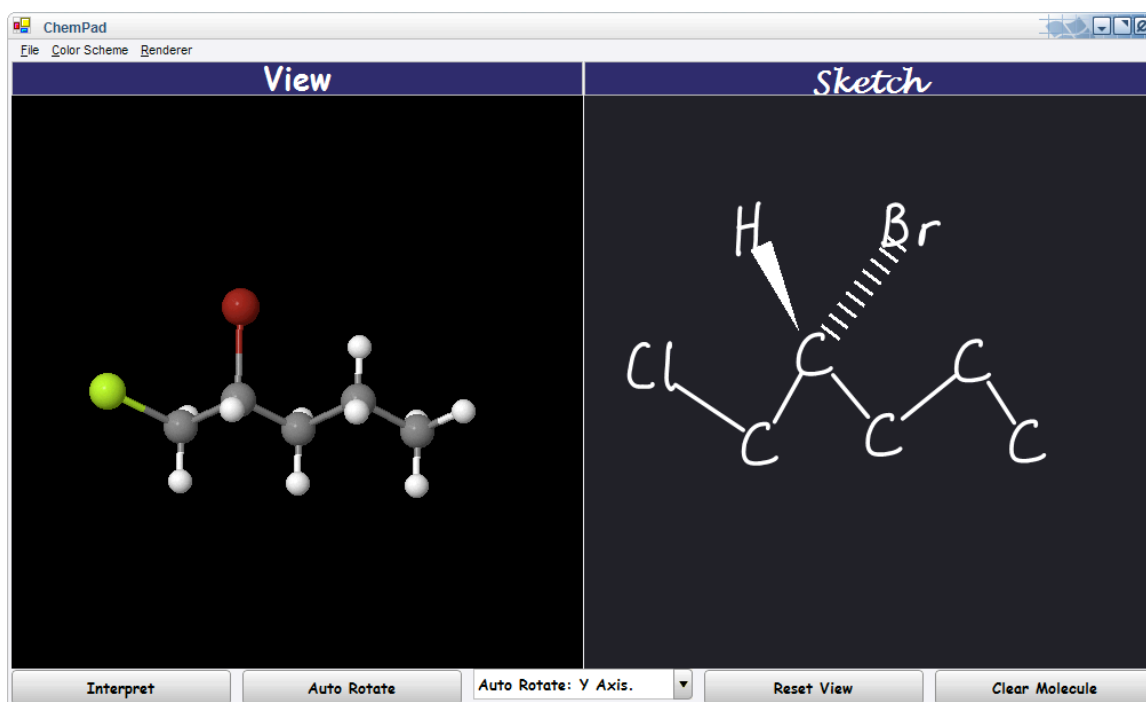

Using ChemPad

a tutorial

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Brown University • Providence, RI • March 7, 2005



General Concepts

The ChemPad Application

The ChemPad application is divided into two parts. On the left are the three-dimensional graphics, marked **View**. On the right is a drawing area, marked **Sketch**; draw chemical symbols here.

Using the Tablet PC and Stylus

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.

