

# Molecular Visualization with JMOL

## What is Jmol?

Jmol is an applet for web browsers that can utilize java, that allows for the visualization of molecular structures on web pages. It is designed to work in Windows, Mac, and Linux environments.

## Working with Jmol on a PC

**Rotating a molecule:** Molecules can be rotated by left clicking and dragging the mouse over the structure.

**Changing the size of a molecule:** Molecules can be resized by holding down the shift key while left clicking and dragging the mouse. To shrink, drag to the upper right; to enlarge drag to the bottom left.

**Translating a molecule:** Molecules can be translated vertically and/or horizontally by holding down the control key while left clicking and dragging the mouse.

**Altering the display type:** To change the display type, click on the word "Jmol" in the molecule window, a pop-up menu will appear. Move down to the word Render and a new menu will appear to the side. Now move the mouse to Scheme and then Ball and Stick. Alternatively after Render, go to Structures then Off. Release and then select a new Structure such as Backbone.

**Other Menu Selections:** The pop-up menu affords you some additional features. Spin will start/stop spinning of the molecule. The options selection provides the ability to remove hydrogens, disulfide bonds, etc. The color selection allows one to change the colors of the atoms. It is best just to play with these features and see what happens.

Standard CPK colors:

Carbon	Gray	Phosphorus	Gold
Nitrogen	Blue	Sulfur	Yellow
Oxygen	Red	Zinc	Steel-blue

## The Jmol Console

The Jmol console window is opened by clicking Jmol, followed by Console and then Open. This enables you to have very detailed control and interaction with your image. We will only be using the console to get reports of measurements we make. Those of you who are interested in becoming an expert with Jmol are encouraged to learn the command line language. It is actually quite intuitive and can be learned in a matter of hours.

## Jmol Commands

Many of the buttons in Jmol windows make the distinction between selecting and restricting:

**Select XXX** leaves all current items in view and selects all atoms that are part of XXX for the next operation. For example, on a protein you can click backbone select, and then change the display of the backbone while leaving all non-backbone (side chain) atoms unchanged. If atoms were not visible before the select button was clicked, they may not become visible until a display mode is selected.

**Restrict XXX** causes all atoms to be hidden from view except those chosen. Make a selection from the display menu to determine how the atoms are to be seen. If atoms were not visible before the restrict button was clicked, they may not become visible until a display mode is selected.