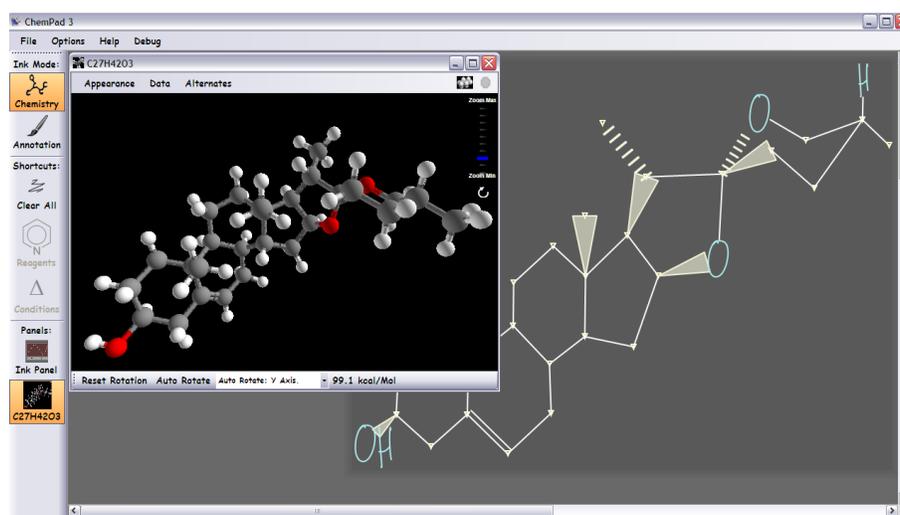


ChemPad3

a tutorial

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1 Welcome to ChemPad!

ChemPad is a Tablet PC application for students learning introductory organic chemistry. ChemPad allows students to draw in molecule diagrams (line diagrams) like those found in their textbooks and tests and ChemPad automatically generates the 3D molecule models corresponding to the diagram. These models can be used to explore concepts of molecule shape, molecule energy in different conformations, and stereochemistry.

1.1 Tablet PCs

ChemPad runs best on a Tablet PC, which is a special kind of laptop computer. The Tablet PC comes with a special pen, called a stylus, which you can use just like a mouse or trackball by pointing directly at the screen where you want the cursor to go. You can also write or draw with the stylus. If you are

uncomfortable with the stylus, you can use the Tablet PC tutorial, which can be found in the Start menu.

ChemPad has been designed to be used exclusively with a stylus. The interface is a little bit different than you are probably used to from standard programs like Microsoft Word and Adobe Photoshop. You give the program most instructions by drawing on the screen, rather than by selecting from menus or typing at the keyboard.

1.2 System Requirements

ChemPad is designed for Tablet PC computers running either Windows XP Tablet Edition, or Windows Vista Business Edition. Additionally, ChemPad can work on computers with Windows XP Professional, Windows XP Media Center Edition, and non-basic versions of Windows Vista. To install ChemPad on an XP Pro or MCE computer, you will first need to install the Microsoft Ink SDK <http://www.microsoft.com/downloads/details.aspx?familyid=b46d4b83-a821-40bc-aa85-c9ee3d6e9699&displaylang=en> and the Microsoft 2005 Recognizer Pack <http://www.microsoft.com/downloads/details.aspx?familyid=080184DD-5E92-4464-B907-10762E9F918B&displaylang=en>

While we highly recommend using ChemPad on a TabletPC, users have reported successfully using ChemPad on desktop computers with low-cost external digitizer tablets such as the Wacom Graphire and the IOGEAR Digital Scribe.

1.3 A Research Project

While we have strived to make ChemPad into a useful tool for organic chemistry students, ChemPad is first and foremost a research project by two graduate students. Given our limited resources to devote to developing ChemPad, we know that it is incomplete, has some bugs, and doesn't always produce the correct answer. Nonetheless, we hope that you find what it does accomplish is useful and welcome bug reports and feature requests sent to chempad@cs.brown.edu.