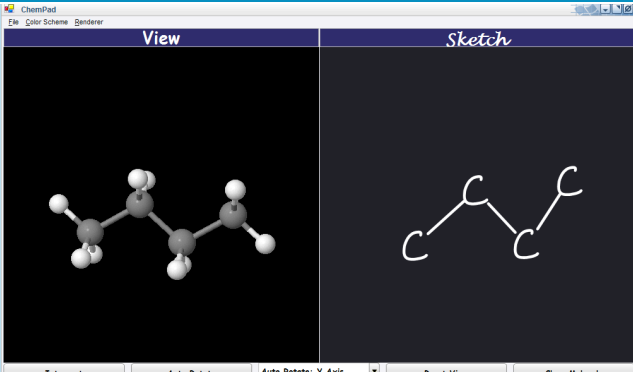
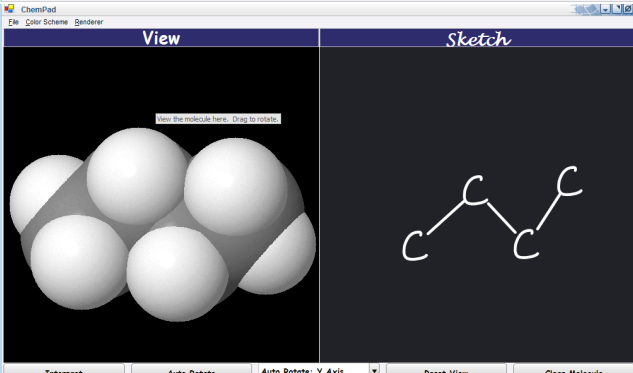
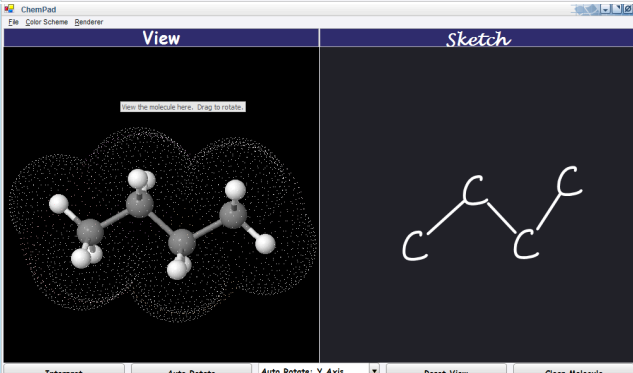
ChemPad has been designed to be used exclusively with a stylus. The interface is a little bit different than you are probably used to from standard programs like Microsoft Word and Adobe Photoshop. You give the program instructions by drawing on the screen, rather than by selecting from menus or typing at the keyboard. You may have to draw things a little bit differently than usual in order for ChemPad to understand them. In particular, draw each chemical symbol without lifting the stylus from the display.

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 screen. The 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 **View** panel. Give it a try and you'll see how easily you can look at a molecule from whatever point of view you choose.



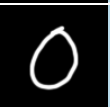





Visualization Styles

The View 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.

Visualization Style	Example
Ball-and-Stick	
Space-filling	
Dots	


Drawing Atoms

ChemPad will only recognize the atomic symbols it understands, which are the most common elements encountered in organic chemistry. Note that hydrogen and fluorine must be written as lower-case, even though the chemical symbol is upper-case. This is because it is hard to write a recognizable (by our system, at least) capital H or F without lifting up the stylus, which is required by the system.

Draw	Think	Element
	Lowercase h	Hydrogen
	Uppercase C	Carbon
	Uppercase O	Oxygen
	Uppercase N	Nitrogen
	Cursive "Cl", uppercase C, lowercase l	Chlorine
	Lowercase cursive f	Fluorine
	Uppercase cursive I	Iodine
	Cursive "Br" with uppercase B, lowercase r,	Bromine

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 (see below for an example scribble gesture) and try again. With a bit of practice you'll learn how to draw atomic symbols that ChemPad can recognize. If ChemPad gets the wrong element, for instance, oxygen when you meant carbon, just tap the stylus on the incorrect symbol. This will bring up a


menu with several atoms listed; pick the one you want, and it will replace the incorrect element with the one you want.

	Erase what I scribbled over
tap	Switch the atom you tapped to another element

See the last page of this tutorial for a guide to all of the letters and gestures which ChemPad understands.

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. To draw a bond between hydrogen and bromine, completing a hydrobromic acid molecule, just draw a straight line where you want the bond to go. ChemPad will recognize the straight line as a single bond, and redraw it as a straight line. In the 3D panel, ChemPad will show you the atoms connected by a bond in the 3D panel.

Starting with this...	Draw this...	Get this...	And this!
H Br	H—Br	H—Br	

Multiple Bonds

ChemPad supports double, and triple bonds. Draw them just like you would on paper: two parallel lines for a double bond, and three parallel lines for a triple bond. (See key at the end of this section for examples.)

