Report On The Development of ChemPad for Teaching Organic Chemistry Students to Visualize Three-Dimensional Molecular Structures

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Note: This document uses chemical terminology, but it is not necessary to understand the terminology to understand the goal and achievements of this study.

1 Introduction

Organic chemistry is a hard course. Early in their college studies, students who wish to pursue a career in medicine must have a solid understanding of organic chemistry and, perhaps more importantly to the students, a good grade in organic chemistry. The difficulty of the material prevents many students from continuing with this career path. One of the major difficulties for students in organic chemistry is understanding the three-dimensional nature of molecules. Students usually have no background in three-dimensional visualization and have great difficulty converting between the two-dimensional drawings used in text books and on classroom blackboards to represent molecules and their three-dimensional structures. Without this understanding, to survive the course, students must memorize a large vocabulary of molecules and rules to fake an understanding of the three-dimensional structures. Although this is possible for some, good students and good chemists tend to learn to visualize the molecules in three dimensions and apply a much simpler set of rules to these visualizations.

To address students' need for three-dimensional visualization in chemistry at Brown, University President Ruth Simmons authorized $50,000 of Atlantic Philanthropies funding to develop a new piece of educational technology targeted at this goal. This resulted in Professor Matthew Zimmt's Chemistry 35 course this spring being equipped with ChemPad, a Tablet PC application shown in Figure 1. ChemPad assists students learning to visualize molecules from standard two-dimensional drawings as a digital substitute for physical ball-and-stick modelling kits. Students can build the same structures they would with the modelling kit and see the same 3D features of the molecules. However, students using ChemPad can construct these models much quicker than with a physical model and receive interactive feedback about their 3D intuitions which would otherwise be unavailable without a TA or a professor available. By using the visualization assistance ChemPad offers to solve a 3D thinking task, students develop the skills to reach correct intuitions without assistance.

2 The ChemPad Application

Using ChemPad consists of drawing a molecule on the computer and observing the three-dimensional structure presented. Instead of selecting atoms and bonds from toolbars and menus the way a chemist does in professional modelling software, students use the Tablet PC stylus to draw a molecule in digital ink on the tablet that looks very similar to the same drawing they would make on an exam or on paper when talking to another chemist about the molecule. These drawings consist of single-stroke symbols representing atoms, bonds, and special pedagogical functions. For example, a student drawing ethanol would draw two C's and an O to represent the two carbons and one oxygen in the molecule. The atoms are

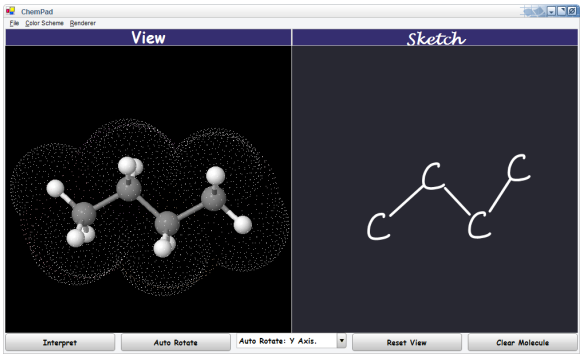

Figure 1 ChemPad visualizing the butane molecule.

then connected with covalent bonds by drawing straight lines between letters. As the atoms and bonds are being drawn, ChemPad displays the balls and sticks of the atoms and bonds being recognized and the student's handwriting is incrementally prettified. Finally, the student indicates that the drawing is complete by tapping the "Interpret" button and ChemPad presents the user with a 3D scene showing the ethanol molecule with implicit hydrogens attached and the molecule oriented in the configuration approximated by the user's drawing.

Understanding that molecules are three-dimensional is a first step towards solving the difficult problem of naming chiral molecules. The ChemPad team focused on making ChemPad not only a general molecule visualizer, but added pedagogical interactions to take students through the steps of naming chiral molecules. A dialog giving the user a chance to reevaluate a naming is shown in Figure 2. Similarly, ChemPad contains visualizations for the naming of cis and trans (Z/E) stereoisomers and visual error reporting for three-dimensional notation mistakes. These visualizations are all aimed at giving students a kind of feedback on their intuitions that would not be available with other studying tools.

3 Use in the Classroom

Professor Zimmt demonstrated ChemPad to his class during the lectures on stereochemistry. Using the lecture hall projector system, Professor Zimmt was able to project several example molecules being manipulated in 3D at a size much larger than a modelling kit would have allowed. Although there are many existing molecule viewers for computers, ChemPad allowed Professor Zimmt to *quickly* adjust the molecules' 2D and 3D representations to respond to, "what if" questions from students.