2 General Concepts

2.1 The ChemPad Application

When opened, the ChemPad application presents the user with a large ink panel where the user can draw molecule diagrams and annotations. As the user creates molecule models, 3D windows will also appear in the ink panel. On the left, there is a strip of buttons for controlling which of these windows is in front, which type of drawing the user is making (chemistry notation, or uninterpreted annotation), and an erase shortcut. Menus at the top of the application allow

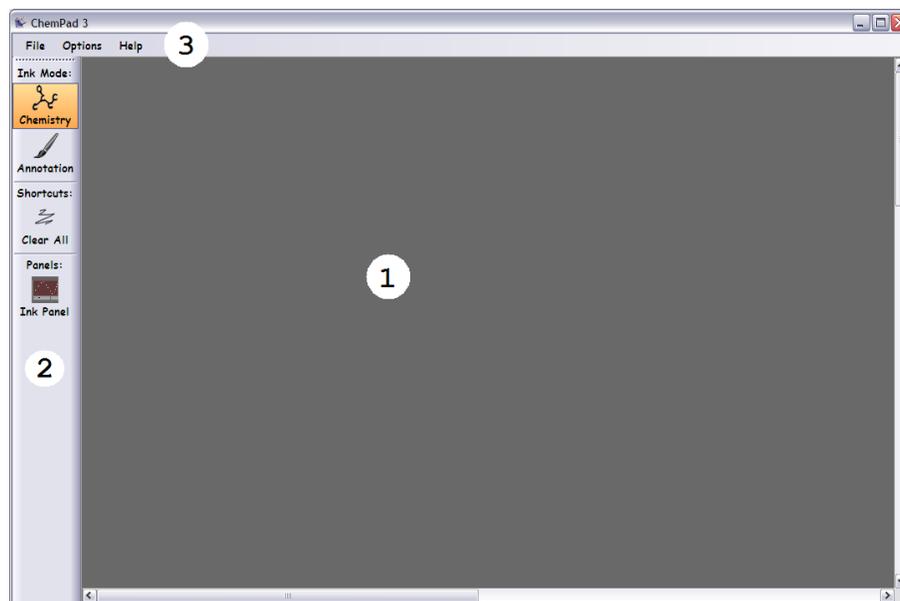


Figure 1: *ChemPad version 3. 1. The main ink panel where molecule diagrams and annotations can be drawn. 2. Control buttons. Here you can switch between the “Chemistry” and “Annotation” modes, select 3D windows or the ink panel to be brought forward, and activate a shortcut which erases all ink in the ink panel. 3. Menus which allow files to be saved and loaded, ChemPad options to be changed, and documentation on ChemPad and its technologies to be viewed.*

the user to change options, save and load files, take image snapshots of their work, and get help and other documentation.

2.2 A Molecule Diagram Example: Butane

To help you get started, this example shows how to draw a diagram of butane in ChemPad and generate the 3D model. Begin by drawing the butane carbon backbone and circle it as shown in the first four pictures of Figure 2. After circling the diagram, it will be given a green highlight and a button will appear to create a 3D model. Clicking the button will bring up a 3D window which, after a moment of processing, will contain the butane model.

2.3 Working with 3D Graphics

3D graphics can help you understand the spatial structure of molecules. To really understand the structure, you should turn it around and look at it from all angles. In ChemPad, there are two ways to do this. The easiest way is to turn on Auto Rotate, using the button at the bottom of the 3D window. The