Incomplete Bonds

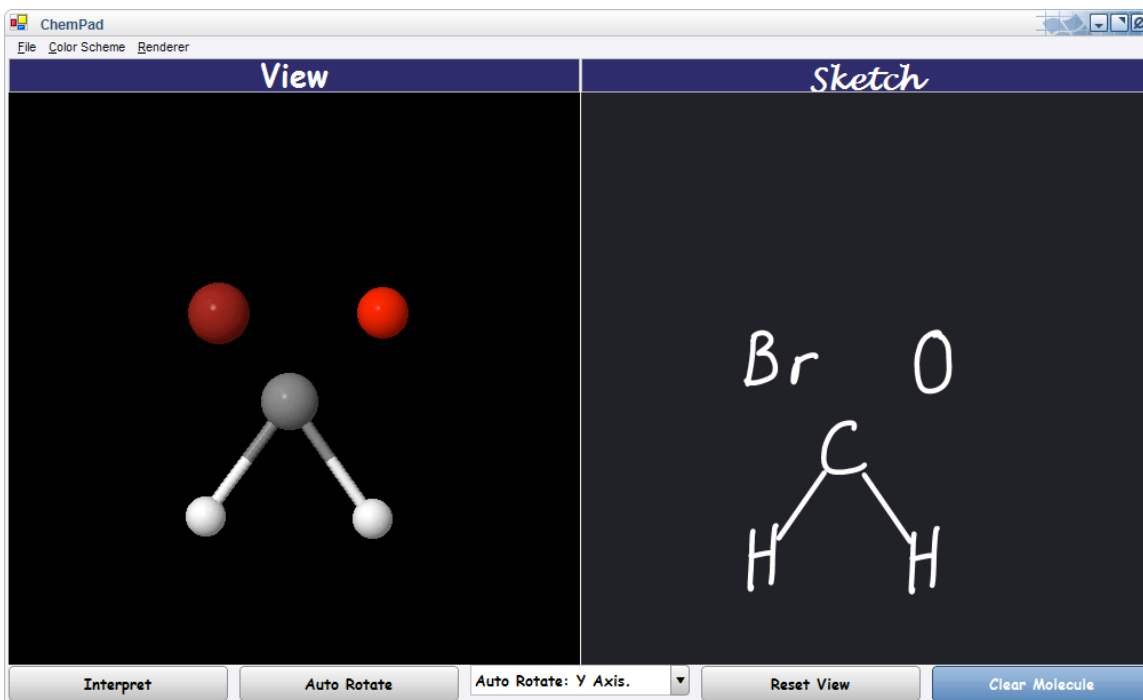
You can draw “atom, bond, atom, bond” rather than “atom atom atom, bond bond bond.” ChemPad will draw a bond which is only connected on one end as half-gray, half white. If you see a half-gray bond, it means that the gray end of the bond is not connected to an atom. Draw an atom at the grey end of the bond, and the bond will connect itself to the atom you just drew.

For example, the image on the left shows an incomplete triple bond. Draw a C (for carbon) at the empty end of the triple bond, and you’ll get a carbon-carbon triple bond, as shown in the image on the right. Notice that the triple bond is now all white, not half-gray.

