws the axial and equatorial positions on a touch-screen and receives a response from the app when the positions have correct angles relative to the cyclohexane ring conformer. She was hopeful that arrow-pushing ideas could also be adapted to a touch-screen device.

Question 2: Could the bond-making and breaking arrows of organic chemistry mechanisms also be used as the tool for moving through a game-based learning experience?

To answer these questions, the first version of the Mechanisms app was designed as the Mechanisms Game (MG); Ms. Winter hired a mobile app consulting firm named Brilliant Chemistry. (Note: The consulting firm's name referred to chemistry only as a metaphor, the principals had no subject matter expertise.) The result of this consulting engagement was a set of slides that included an early version of the visual design (Figure 1a). The other slides were the images to create the blueprint for the user interaction model of the game, called wireframes. In the case of the MG, each reaction event was given an image. Two of these wireframe images are shown (Figure 1b), showing the steps of a nucleophilic substitution reaction.

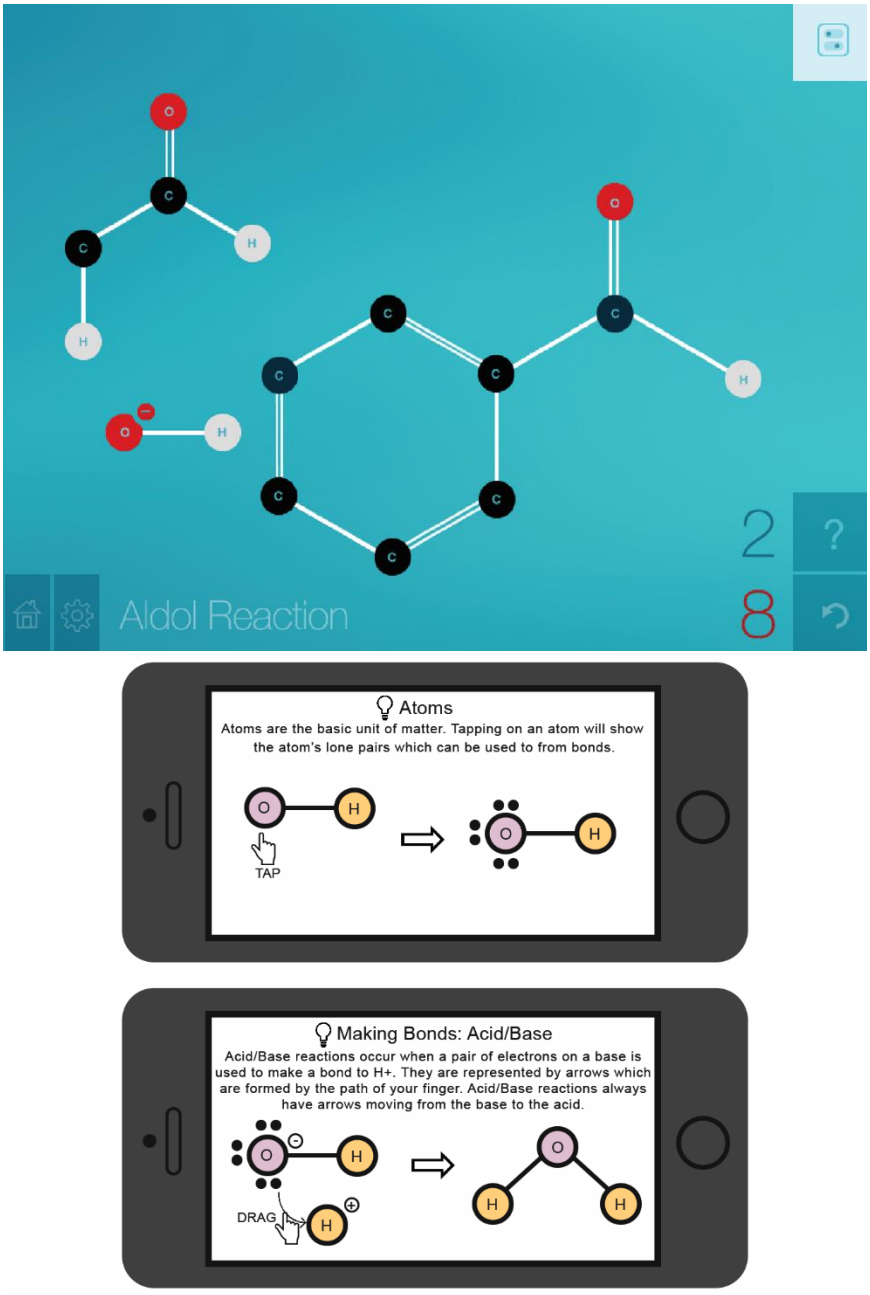


Figure 1a: Visual design of the MG, 1b: Example of Wireframe images

At the conclusion of the consulting work in early 2014, not a single line of code had been written, but the MG was ready to be handed over to software developers. When vetted by a series of game studios the price tag to produce a Minimal Viable Product (MVP) of the game was well into the six-figure range. The project stalled at this point due to lack of funding.

This preliminary design work, however, was used as the basis for a Small Business Innovative Research (SBIR) grant from the National Science Foundation (NSF), which was awarded to Julia Winter, as the Principal Investigator, in January 2016. With the start of the SBIR Phase I grant, the company Alchemie was incorporated and Julia Winter left Detroit Country Day School to build the Mechanism Game.

NSF SBIR Phase I: UX/UI development and early testing

The first phase of SBIR funding is used to prove the commercial viability of an idea. The NSF funds concepts that are deemed too risky for traditional investors, such as angel investors and venture capitalists. During this phase of development, a prototype of the Mechanism Game, now called Mechanisms, was built and tested.