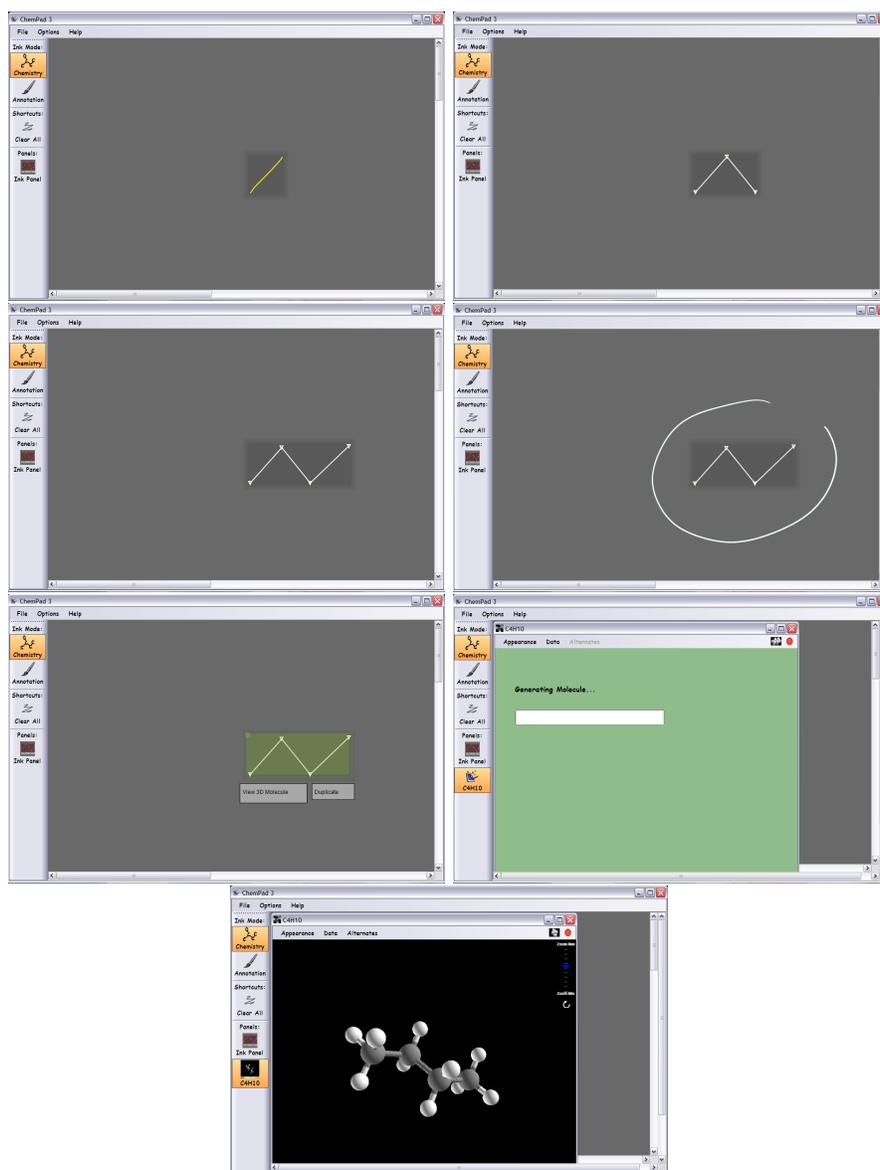


Figure 2: Drawing the butane carbon backbone. Draw three lines in a zig-zag fashion. As they are recognized, they will be prettified into straight lines. Circle the diagram to recognize it. Clicking the “View 3D Molecule” button brings up the 3D model.

molecule will rotate around as if it were on a pedestal. You can also roll the molecule around by dragging with the stylus over the 3D window. Give it a try and you'll see how easily you can look at a molecule from whatever point of view you choose.

2.3.1 Visualization Styles

The Appearance menu gives you three ways to visualize the molecules you draw. **Ball-and-Stick** is the most familiar style, representing the atoms as small spheres stuck together with thin cylinders. Two other drawing styles remind you that molecules aren't really made of small spheres with hard shells, though. **Space-filling**, shows the sphere of each atom extending to 100% of the van der Waals radius. Molecules drawn in this style look like pool balls glued together. The **Dots** rendering style combines both modes, showing the ball-and-stick model surrounded by a cloud of dots representing the van der Waals surface.

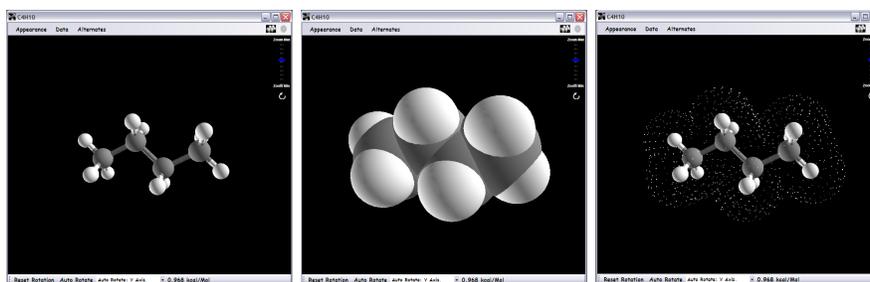


Figure 3: 3D visualization styles in ChemPad. The left is the **Ball-and-Stick** visualization. The middle is the **Space-filling** visualization. The right is the **Dots** visualization.

3 Drawing Molecule Diagrams

3.1 Drawing Atoms

Beyond carbon backbones, users can add different atoms to their molecule diagrams by drawing atomic symbols from the periodic table. ChemPad will only recognize the atomic symbols it understands, which are the most common elements encountered in organic chemistry. Those elements are: Hydrogen (**H**), Carbon (**C**), Oxygen (**O**), Nitrogen (**N**), Fluorine (**F**), Chlorine (**Cl**), Bromine (**Br**), Iodine (**I**), Phosphorus (**P**), Sulfur (**S**), and Boron (**B**)¹. These letters can be drawn in upper or lower case as well as print or script. You can also

¹Boron is not fully implemented in ChemPad as of this writing and ChemPad can only handle a small number of Boron-containing molecules.

change an element in a diagram by circling a non-carbon backbone atom. The menu in Figure 6 will be brought up which allows a different element to be selected.