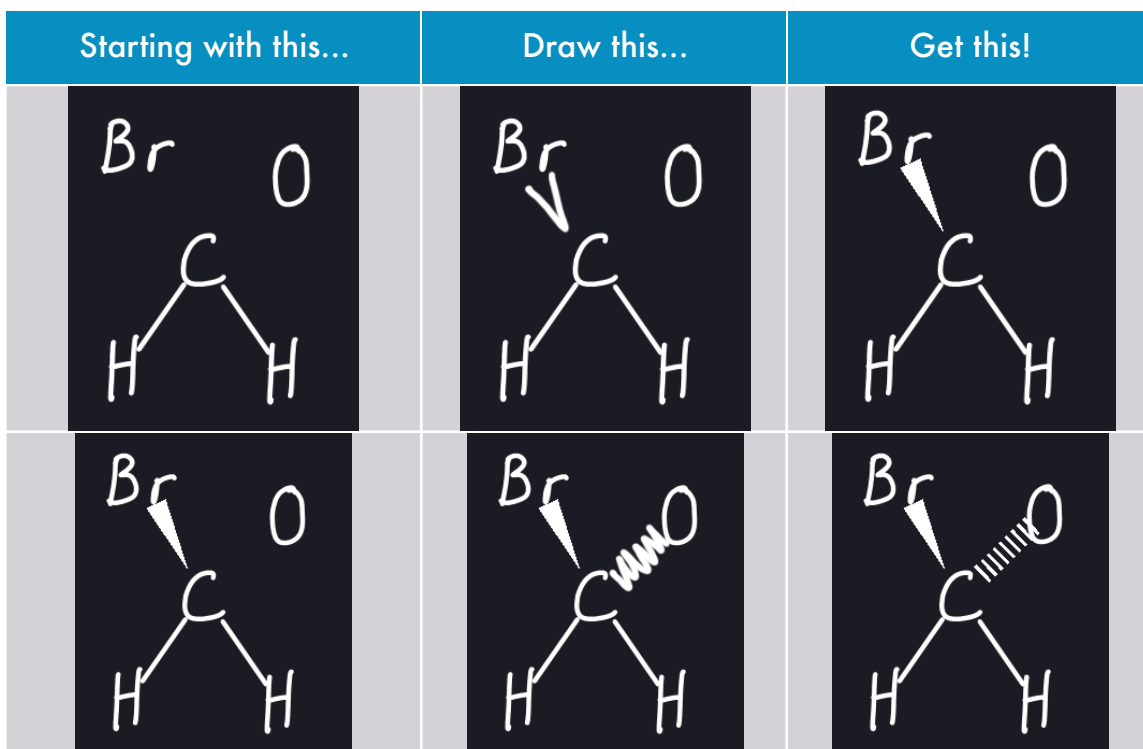


Wedges and Dashes

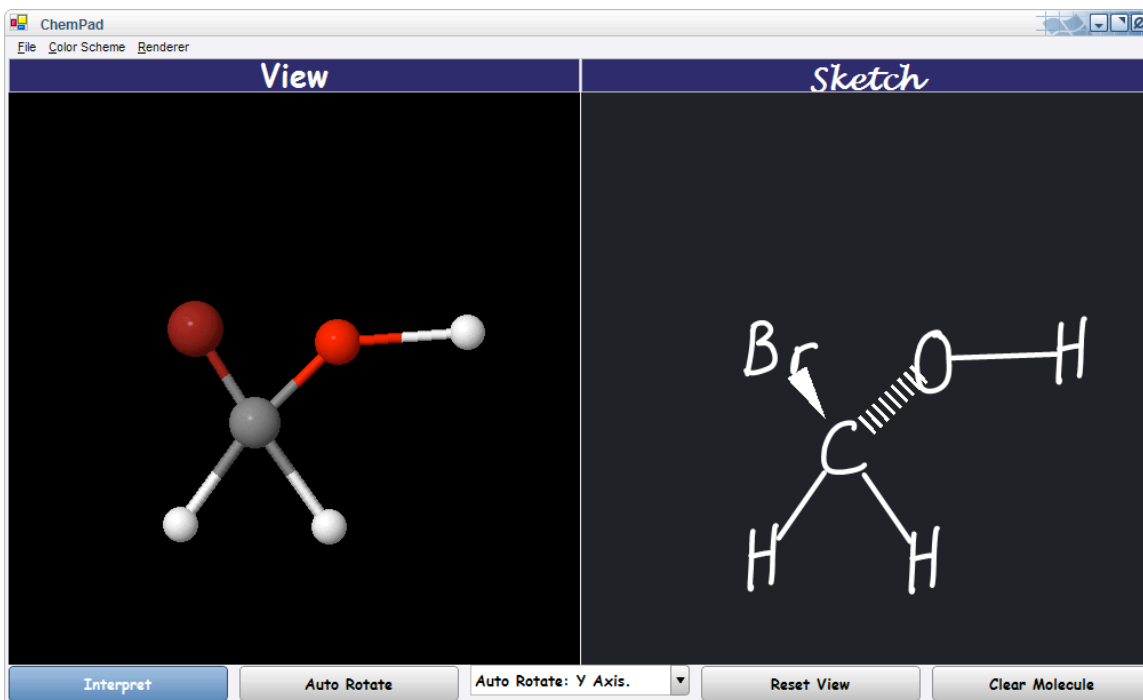
If you have drawn the molecule and atoms shown below, and you want to bond the bromine and oxygen atoms to the central carbon, you will need to indicate stereochemistry with wedge-dash notation.



