ChemPad: Generating 3D Molecules From 2D Sketches

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1 Introduction

Molecules are inherently three-dimensional (3D) objects that are represented by chemists on paper and classroom blackboards by a system of two-dimensional (2D) notations. ChemPad, a new Tablet PC application with a pedagogical focus, generates 3D molecular structures from hand drawn digital ink rather than from traditional molecule construction interfaces. Leveraging the gestural power of Fluid Inking [Zeleznik et al.], ChemPad allows chemists to input molecules in a quick and natural fashion to generate models viewable by the open-source JMol[1] molecule viewer. This capability gives ChemPad pedagogical value as shown by our user study of a hundred organic chemistry students who had difficulty with 3D chemistry thinking and used ChemPad to overcome that hurdle.

2 Model Generation From Handwriting

Using ChemPad consists of drawing a molecule in a Sketch panel and observing the three-dimensional structure in a View panel. Instead of selecting atoms and bonds from toolbars and menus the way one does in professional 3D molecule modelling software or ACD Lab's ChemSketch, ChemPad users 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 paper when talking to another chemist about the molecule. These drawings consist of symbols representing atoms, bonds, and pedagogical functions that have been designed in a Fluid Inking [Zeleznik et al.] grammar. When the user chooses to interpret the drawing, an appropriate 3D representation of the molecule is generated and displayed. The 3D molecule generation is accomplished by using the technique of reducing the problem to one of calculating torsonial angles, as noted in [P. Finn 1996], and then satisfying the constraints of the user's drawing with rules inspired by human motion tracking solutions.

3 A Pedagogical Focus

A major hurdle for aspiring chemists in college Organic Chemistry courses is to be able to visualize the actual 3D structure from the dimensionally-deficient 2D drawings. These students usually have no background in three-dimensional visualization and many otherwise bright students have great difficulty converting between the two-dimensional drawings used in "flatland" to represent molecules and their three-dimensional structures. ChemPad's initial pedagogical intent is to scaffold students who have difficulty with this mapping between 2D drawings and 3D molecules. By using the visualization assistance ChemPad offers to solve a 3D thinking task, students develop the skills to reach correct answers without assistance. In many ways, ChemPad acts 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.

ChemPad was used by 100 students in Brown University's Organic Chemistry course this spring. Professor Matthew Zimmt used the program in lecture, and lab sections were held twice a week over four weeks for students to use the software to work through example problems in their own time. Feedback from students and Zimmt was generally positive and has exposed to the research team how difficult it is for some students to visualize three-dimensional structures. Students who were identified as having difficulties with 3D visualization were contacted and encouraged to attend the ChemPad labs. Of these target students, those that used ChemPad generally performed better on exam problems requiring three-dimensional visualization skills than target students who did not use ChemPad. It was particularly encouraging that these exam questions were beyond the scope of the basic stereochemistry exercises focused on in the ChemPad lab sections and that users of ChemPad had thus developed further intuitions into 3D thinking.

4 Conclusion

ChemPad is an interpreter of chemical sketching that has already demonstrated itself to be effective at the pedagogical task of helping students develop three-dimensional mental models of molecules. Continued development of ChemPad will integrate additional visualization tools to address pedagogical goals such as confirmation and reactivity. Beyond pedagogy, ChemPad will be expanded to be a more general chemistry sketching interface as inspired by [LaViola and Zeleznik 2004]. Indeed, integration of ChemPad with [LaViola and Zeleznik 2004] would create an even more general tool which could be not only an integral part of the entire first year of chemistry studies but become be a regularly used test bed for professional chemists to sketch out their ideas and intuitions.

References

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[1] http://jmol.sourceforge.net/