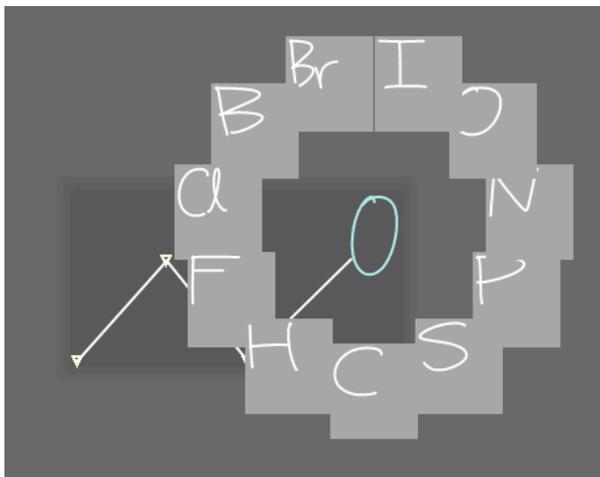


Figure 4: Radial menu for selecting atom element.

If ChemPad recognizes the atomic symbol you drew, it will re-draw it in its own handwriting. If ChemPad doesn't recognize the symbol, it will stay in your handwriting. Scribble it out (scratch over the symbol with the stylus several times) and try again. With a bit of practice you'll learn how to draw atomic symbols that ChemPad can recognize.

3.2 Drawing Bonds

To draw bonds in the plane of the screen, as opposed to wedge and dash bonds, described below, just draw a straight line connecting two atoms. The software will recognize this as a bond, and redraw it with a perfectly straight line. If it is not recognized as a bond, erase it by drawing a squiggle over it, then try again.

Of course, ChemPad supports double, and triple bonds as well. Draw them just like you would on paper: two parallel lines for a double bond, and three parallel lines for a triple bond.

ChemPad also supports wedge and dash bonds, which are used to indicate stereochemistry. A wedge bond can be drawn as either the wedge triangle (not filled in) or just the "V" of the wedge in a single stroke. A dashed bond is made

by drawing three of the bond dashes. Once the third dash is drawn, ChemPad should recognize the dashed bond and fill in full bond.

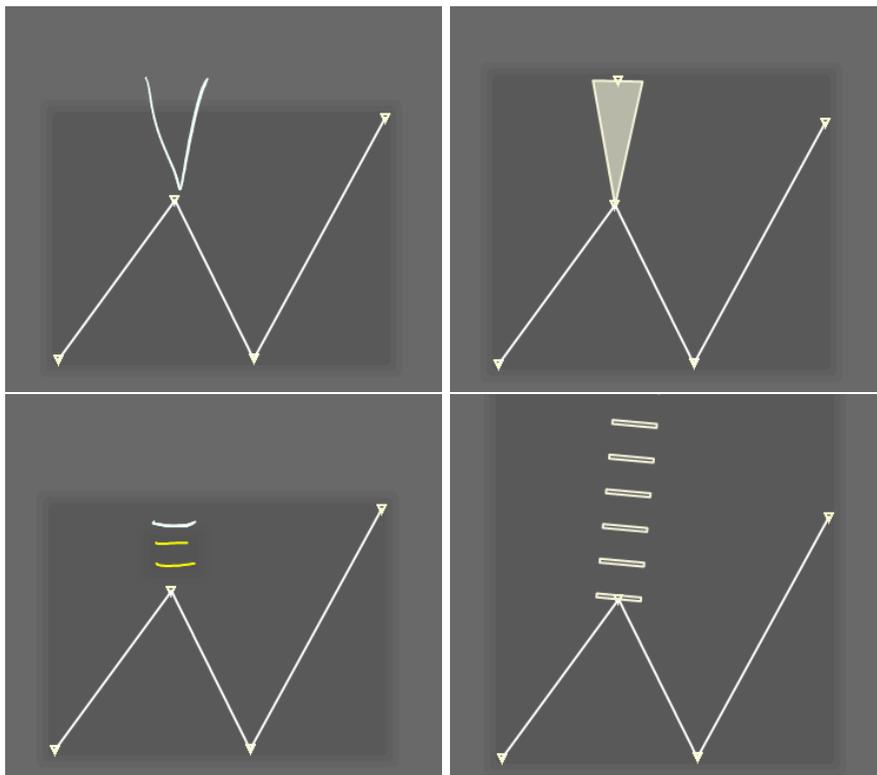


Figure 5: *Drawing wedge and dash bonds. A wedge bond can be drawn with the “V” of the wedge. A dash bond can be drawn as three dashes of the bond.*

4 Interpreting your Drawing

When you hit the “View 3D Molecule” button, ChemPad tries to make sense of the molecule you drew. If you drew a valid molecule, ChemPad can usually understand it, and give you a three-dimensional model that matches the molecule you drew. Sometimes the molecule you draw doesn’t make sense or ChemPad doesn’t know enough about the molecule to be able to make a matching 3D model. If ChemPad can’t create a 3D model for a diagram, try drawing the diagram again (to make sure there aren’t any problems with the diagram) and give ChemPad as second chance.