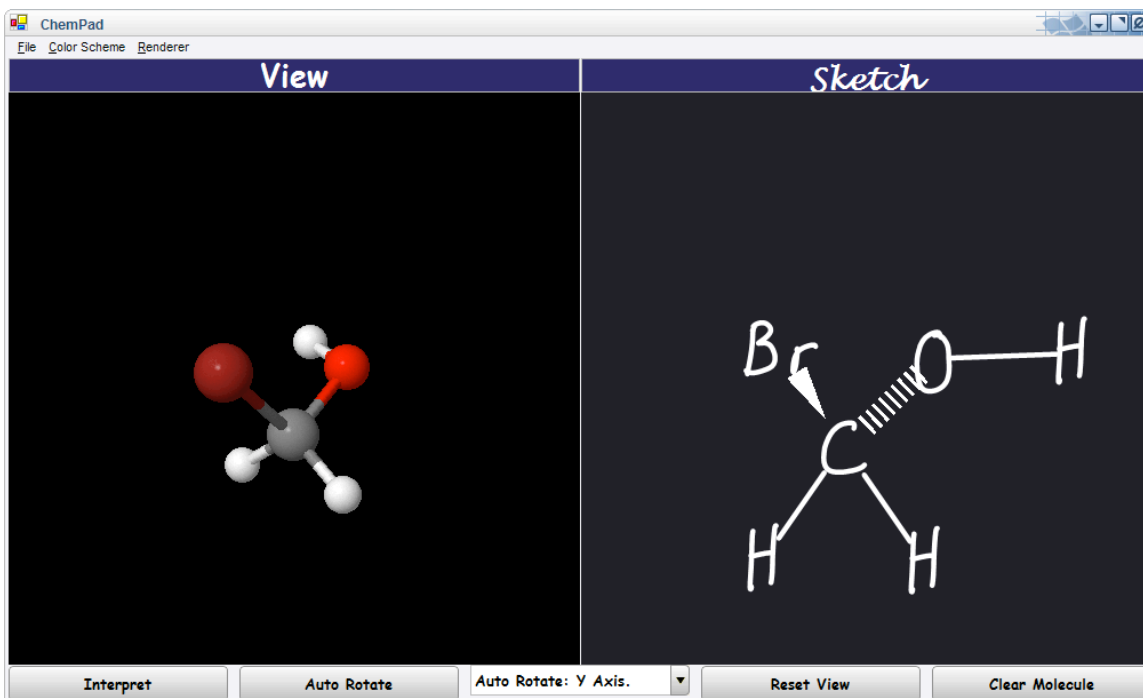
In ChemPad, you draw a gesture which means "put a wedge bond here" or "put a dashed bond here," rather than drawing the bonds themselves. The symbol for "put a wedge bond here" is a long skinny "v," as if you were drawing the two long sides of the triangle. The symbol for "put a dashed bond here" is a zig-zag. The zig-zag is different from the "scribble" gesture in that the zig-zag has sharper corners.



Add a hydrogen to the oxygen, to complete the hydroxyl group. Now the screen should look like this:



The molecule's representation in 3D looks odd; we expect tetrahedral geometry, but all the atoms seem to be in the same plane. To make ChemPad figure out the molecule's correct geometry, hit the **Interpret** button. This calculates the molecule's geometry. Now the 3D panel shows the molecule in 3D, with the stereochemistry you indicated. Note that the wedge bond makes the dark red bromine atom appear closer to you, coming out of the screen, and the dash bond makes the red oxygen atom appear farther away from you.

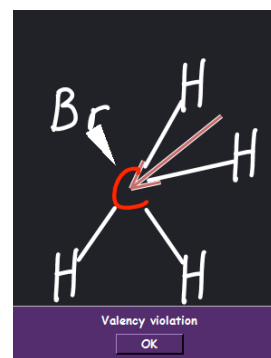


Interpreting your Drawing

When you hit the **Interpret** 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. ChemPad checks for errors when you hit **Interpret**, and alerts you of errors. Currently, there are three kinds of errors which ChemPad recognizes. These errors will only make sense to you if you know some chemistry; if you don't, just trust us that these are errors.