After the initial lectures on stereochemistry, the ChemPad Lab was opened to students who wanted to use ChemPad to work on their three-dimensional intuitions. Lab sections were held twice a week for two and a half hours per session over the course of the four weeks immediately preceding the midterm exam. The lab was

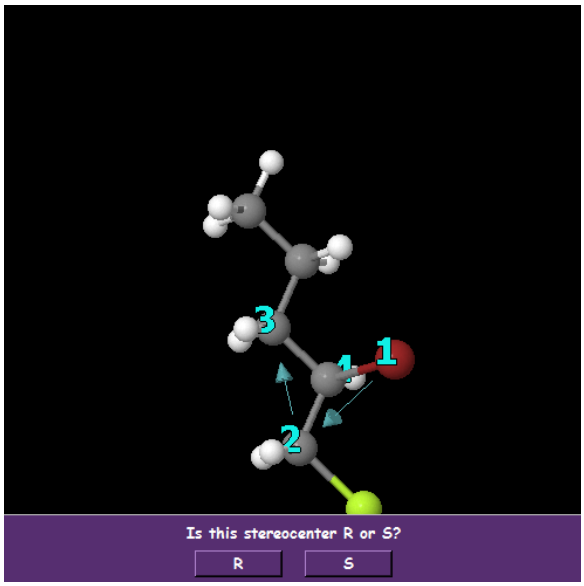

Figure 2 Visualizing stereochemistry rules in ChemPad

equipped with twenty Tablet PC computers graciously donated by Hewlett-Packard. Professor Zimmt prepared a series of three worksheets on stereochemistry for the students to work on in the lab and also made them available on the course website for students not attending the lab. Each lab section was staffed by two to three undergraduates in chemistry who helped answer chemistry questions and one to two members of the software development team who developed ChemPad to help with technical difficulties as they arose.

Over the course of the four weeks, a hundred students came to the lab sections to use ChemPad and a quarter of them returned at least a second time to get more practice. Students typically spent an hour to an hour and a half working on each worksheet. The tablet interface proved to be mostly intuitive and only required about five minutes to master for most students. Lab sections quickly became a mess of tablets, course notes, and textbooks as students pulled out their various resources and began forming mental connections between them. Many of the lab sections had a collaborative atmosphere with students discussing their intuitions and problems with both the chemistry staff and their neighbors.

Students' responses in anonymous surveys were very positive as shown in Figure 3. Whether using ChemPad to overcome the visualization hurdle or as additional reinforcement, students spoke positively of the experience. A number of students did voice complaints about the robustness of the handwriting recognizer, but only four students had consistent difficulty with the software being unable to recognize their handwriting. Students also expressed interest in ChemPad being available as a tool they could use in their daily studies; a worthy goal for future ChemPad development.

Professor Zimmt used early quiz scores to identify students struggling with three-dimensional visualization and emailed them invitations encouraging them to attend the ChemPad lab sections. Analysis was performed on exam scores of students who initially did poorly with stereochemistry to determine the effects of attending the ChemPad lab sections on their exam scores. Of students who received less than half credit on the stereochemistry quiz, those who attended the ChemPad Lab section did better on three-dimensional thinking questions on the midterm exam three weeks later. The

- "There's nothing that I dislike about ChemPad. I'm glad Brown is putting some extra effort into such programs like this. Thanks."
- "I think its very easy to use and easy to learn. It's very self-evident to me what commands do what."
- "I like being able to flip the molecules to see it in the right orientation."
- "Having a 3-D representation of the molecule for learning purposes is extremely helpful...much better than on paper."
- "I like that it shows the C.I.P. numbering so that you can see if it is clockwise or counter-clockwise very easily."
- "It helped me understand rotation better. It also helped me visualize which atoms were stereocenters."
- "I learned how the molecules looked realistically, rather than just on paper."
- "It makes a world of difference for me because I have a hard time visualizing 3D structures."
- " (I like that) I can see my mistakes."

Figure 3 Highlights of student feedback regarding ChemPad

score averages are shown in Figure 4. This is particularly pleasing to the research team since the questions on the exam were *not* similar to the exercises provided on the lab section worksheets and required a more complex set of three-dimensional intuitions.

4 Future Work

Over the past twelve months, ChemPad has already been developed into a tool that is useful for organic chemistry students at Brown. Mention of ChemPad in publications and demonstrations at conferences has already lead to emails of interested chemistry instructors from high schools, colleges, and universities. Based on this success and interest, the research team hopes to continue developing ChemPad into a tool useful to more areas of Chemistry education and plans to freely release the software later this summer. Immediate plans for ChemPad involve integrating the mathematical sketching and simulation research done here at Brown and adding a more sophisticated chemistry engine so that ChemPad can handle more complicated molecules, reactions, and simulations.