The Alchemie team worked with Schell Games of Pittsburgh, an independent game studio that specializes in educational or "transformational" games, and has also earned its own SBIR funding for chemistry projects from the Department of Education, for Happy Atoms (*2*) and HoloLAB Champions (*3*).

The Schell Games method includes what they call the Transformational Framework, a tool set for designers to guide games that are, as they define it, "developed with the intention of changing players in a specific way that transfers and persists outside the game," (*4*). Since designing a successful transformational game requires additional planning and resources beyond entertainment-only games, Schell Games developed the Framework to guide the process of pre-production and to help pre-emptively answer questions that commonly arise during the transformational game development. Transformational pre-production work for Mechanisms included:

1) Creating design pillars
2) Describing audience and context
3) Identifying barriers to success
4) Defining the high-level purpose and players' transformational goals
5) Developing the software with iterative design feedback

Creating design pillars

The creation of design pillars was a core facet of the pre-production process. Design pillars are two to four key phrases that the team develops to encapsulate the core of a game's experience. At the beginning of a project, they help the team to solidify the high-level design goals. They also serve as design touchstones for the remainder of the project. After a team decides on the key phrases, the artists and designers draft posters to use as project references (Figure 2). For Mechanisms, the team developed two design pillars:

- New Touch New Experiment: Every interaction that the player has with the game should grant them a new piece of information. The player should be able to form hypotheses that they can test using the game.
- Responsive Models for Mastering Chemistry: The core of what makes this game unique as a learning tool is that it can give players feedback and new information based on their inputs. With that in mind, its design should follow pre-existing chemistry standards that professors use in their classrooms.

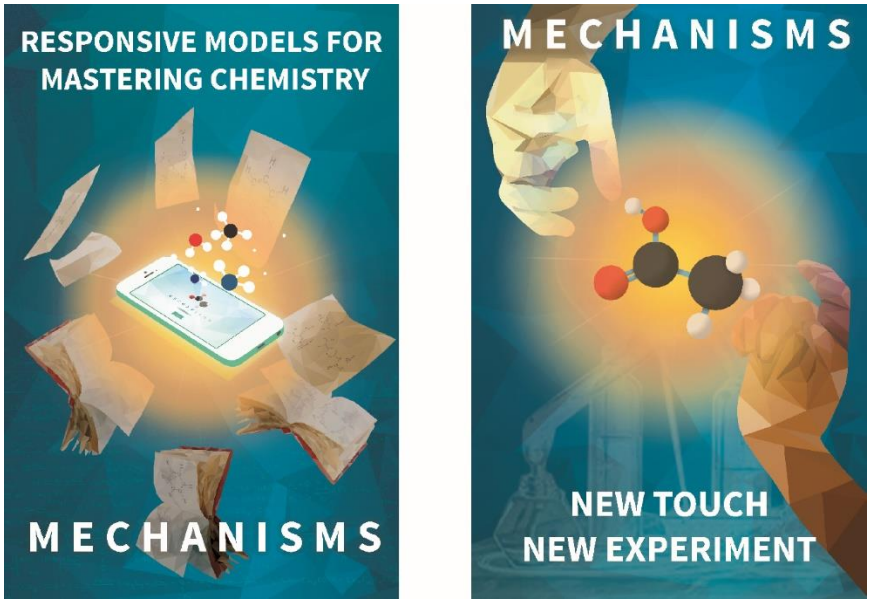


Figure 2: The Design Pillar images for Mechanisms

Describing audience & context

It was important at this stage to make the distinction between short- and long-term audiences. The Phase I grant identified that before testing with students, there needed to be confirmation with organic chemistry professors that the proof-of-concept was a useful tool worth pursuing further. With that in mind, while in the long term the primary audience of Mechanisms will be students, for the Phase I prototype the main target audience were organic chemistry professors. It was therefore assumed that target users would have a solid grounding in organic chemistry, and some of the scaffolding and tutorialization necessary for student learners could be omitted in the prototype. It should also be noted that in the long term, professors would still be part of the audience since they, and other policy makers at universities, are responsible for recommending useful tools and software to students. The data from both professors and students used to evaluate the technical objectives of the NSF Phase I project were collected in accordance with and after receiving approval from the institutional review boards of participating institutions.

Identifying barriers to success

While chemistry professors were the main audience for Phase I, most of the research focused on identifying and addressing the existing barriers that students encounter while they are learning organic chemistry. For instance, the rules of organic chemistry are consistent, but they are highly context-dependent so it can be difficult to know when to apply them. As a result, there is no easy step-by-step rule-set for solving a given mechanism. Instead, solving an organic chemistry mechanism usually involves weighing several likely options. The language of organic chemistry is complex, so it is difficult for students who do not understand the language to know what questions to ask. On a similar note, there is a relatively long turnaround time between solving a problem and getting feedback from assessments such as exams, so students may find themselves trying to learn new material building on concepts they do not fully understand.

Defining the high-level purpose and players' transformational goals

In the long term, the stated goal of the Mechanisms app was to increase meaningful learning of difficult organic chemistry concepts. With that in mind, for this prototype two short-term transformational goals were defined. First, to allow players to experiment with organic chemistry concepts and receive immediate and helpful feedback. Second, to show college professors through the proof-of-concept that a complete game was worth pursuing.

Organic chemistry is an enormous field and there are plenty of barriers to entry, so for this prototype the scope was narrowed to solve a specific set of three problems, targeting acid-base chemistry, resonance, and acid-catalyzed hydration of an alkene. The transformational goals for players were threefold. First, after playing the game, players should understand how mechanisms can be used as a tool in organic chemistry. Second, players should gain an instinctive understanding for the rules systems that govern mechanisms. Finally, they should be able to solve a given mechanism.

