OrganicPad: a freehand interactive application for the development of representational competence.

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One reason chemistry poses a challenge to both learners and teachers is that, for robust conceptual understanding, students must understand how and why molecular level structure affects reactivity and properties. Much has been written on the difficulties students have in translating between a symbolic, molecular, and macroscopic understanding of chemistry (1, 2) and most modern texts go to great lengths to provide multiple representations to students.[1] Lewis structures are probably the most important of the symbolic representations that students encounter. Students must master not only what the representations mean, but also how and why they are constructed, and what they are used (and useful) for. Unfortunately, many students have great difficulty both drawing and using Lewis structures. For example in our work we have seen that the majority of students (even in an organic chemistry course) do not appear to use structures to predict properties in a meaningful way (3). Many students (and perhaps some instructors) confuse the rules for drawing structures with the concepts that underlie bonding, resulting in students who believe that bonds form because atoms "want" or "need" an octet (4, 5). Indeed the idea that Lewis structures are symbolic representations may well be lost on many students (for example: if asked what the bond angle is in methane, when presented with a typical Lewis structure, many students will answer 90).

These problems notwithstanding, learning to draw and use Lewis structures accurately and effectively remains an integral part of most general chemistry courses, and is an especially important skill for those students planning to move on to organic chemistry. The development of these skills during general chemistry is all the more important since many organic chemistry instructors assume (erroneously as our work has shown) that students have mastered this skill before they begin the course (3).

There is a fairly large literature on "improved" ways for students to learn to draw structures, but unfortunately this is one of those tasks that requires "bootstrapping" as Taber calls it (6). For many structures, it is difficult to elucidate the connectivity between the atoms correctly unless you already know what the structure should look like. In other words, the students are caught in a kind of "Catch 22". The solution to these problems is practice and a growing familiarity with the typical types of structures that are normally encountered in introductory chemistry courses. This familiarity is often difficult to obtain if beginning students are required to draw the many exceptions to the "rules". Another common approach is to require students to draw only structures where there is one central atom (noble gas compounds, inter-halogen ions and the like - many of which they will never meet again), which results in our distressing finding that many organic chemistry students have significant trouble drawing organic molecules with more than one carbon atom (3). Ideally, in order to master the basic skills, students need practice and immediate feedback that prompts them to think critically about what they are doing, rather than simply providing the correct answer.

Since Lewis structures are in fact rule-based representations, technological solutions are clearly appropriate, and there have been a number of systems developed that will recognize and grade input from students. While many of these systems are widely adopted and have been incorporated into publishers' course management systems, there remains the problem that the interface is typically not naturalistic, and students (who are already struggling with learning to draw structures) must also face fairly steep learning curves as they drag and drop atoms and bonds, choose items from a template, and place them in fairly limited positions on the screen.

It was in this light that we developed *OrganicPad*, (Figure 1), a freehand interactive tablet-PC based program that can recognize and respond to student input in a variety of ways and a variety of settings

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Figure 1. OrganicPad with examples of some of the representations that can be drawn.

Overview

The current version of *OrganicPad* is a PC-based program designed for use on tablet PCs or for use with a Wacom slate; however, it can also be used with a mouse or trackpad. A web-based version is currently under development. This paper describes the PC-based system now in use and how we plan to extend it to the web.

OrganicPad has a number of features. Using the draw mode, the program can recognize atomic symbols, bonds, lone pairs and charges. Once a structure is drawn, it is possible to convert it to a 3D representation, as shown in Figure 2. The 3D mode allows student to convert a structure to ball and stick, space filling models and/or electrostatic potential maps. In the pen mode the screen is just like a blank sheet of paper allowing teachers and students alike to annotate the structures that they are creating. The push tool allows students to draw curved arrows when they are representing electron flow during organic chemistry mechanisms. It is important to note that in draw, pen, and push modes the students' input is recorded in a database for further analysis.