The author of this report, a graduate student in Computer Science, satisfied the Computer Science Department's research requirements for advancing to Ph.D candidacy by designing and implementing the chemistry recognition system in ChemPad. With the complexity and pedagogical value of electron orbital and molecular dynamics visualizations, the author hopes to find a dissertation topic through continued work on ChemPad.

5 The Team

ChemPad was developed through the collaboration of Professor Zimmt, graduate student Dana Tenneson, and members of Professor Andries van Dam's Graphics Group Sascha Becker, Loring Holden, and Robert Zeleznik. The ChemPad Lab sections were also staffed by undergraduate students Courtney Nelson, Katherine Husk, Addie Peretz, Jennifer Paul, Kimberly Martinod, and Christoper Maloney.

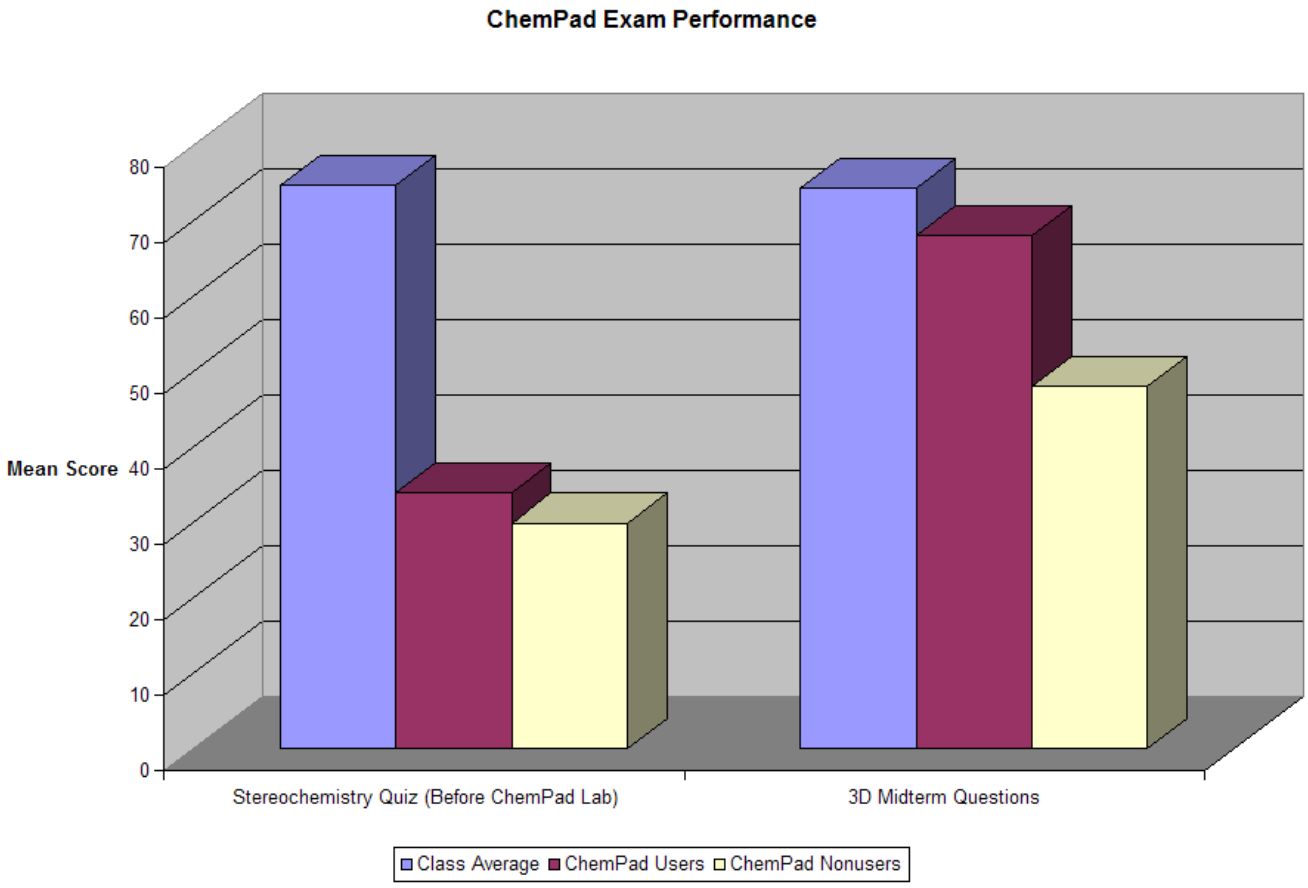

Figure 4 Exam score comparison of ChemPad users and nonusers amongst students who scored less than half credit on the stereochemistry quiz.