Developing the software with iterative design feedback

Since this project was geared toward researching new forms of gameplay and feedback, the development cycle was structured to allow the programmers to build well-defined systems while the design team produced documentation for the next round of features. The project began with the implementation of basic functionality. These interactions with the touch screen are referred to as User Interactions or UI. Specifically, at the end of this stage of development in the UI, the player would be able to see and move a molecular system on the screen, to see whether an atom had a formal charge, to tap on an atom or a bond to reveal hidden information like the number of available electrons, and to break and form bonds by dragging electrons with their finger.
All the UI was defined in extensive game-design documentation before integrating into the software (Figure 3).

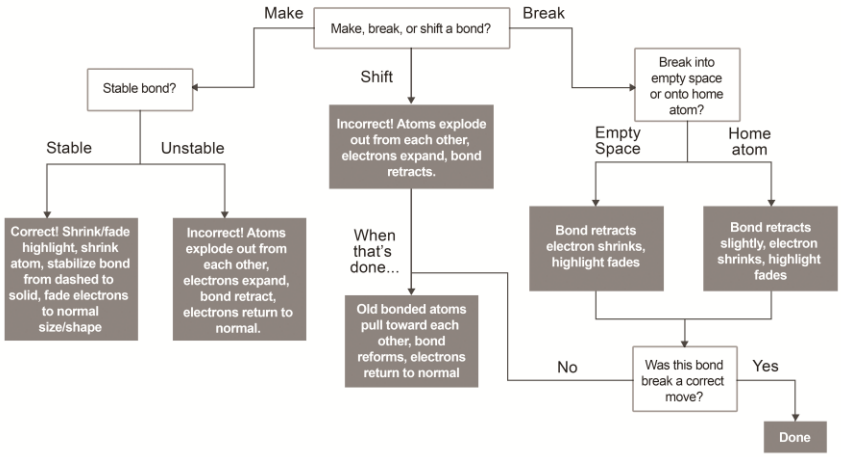


Figure 3: A flowchart of UI for Mechanisms

Throughout the project, feedback was sought from multiple sources to understand the user experience, or UX. Students helped to determine which concepts were most difficult. Professors were interviewed and performed prototype play-throughs to give a subject matter expert's opinion of the UX. They also provided expertise on the overall rule-sets: which bond could or could not be made or broken. Professors were also consulted on the visual feedback, that is, whether the chemistry "felt" right or not. Non-chemistry game designers were frequently involved to improve general gameplay. Feedback from play-testers without expertise in either chemistry or game design was solicited to identify UI features which did not feel intuitive or encouraging to game exploration.

The prototype was built in six two-week development sprints in iterative cycles; as feedback was collected, it was incorporated into development and the process repeated itself every two weeks. At the end of this three-month period, the Mechanisms prototype had a tutorial section, and three separate puzzles: Acetic acid and hydroxide, 4-hydroxy benzaldehyde and hydroxide, and acid-catalyzed hydration of 1-methylcyclohexene.

Testing of the prototype with chemistry professors and students

There was one metric for the success of Phase I development: support from college faculty to use the product with their organic chemistry students. As defined in the Phase I technical objectives, a successful prototype would garner a positive recommendation from at least 50% of the group of faculty we planned to survey and interview. A group of twenty-five faculty and instructors were recruited to use the app on own their own device and complete a survey and video-conference interview. Of the twenty-five-faculty surveyed, twenty-three said that they would recommend the product to their students, indicating that the Phase I criterion had been met and providing encouragement for the Phase II grant proposal**.**

The instructor interviews yielded more detailed information about specific uses the twenty-three faculty envisioned for the product, and the reasons why two faculty would not recommend its use. The interviews also provided insight into what elements of the product they enjoyed and did not enjoy, as well as suggestions for future development. These comments fell into three categories: technical, chemical, or pedagogical. Technical comments were about the performance of the product. Chemical comments were regarding the way chemical phenomena were represented in the product. Pedagogical comments pertained to the utility of the product as a teaching and learning tool.

The interview participants represented a wide range of educational institutions. Most were schools and universities, although several instructors identified their current institution as private, for-profit entities. The participants' affiliation included twelve institutions in the United States, eight in the United Kingdom and one each from Canada, France, and Thailand were also represented by the participants. Of the schools and universities, fourteen were public and five were private institutions. This institutions also varied in enrollment size. Five had enrollment of greater than 30,000, five had enrollment between 20,000 and 30,000, six had enrollment of less than 10,000, two had enrollment between 10,000 and 20,000 and six had no student enrollment.

Instructors valued the app's potential as a tool that addressed their students' learning needs. They appreciated its open-endedness and freedom to make mistakes (n=6) "I did like the option to make mistakes or break bonds in the wrong direction, because there aren't many tools that do that." Another instructor emphasized the same point: "I really liked the aspects where you allowed them to make mistakes and coached them back in, so they can think about the other possibilities and evaluate them. That's an important part of critical thinking that I don't see in too many other places." Other descriptors that instructors used for the game were: dynamic, intuitive, tactile, fun, and powerful.

The primary critique that the faculty offered was that there was not enough scaffolding for naïve learners, and that students might struggle without additional support built into the game (n=16). This suggestion was not without merit; the prototype that the faculty tested was intended for users with chemical expertise. However, the instructors offered specific ideas that the scaffolding should include, such as clues about formal charges and electronegativity, explanations for moves that are disallowed, and greater specificity for the goal for each puzzle task.