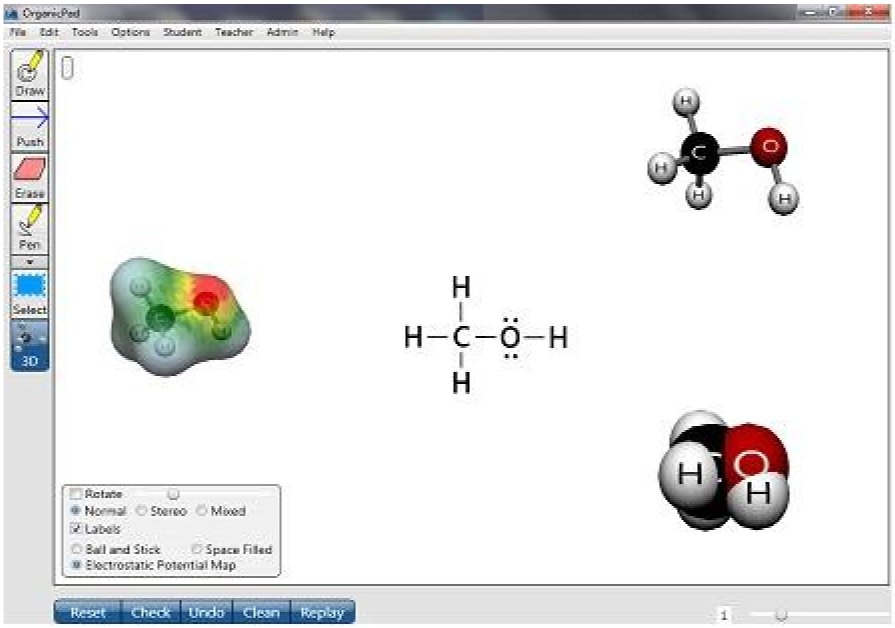

Figure 2. Types of 3D representations that can be produced with OrganicPad.

OrganicPad for teaching and learning

The simplest way to use *OrganicPad* is to draw structures as you normally would onto the tablet screen. The program can recognize the "common" atoms, that is, H, C, N, O, I, Cl, Br, F, S, P, Na, Li, Mg, Al, B. There are as few constraints as possible placed on how the student draws the structure - the system is flexible and students need not place their structure in any particular orientation or draw it in any order. When finished, the student can hit the check button, and the program will indicate whether the structure is correct, or if there are problems, where they lie as shown in Figure 3. In this example, both the hydrogen and carbon atoms have been boxed in red to indicate that the student has drawn too many bonds to both.

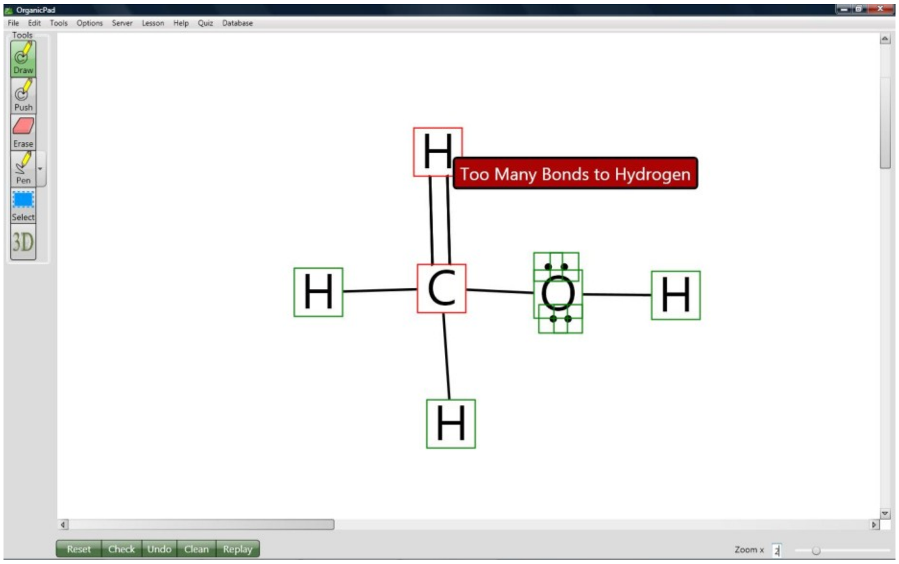

Figure 3. An example of feedback.

While this mode, in itself, can be very useful, we have developed a more sophisticated feedback system, for a limited set of structures, in which contextual responses have been developed to provide the student with increasingly directed feedback as they move through the task of structure drawing. An example of this is shown at (http://www.youtube.com/watch?v=CAqCashseYI). The feedback is based on our studies of how students often proceed as they write Lewis structures, and common errors that they make (3). We are currently conducting studies on how working with this kind of contextual feedback impacts student abilities.