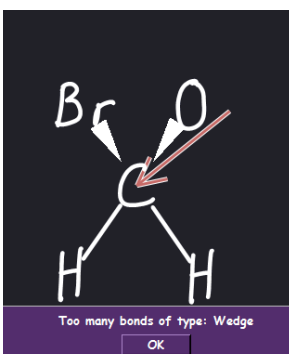
Valency Errors

In a neutral molecule, each element must participate in a particular number of bonds for its valency to be complete. Carbon requires four bonds, hydrogen one, oxygen two, and nitrogen three. The halogens (chlorine, fluorine, iodine, and bromine) all need one bond.



Impossible Structure Errors

Each bond between atoms of each element makes a bond of a particular shape. When drawing the molecule, you must indicate the proper shape for the bond using wedges, dashes, and in-plane bonds. If you drew, for instance, a carbon with four wedges coming out of it, ChemPad would tell you "Too many bonds of type wedge." In ChemPad, only one wedge bond is allowed, although sometimes it makes sense to draw two wedges from a single atom. If you see the error message, "Too many bonds of type..." use your knowledge of chemistry to figure out what's wrong and how to fix it.



Elements that form bonds to more than one additional atom encounter specific geometric restrictions. As an example, carbon bonded to four other atoms is tetrahedral: the four bonds to the other atoms are directed to the corners of a tetrahedron. ChemPad assumes that atoms you bond by simple lines lie in the plane of the screen. When you draw a molecule in which more than two atoms are attached to a C or N, you must specify which of the specified atoms is not in the plane of the screen. You do this using wedge or dash bonds. If you make a mis-

take, you will get a message such as “Too many bonds of type...” Use your knowledge of chemistry to figure out what’s wrong and how to fix it.

Incompletely Specified Structure Errors

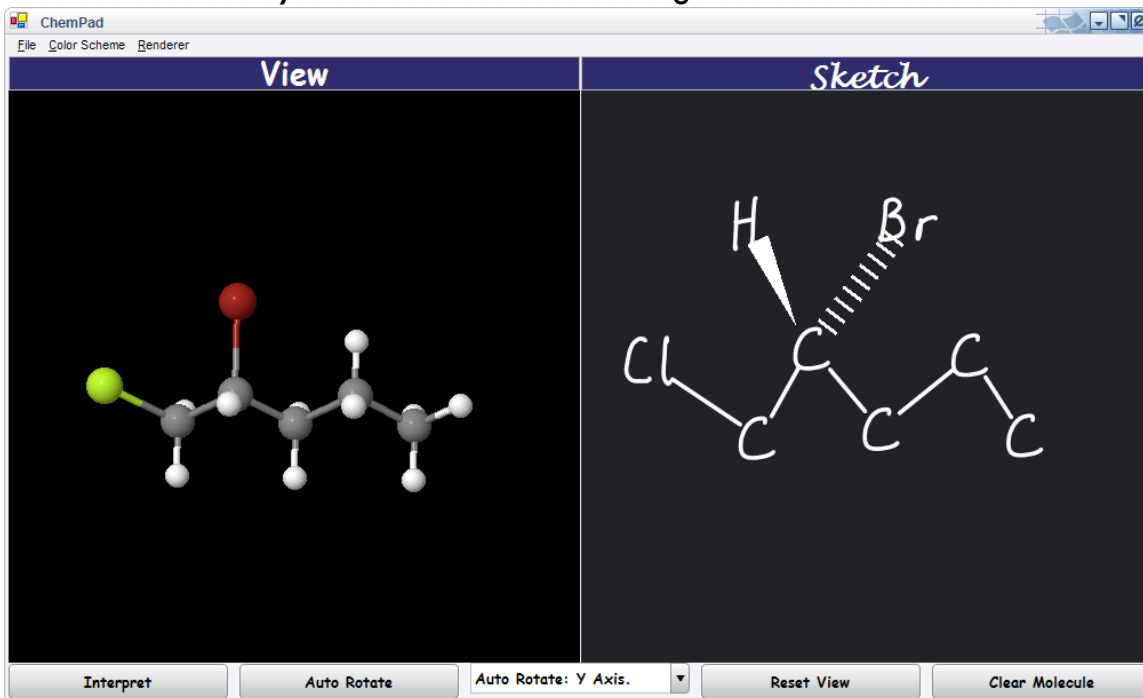
These are a special kind of impossible structure errors; you put too many bonds in the plane, when really one or more of those bonds has to be out of the plane, either into or out of the screen. This is flagged as “Incompletely Specified Structure.” If you get this error, think about the physical structure of the molecule. Have you drawn some bonds with just a normal straight line which should be drawn as a wedge or a dash?