To test the playability of the app and investigate potential for impacts on student learning, nine students were recruited for one-on-one interviews during Phase I research and development. The students attempted three paper-and-pencil organic chemistry problems that were analogous to the puzzles in the app, then engaged with the app, and finally, re-attempted another set of analogous paper-and-pencil problems. They were asked "What did you think of the game?", "What did you like?", and "Was there anything you found difficult or confusing?"

A study was performed on the data collected for the prototype app in the summer of 2016 during Phase I. The goal was to answer the following research questions:

- How does students' electron-pushing when using Mechanisms compare to their use of curved-arrow notation on paper-and-pencil mechanisms?
- Does interaction with Mechanisms help students to improve their performance on paper-and-pencil mechanisms problems?
- How do students use immediate feedback on their organic chemistry reaction mechanisms to direct their next move?

The most prevalent errors from the students' interaction with Mechanisms app were coded according the scheme shown in Figure 4. The types and frequency of unique errors committed by each student is shown in Table 1, names have been changed. The errors observed in the students' game play corresponded to errors previously described in research about students' understanding of organic mechanisms (*5*). For example, errors b and f correspond to the previously reported idea that curved arrows indicate the movement of an atom, rather than the flow of electrons *(6, 7)*. Errors a and d showed that students were not considering the convention that arrows be drawn from electon "source" to "sink" *(8)*.

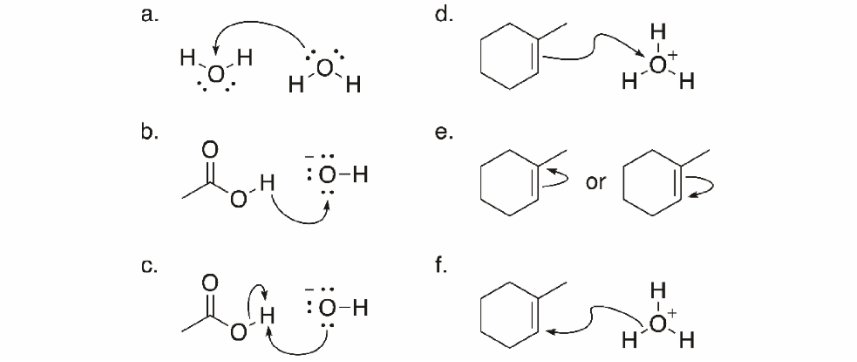


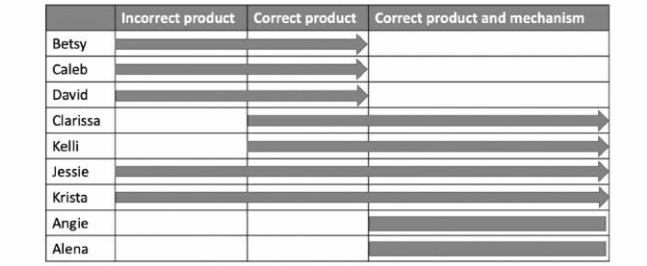
Figure 4: Coding of errors committed by participants during summer 2016 study of prototype app a.) formation of a peroxide, b.) arrow moving atom instead of electrons, c.) electrons flow to wrong atom during heterolytic bond cleavage, d.) oxygen with a positive charge is an electrophile, e.) heterolytic cleavage of π-bond to form carbanion or carbocation, f.) addition of hydride to alkene carbon.

Table 1: Type and frequency of mechanistic errors among participants in summer 2016 study of prototype, with error codes a-f as defined in figure 4.

	Error Code						
Participant	a.	b.	c.	d.	e.	f.	Other
Angie	1	3	2	1		2	
Alena		1	2				
Jessica			1		1	1	
Krista	1	2		1			1
Kelli		1	4	1	1	2	1
Clarissa		1	2				1
David		2	1	2	2	2	1
Betsy		5	3	1		1	3
Caleb		1	1	1	1	1	1

Despite the errors committed while using the app, most students improved their ability to draw the paper-and-pencil mechanisms afterward as shown in Table 2. Three students shifted from an incorrect mechanism and incorrect product to being able to correctly identify the product. Two students were able to improve from only able to identify the product during the pre-test, and being able to draw the mechanism for that correct product in the post-test. Two additional students progressed from not being able to predict the mechanism nor product, to being able to correctly draw both mechanism and product. Finally, two students identified the correct mechanism and product during the pre-test. Of all of the students who did not initially draw a correct mechanism on the pre-test, each student made some gains on the post-test after engaging with three puzzles on the app.

Table 2. Participants' level of correctness for paper-and-pencil mechanism question, with the arrow tail indicating each participant's level of correctness before engaging with the app and the arrow head indicating the same participant's level of correctness after engaging with the app. A rectangle indicates no change was observed.



Though brief gameplay and a small sample size limited this preliminary study, early conclusions indicated that undergraduate students interpret Mechanisms app representations similarly to paper-and-pencil curved-arrow notation. This was evidenced by the similarity of misconceptions about electron-pushing observed during app use to the misconceptions reported by previous studies where students drew mechanisms with curved-arrow notation (*5-8*). The change in students' abilities to answer a paper-and-pencil mechanism question after using the app indicates that performing analogous tasks in Mechanisms may improve students' abilities to draw mechanisms with paper-and-pencil.

The results from the development of the app prototype and the research with both instructors and students completed the six-month Phase I project. The Phase II grant was awarded to Alchemie with a start date of March 2017. The technical objectives of this grant included transforming the prototype to a full commercial product, which would include creating a pedagogical puzzle system with an assessment method, and building a machine learning analytics framework.