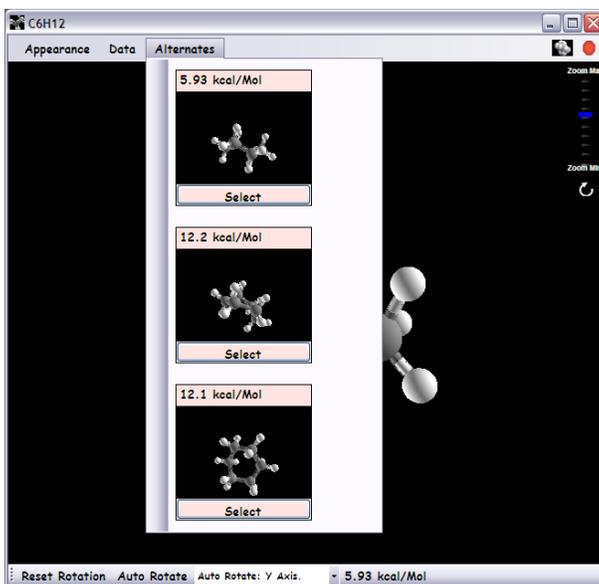


Figure 6: Some diagrams have multiple interpretations. These interpretations can be accessed from the “Alternates” menu.

Often, ChemPad will be able to find multiple 3D models which match a given diagram. After creating the 3D model initially presented, ChemPad continues to try to find other 3D models which match the diagram. You can tell ChemPad is still working on this by the spinning molecule icon in the upper right corner of the 3D window. When an alternate model is found, it will appear in the “Alternates” menu. Clicking “Select” on an alternate will move it to the 3D window.

5 Learning Stereochemistry with ChemPad

5.1 What is stereochemistry?

If you don't already know what stereochemistry is, the rest of this section won't make any sense to you. If you've heard of stereochemistry, read about it, sat in class and listened to lectures on it, but it still hasn't quite clicked, ChemPad is your new friend. You will learn to visualize and distinguish between R and S stereocenters with ChemPad.

5.2 The Stereochemistry Self-Quiz: Absolute Configuration

ChemPad is designed to help you quiz yourself on stereochemistry. You draw a molecule which has a stereocenter, then try to determine its absolute configuration (shape) just by looking at the drawing – because in the real world, your exams and your notes will all have flat diagrams, not fancy 3D graphics. Then, to see ChemPad’s visualization, circle the stereocenter and click “Yes” to the prompt asking if you want to see the stereochemistry in 3D.

Now look at the 3D rendering. ChemPad has labeled each of the four ligands with their Cahn- Ingold-Prelog priority numbers. Rotate the molecule until the ligand numbered 4 is facing away from you; this is the orientation from which you can most easily determine the stereocenters absolute configuration.

ChemPad will ask you, Is this stereocenter R or S?

Reply by hitting the R or S button, and then the correct stereochemistry will be revealed.

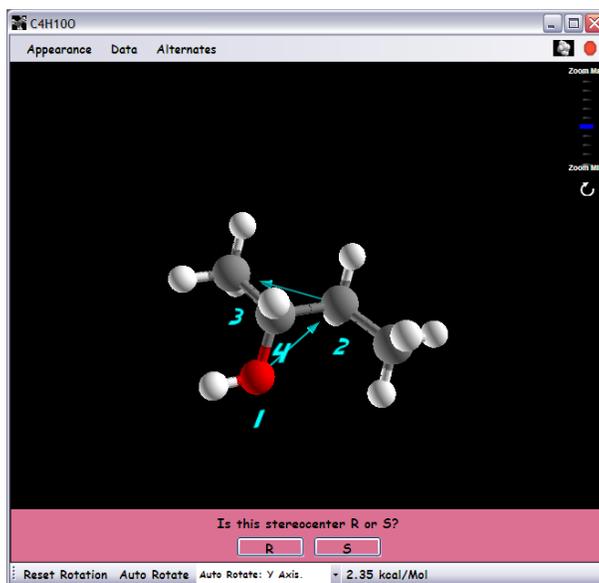


Figure 7: Using ChemPad to explore chirality.

6 More Information

To learn more about ChemPad, report bugs, or get an updated version, visit the ChemPad website <http://www.chempad.org> or send email to the ChemPad team (chempad@cs.brown.edu).

7 Thanks

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