Learning Stereochemistry with ChemPad

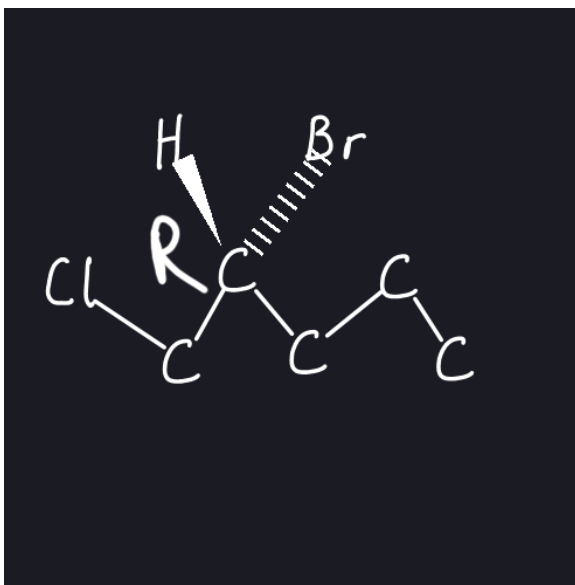
What is stereochemistry?

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.

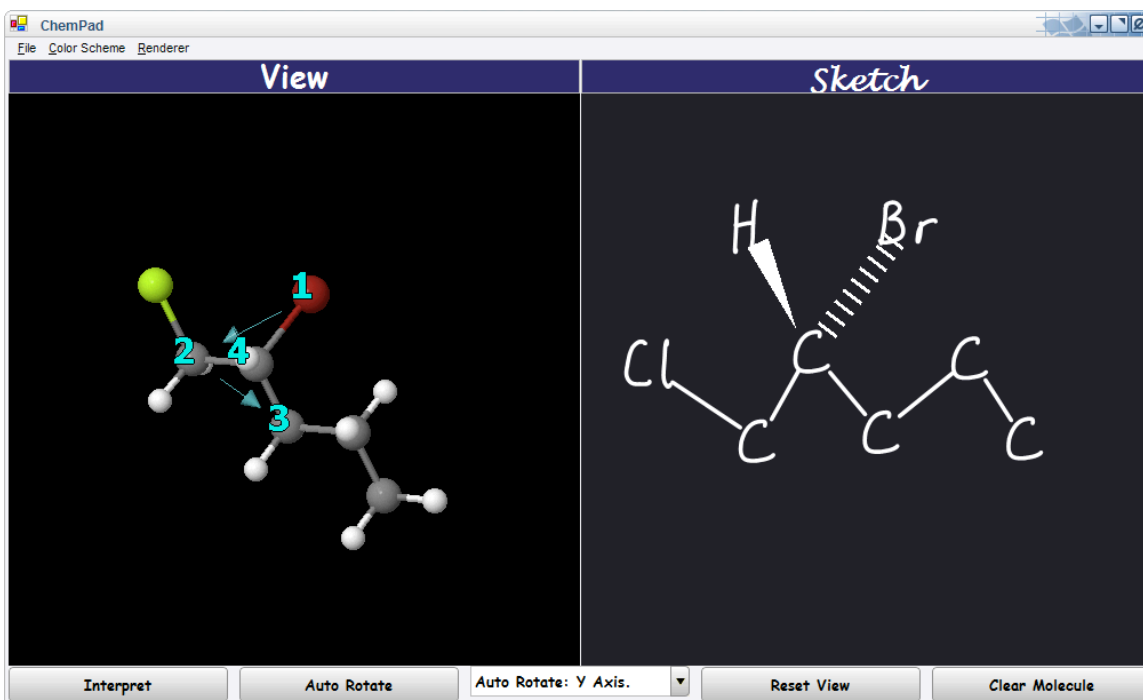
The Stereochemistry Self-Quiz: Absolute Configuration