NSF SBIR Phase II: Authoring tool development

During the first stage of Phase II development, systems were created for structure recognition, molecular layout, and database architecture. A problem that remained unresolved during Phase I was the creation of a back-end system to rank and predict the numerous possibilities of the organic chemistry reactions. It was decided early in the Phase I development process to hand-code the reaction choices into the puzzles, this method was not scalable in terms of software development.

The Mechanisms Authoring tool allows chemistry content experts to act as designers. These experts can create Mechanism puzzles, designating which bonds to make and break as well as the order in which the bonds can be manipulated, all without requiring the designer to create the software code by hand. By allowing the designer the freedom to choose the method by which the puzzle is solved, there was no need to build in additional chemical algorithms. The development effort from Phase I shifted from hand-coding by software developers to a user-friendly design interface for chemistry subject matter experts.

One of our pedagogical goals with Mechanisms was to encourage students to focus on finding the most reasonable move, mechanistically, one step at a time. Traditionally, students are given a reaction scheme which essentially gives them the goal end structure. Recent research has shown that, when given the product,

students tend to use an end-means analysis to solve a mechanism rather than rationalize individual steps (9). To facilitate students' forward reasoning through the steps of the mechanism, the design team decided to include actionable goals for each puzzle that guide students through the mechanisms. As goals are achieved, the player earns stars, regardless of the number of mechanistic moves in the path the player chooses. The puzzle is complete once all goals are met, which the game indicates by awarding all three stars.

The authoring of goals followed three guidelines. First, the goals should start with an action verb. This helps preserve a game-like feel and ensures that it will help inform what the next step should be. Second, when a reaction is first introduced, there are more goals, and the goals are more detailed. The intent was to build guided practice into the problem without labeling it as such. Then as expertise is gained, the goals become fewer and less explicit. Third, the goals were to use the language of organic chemistry. For a new learner the terms may be intimidating, however when learning any language, using the new terminology is essential to build proficiency.

Strategically, the goals were designed to be accessible within the puzzle from the menu in the upper left-hand corner. Additionally, once a goal was achieved, a button appeared in the lower right-hand corner, that when tapped on would show which goal had been achieved and which goals were still unmet. It was intended to give the player the freedom to explore their own chemical intuition without the influence of knowing the end product or goals. However, after instructor and student feedback, we found the goals were not quite visible enough. As a remedy, a button to access the goals was placed on the task card, which is the initial image a user sees when a puzzle is selected (Figure 5).

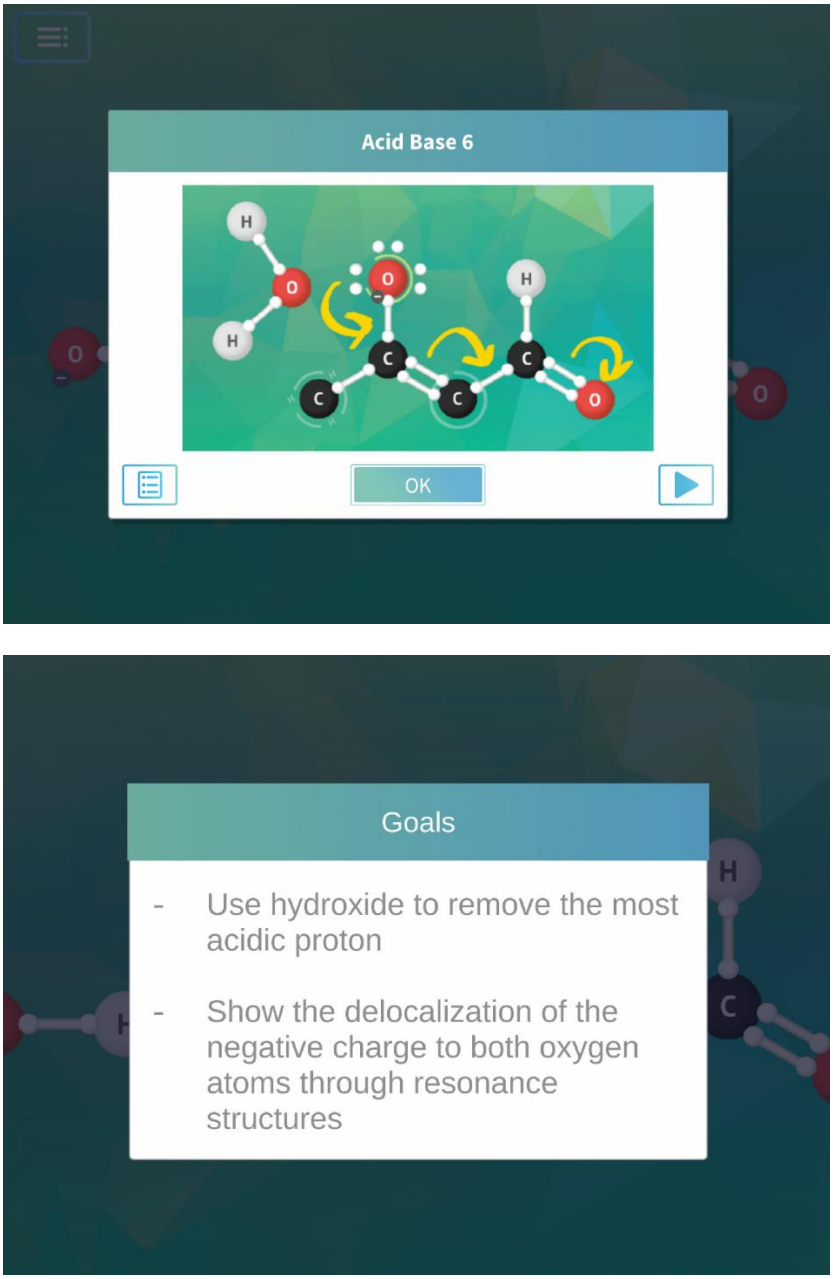


Figure 5: A task card and list of goals from a Mechanisms puzzle

In addition to goals, the inclusion of in-game hints were determined to be another essential pedagogical feature by instructor recommendation. The puzzle authors drew on their experiences from teaching and tutoring organic chemistry to identify common errors that were prime candidates for hints. Hints were then written to identify why the attempted move was not allowed and what a more reasonable move involved. Once the hint feature was introduced, students overwhelmingly requested that even more hints be included. In response, hints were used to highlight key aspects of a mechanism. For example, to emphasize why electron donating groups are *ortho/para* directors, the Electrophilic Aromatic Substitution Puzzle 2 has a hint that highlights the resonance stabilization gained by being able to delocalize the positive charge to the alcohol (Figure 6).