OrganicPad as a classroom activity

There are a number of ways, both synchronous and asynchronous, that instructors can use *OrganicPad* in their classrooms or labs. Students can log-in to the system which then allows the instructor to send asssignments to them. The instructor can draw or choose a correct answer from the students responses and the program will grade the structures the student has drawn and send feedback to each individual. The instructor can also view what a specific student has drawn and provide further feedback to that student if necessary. If a number of students have a common error, the instructor can show an anonymous version of the structure and initiate class discussion on how it might be improved. A video of this mode is at (http://www.youtube.com/watch?v=Pbq0Dsderek) (n. b. this video shows a slightly older version of *OrganicPad*.) Quizzes or assignments can be given out of class, and graded automatically with feedback. *OrganicPad* recognizes full Lewis structures (showing all bonds and lone pairs), and line structures, depending on the circumstances. Students can draw other forms such as condensed structures (CH3CH3) with the pen, and the system will record their drawing.

OrganicPad as a research tool

We believe that one of the most important features of *OrganicPad* is the ability to record student actions, store, analyze and replay them. While there are a number of qualitative studies (7, 8) on how students construct and use representations, it may well be that the study itself could perturb what students do. Interviewing or observation of students is quite time consuming and the subsequent analyses can be difficult and complex. There is a growing understanding that studies done under controlled circumstances may not always be applicable to "real life" (9); we are interested in what students do "in the wild, and on the fly," that is, under circumstances that are as close to normal as possible. Our approach is to, combine studies using large amounts of student data (quantitative studies) with interviews (qualitative studies) to investigate how students develop representational competence. We have collected tens of thousands of exemplars of how students construct Lewis structures for many common structures. We can cluster them using Markov Modeling (10) to elicit common pathways and points where students make errors. The Markov models are based on the probability that students will move forward from one state to the next using a particular pathway. Figure 4 shows a Markov model for ammonia.

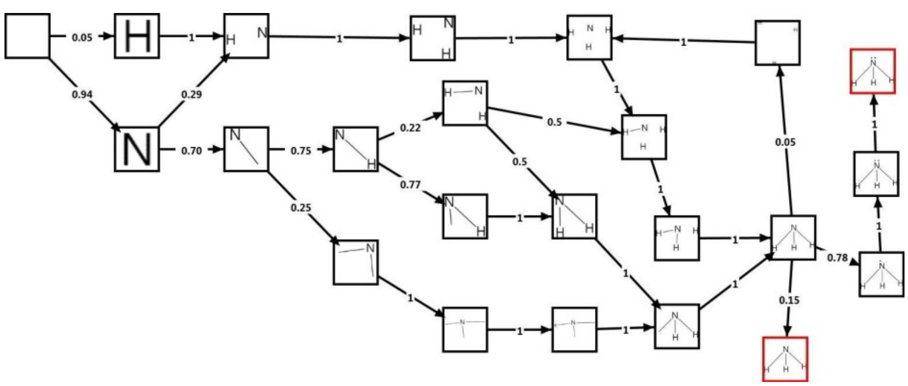

Figure 4. A Markov Model for Ammonia.

In addition to providing us with an indepth knowledge of the likely pathways students may utilize in creating their structures, the Markov models obtained through the use of OrganicPad also provide us with actionable information which we have used to create the contextual feedback system described above.

We have also used *OrganicPad* extensively to investigate how students draw mechanisms for organic reactions. Most organic chemists teach mechanistically, and assume (hope) that students will, in passing, learn to use the tools necessary for them make sense of the huge amount of material. We are currently analyzing data and preparing manuscripts on that analysis - but preliminary indications are that most students in organic chemistry do not spontaneously use mechanisms to guide their approach to predicting products of reactions. Those that do appear to be better equipped to solve far transfer tasks provided to them.

Future Directions

As previously stated, we are currently developing a web based version of *OrganicPad* that will be incorporated into a suite of tools that are currently under development. Foremost among these tools is *SocraticGraphs*, a graphical analysis tool that can recognize and respond contextually to student freehand input. We also continue to use *OrganicPad* as a robust assessment tool for a number of projects that we have initiated to help students better develop representational competence. For example: our new general chemistry curriculum development project, *Chemistry, Life, the Universe and Everything (CLUE)*, (in collaboration with Mike Klymkowsky, see http://virtuallaboratory.colorado.edu/Chemistry/index.html) is designed using research-based principles. OrganicPad will be an integral part of SocraticGraphs and, with activities based on graphical analyses, will be integral to CLUE-based instruction. OrganicPad is currently a free computer program and can be downloaded at http://www.clemson.edu/organicpad.

Acknowledgements: This work is funded by NSF grant DRL-REESE #0735655 and NSF-CCLI #0816692.

Footnotes

[1]Although the efficacy of this approach is debatable and not well documented. Alex Johnstone (11) has pointed out that while experts can translate seamlessly between the different levels and representations, beginners must first learn to operate along the edges of his famous triangle. It may be that presenting students with such a profligate set of representations may only serve to overload their working memory.

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