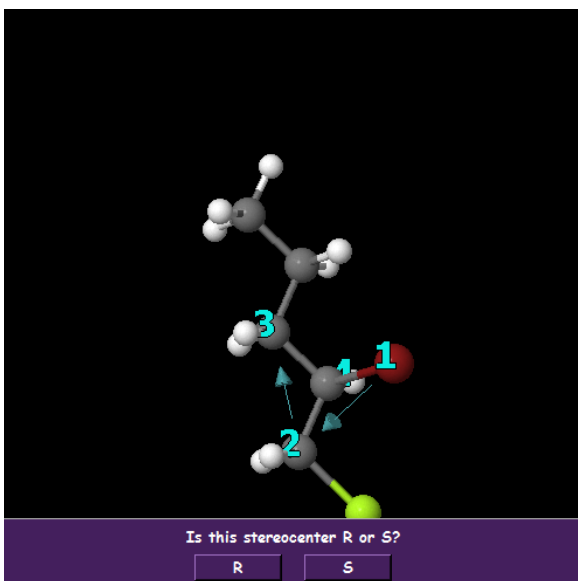
ChemPad is designed to help you quiz yourself on stereochemistry. You draw a molecule which has a stereocenter, then try to determine its absolute configuration (shape) just by looking at the drawing – because in the real world, your exams and your notes will all have flat diagrams, not fancy 3D graphics. Label the chiral center by drawing R or S near the C representing the chiral center, in the **Sketch** panel.



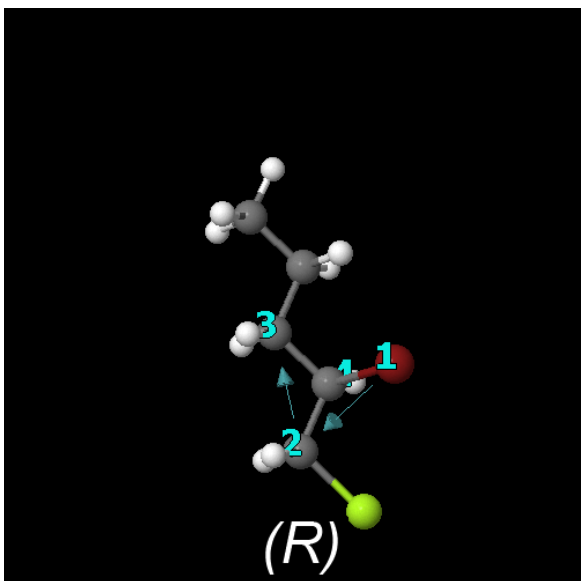
Now look at the 3D rendering. ChemPad has labeled each of the four ligands with their Cahn-Ingold-Prelog priority numbers. Rotate the molecule until the ligand numbered 4 is facing away from you; this is the orientation from which you can most easily determine the stereocenter's absolute configuration.



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.



Stereochemistry of Alkenes

ChemPad also lets you quiz yourself on the stereochemistry of alkenes. This works much the same way as the stereochemistry described above. To see how this works, draw a carbon-carbon double bond, with one bromine attached to each carbon. Is the molecule you drew the *Z* (zusammen) or *E* (entgegen) geometric isomer? Draw a *Z* or lower case e next to it, and the answer will be revealed in the **View** panel.

Gestural Commands

	Lowercase h	Hydrogen
	Uppercase C	Carbon
	Uppercase O	Oxygen
	Uppercase N	Nitrogen
	Cursive "Cl", uppercase C, lowercase l	Chlorine
	Lowercase cursive f	Fluorine
	Uppercase cursive I	Iodine
	Cursive "Br" with uppercase B, lowercase r	Bromine
	Scribble what you want to erase	Erase
	One straight line segment	Single bond
	Two straight line segments	Double bond
	Three straight line segments	Triple bond
	Zig-zag	Dashed bond
	Wedge	Wedge bond
	Tag the nearest carbon as an R stereocenter	
	Tag the nearest carbon as an S stereocenter	
	Tag the nearest carbon as a Z (cis) stereocenter	
	Tag the nearest carbon as an E (trans) stereocenter	
tap	Switch the atom you tapped to another element	

More Information

To learn more about ChemPad, report bugs, or get an updated version, contact Sascha Becker (sab@cs.brown.edu) or Loring Holden (lsh@cs.brown.edu).

ChemPad is sponsored in part by a grant from Atlantic Philanthropies to encourage academic innovation.