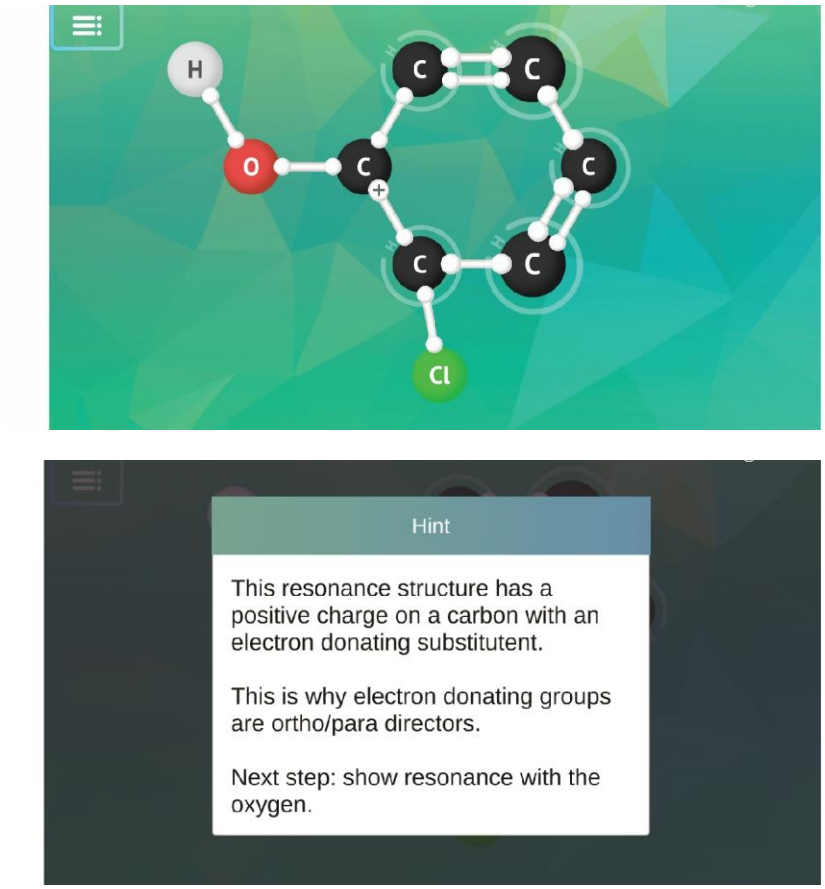


Figure 6: A resonance structure from EAS Puzzle 2 and its corresponding hint.

The most recent pedagogical update is the inclusion of expert mode. In expert mode the goals are hidden until they are achieved, and no hints are available. While the goals and hints are useful tools for independent learning of mechanisms, both student and instructor users requested opportunities to evaluate their mastery of the content. To this end, expert mode is useful for quiz-like experiences and for practicing prior to exams. This mode is also intented to be used in active learning spaces where students are encouraged to work together to rationalize why each move was or was not allowed.

Use cases and research studies

As of January 2019, the Mechanisms app included 250 reaction puzzles and has been implemented at over 50 institutions and incorporated into various active learning settings. As a part of Alchemie's efforts to improve content for its users, instructors were asked how they used Mechanisms in their class. In the spirit of this book, examples have been included which made use of Mechanisms in small break-out sections during class. Additional activities suited for active learning environments have also been proposed.

The first example came from a private small liberal arts college on the east coast. The students first attended a class session with a traditional lecture and then met in a selected subset for two hours in a section called the intensive session. Here, the material is summarized and general questions are answered by the professor before the students break into small groups of two or three to work problems. It was during these small sessions that the instructor used Mechanisms. Students were first introduced to the app and given a chance to familiarize themselves with its functions through resonance and acid-base puzzles.

The students were able to easily download the app to their phones and begin to use it. There was a bit of a learning curve to select the lone pairs, especially on smaller touchscreens such as on phones. Once students got over that activation barrier, they were readily able to manipulate the bonds and electrons in the puzzles. The majority of the students reported that they enjoyed the app and found it fun. However, it was difficult to determine whether this student experience would transfer to their ability to accurately draw mechanisms on paper. One method that proved effective to create the link between finger and screen to paper and pen, was to use Mechanisms in combination with a worksheet. For example, a guided practice for a pre-selected set of S_N2/S_N1 and E1/E2 puzzles asked students to identify the leaving group, the type of carbon undergoing attack (for S_N2/S_N1), the nucleophile (or base), and the mechanism. Then students had to generalize the difference between S_N1/S_N2 or E1/E2

mechanisms. With a more guided way to use the app, the students were more able to communicate and translate organic chemistry jargon to the assigned problem and this led to more effective communication with peers and the instructor. This exemplifies how a scaffolded activity can provide scaffolding for the use of Mechanisms and allow students to engage in learning of organic chemistry concepts without direct instruction.

Mechanisms was also used at a public research (PhD) university on the west coast. For this class, students attended a large-attendance lecture class session with the professor and a smaller-attendance quiz session run by teaching assistants (TAs). During quiz sessions the students worked in small groups of three or four, on worksheets and quizzes. A study was implemented as part of the instructors' regular course of instruction. All student artifacts were de-identified before being shared with researchers and as such did not meet the criterion for human subjects research. As a control, the first mechanisms the students learned, addition reactions, were taught following a traditional lecture format without the use of the Mechanisms app. Later, for substitution and elimination reactions, the students used the app during quiz sessions. The TAs, who led the quiz sessions and circulated around the room while students were working, reported that students were able to picked up on how to use the app even without a demonstration. Additionally, students assisted each other for most questions related to using the app. The student artifacts provided preliminary insight into the ability for students to translate the movement and representations in the Mechanisms app with the symbols used to draw mechanisms on paper.

The quiz session activity contained ten problems that required use of the app. Students were prompted to play specific puzzles in Mechanisms and to write their answer, for the puzzle, on paper by drawing a complete mechanism using bond-line diagrams and arrow pushing notation. To investigate preliminary results, we chose to analyze just the students' answer for the first S_N1 puzzle, a substitution of a tertiary alkyl bromide with water. This problem came half-way through the activity, so by this point students were familiar with the app and we wanted to see how students solved a mechanism that was more than one-step. Another interesting facet was that students had learned the S_N2 mechanism in lecture but not the S_N1 mechanism prior to the activity. Out of seventy-five groups, thirty-five groups (47%) gave a complete mechanism, nineteen groups (25%) gave only the product, twelve groups (16%) wrote down only the first intermediate, and nine groups (12%) did not attempt the problem.

The use of the Mechanisms app did not seem to disrupt the ability to draw mechanisms on paper. From the thirty-five groups that gave a complete mechanism, there were only two instances (6%) where student drawings conflicted with traditional electron-pushing formalisms. One group drew the

molecules as they appear in the app rather than in line-angle notation, and another three groups (9%) neglected to include the straight arrows that separate steps in a mechanism. Interestingly, before use of Mechanisms (based on answers given for an addition mechanism on a quiz earlier in the semester), twenty-eight groups (36%) showed all lone pairs, on all heteroatoms and on all intermediates while working through a mechanism on paper. However, after introduction of the app, this dropped down to one group. Instead, students chose to focus on showing primarily the lone pairs for the atoms from which the arrow began (the electrons that were directly involved in the mechanism). This indicates that the app is helping to focus student attention to where the action is taking place in the mechanism.

Remarkably, even though students had not yet been taught the S_N1 mechanism in lecture (only S_N2), fourteen of the thirty-five groups (40%) that gave a complete mechanism, were able to correctly show the substitution as a two-step process. Additionally, of the twelve groups that stopped writing the mechanism at an intermediate, eleven drew a S_N1 mechanism. Potentially, this means that a majority of students (57%) were able to identify the difference between S_N1 and S_N2 reaction mechanisms based on the presentation of information in the app. Another intriguing result, is that eleven groups (15%) stopped drawing the mechanism at the highly reactive carbocation intermediate. Remember, students are not given the product of the reaction on the task card, so it would be interesting to further probe why they chose to stop at that intermediate. It should also be noted that, reassuringly, only one group of all the samples wrote out the "decision point" in their mechanism. The decision point is a cue within the app to show the concerted nature of a two-arrow move where the screen is darkened and only two moves are possible: the reversal of the original move or the allowed move forward in the mechanism. This result suggests that the darkened screen during a decision point successfully cued students that the structure of a decision point is not an intermediate. This preliminary data warrents future studies that look at how students identify intermediates in Mechanisms. On a similar note, it would be interesting to see if students view resonance structures in the app as intermediates rather than contributors to an overall structural hybrid.

Overall, this case study provides some initial evidence that students are able to translate between the movement of electrons in Mechanisms and the representation of the electrons using arrows on paper. The conclusions of this study are limited by the fact that students worked in groups, the activity was graded only for completion, game play was brief, and it is not known which or if students read the textbook to learn the S_N1 reaction. Therefore, more work needs to be done to understand how successful students are at defining intermediates

and distinguishing the difference between a one-step and a two-step mechanisms (like S_N1 and S_N2) by using the app Mechanisms.

To help support instructors, chemistry content specialists at Alchemie have designed both independent self-assessment worksheets and active learning activities for course-based discussion facilitation. These resources are available on the company website and are free to use. The worksheets utilize Mechanisms to review key concepts, such as resonance and acid-base theory. These are designed to be used as a refresher of key concepts throughout the course as well as a study aid for final exams. The active learning activities are designed to promote discussion among students working in small groups.

Another feature requested by instructors for use with active learning pedagogies was the ability to control when an assignment could be completed by adjusting start and end times of an assignment window using the web-based instructor dashboard. When these times corresponded with actual class times, the Mechanisms app could be used like a clicker-system, alternatively when the assignment window occurs just before a class period, the usage could be as a warm-up activity before class.

Next steps: Pattern recognition from data

Organic chemistry textbooks and lectures cover the general mechanism for many standard reaction types. On their own, students work through examples and check their proposed mechanism against these examples. However, unless a student comes to office hours, or the instructor circles through an active learning class, the instructor does not have the chance to see what students' initial mechanistic instincts are. What is unknown is how much thought do students put into understanding why their proposed mechanism is incorrect. What if instructors could see what the common initial mistakes are among students? Could they provide more clarity to students in lecture or extra feedback on an answer key? Would this information lead to a major advancement in identifying and breaking down barriers to understanding mechanisms? These are compelling questions, but there are limited assessment tools that give instructors acces to realtime student thinking. Perhaps one of the most exciting features of Mechanisms for instructors is the app's ability to record ALL the moves students attempt. To date, the database of Mechanisms has collected approximately 250,000 user sessions from the app, with all moves coded as to sequence and type, such as nucleophilic attack or deprotonation.

Initially, Alchemie's chemistry content experts were surprised by some of the emerging common errors in the student data. From the lens of a novice though,

these moves begin to make sense and reveal where more guidance and explanation is required. For example, reviewing data from Addition Puzzle 2, hydration of 2-butene, exposed the belief that an oxygen with a positive charge is an electrophile (Figure 7). This error was observed in both the first step, addition of a proton to the alkene, and in the last step, deprotonation. For an expert, the hydronium is first-and-foremost a Brønsted-Lowry acid, so arrows would move initially to the hydrogen atom. If, however, the acidity of hydronium is not recognized, then this is actually a fairly logical step that follows the commonly used saying "electron rich attacks electron poor."

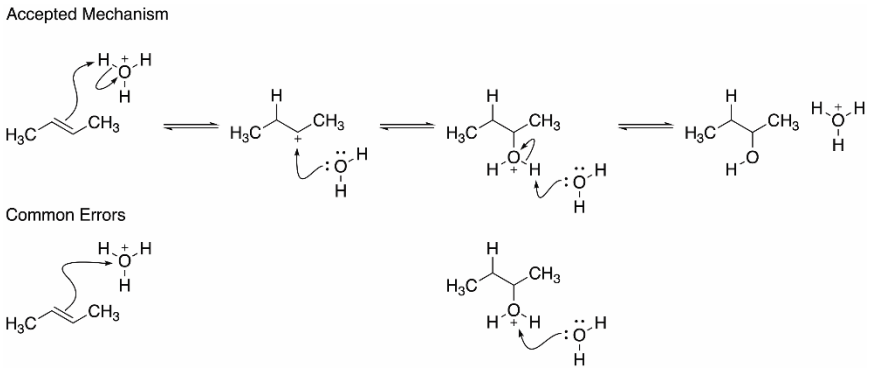


Figure 7: The accepted mechanism of Addition Puzzle 2 in the Mechanisms app. Student attempts at using oxygen of hydronium as the electrophile shown below the corresponding steps.

Addition Puzzle 2 also revealed that, students struggle with how to show proton transfers in a mechanism. Multiple times students tried to have a proton leave without the facilitation of a base (Figure 8a) or started the arrow from the hydronium oxygen-hydrogen bond (Figure 8b). Perhaps students are trying to complete the puzzle in the most efficient number of steps but then that means they are do not fully understand why the flow of electrons follows the patterns it does. Overall, data collected from Addition Puzzle 2 suggests students struggle to recognize when to use the acid-base steps traditionally learned early on in organic chemistry courses. Without a firm basis in this foundational chemistry concept, more advanced mechanisms that include an acid-base, such as those involving carbonyls, are going to be even more challenging for student. Ongoing research carried out at two midwestern research intensive universities are exploring these hypotheses with think-aloud studies of individual students using the app.

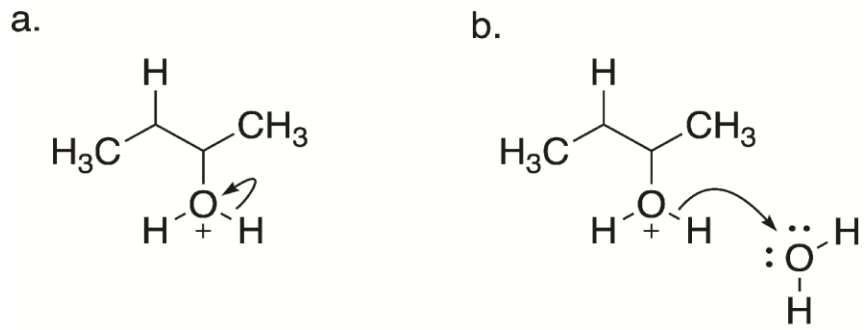


Figure 8: Common errors for deprotonation attempts a.) loss of a proton without the assistance of a base and b.) movement of electrons from the hydronium oxygen-hydrogen bond onto the base.

As more students continue to use the app and play through the puzzles, it is anticipated that more unexpected common errors will be recorded. Moving forward, we plan to use this data to identify where students would benefit from more hints and explanations. The inclusion of this automated guidance through advanced analytics and machine learning will provide individualized feedback for students and concept-based assessment for instructors, and is the ultimate goal of the NSF SBIR research and development effort. As we continue to improve the content and pedagogy of Mechanisms based on user feedback, our hope is that we can give all students the guidance they need to succeed in organic chemistry.

Acknowledgments:

We would like to thank Professor Brian Coppola of the University of Michigan for early and ongoing support of the development team, lending his pedagogical insight and expertise for the Alchemie Mechanisms project.

This work has been supported, in part, through grants to Alchemie from the National Science Foundation Small Business Innovation Research program, Phase I #1548225 and Phase II #1659983. Research by Dane DeSutter has been supported by the NSF Non-Academic Research Internships for Graduate Students (INTERN) program to supplement NSF grant #1661096 awarded to Professor Mike Stieff of University of Illinois at Chicago.

Competing Interests:
Authors Julia Winter, Sarah Wegwerth, Brittland DeKorver, and Layne Morsch have received compensation for work performed as employees, contractors, or consultants of Alchemie, the producer of Mechanisms.

Authors Dane DeSutter, Lawrence Goldman, and Lauren Reutenauer declare no competing interests.

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