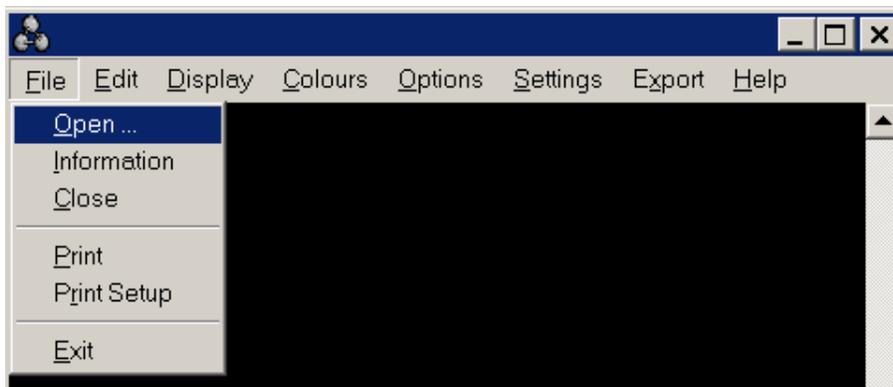


## Quick Guide to RasMol

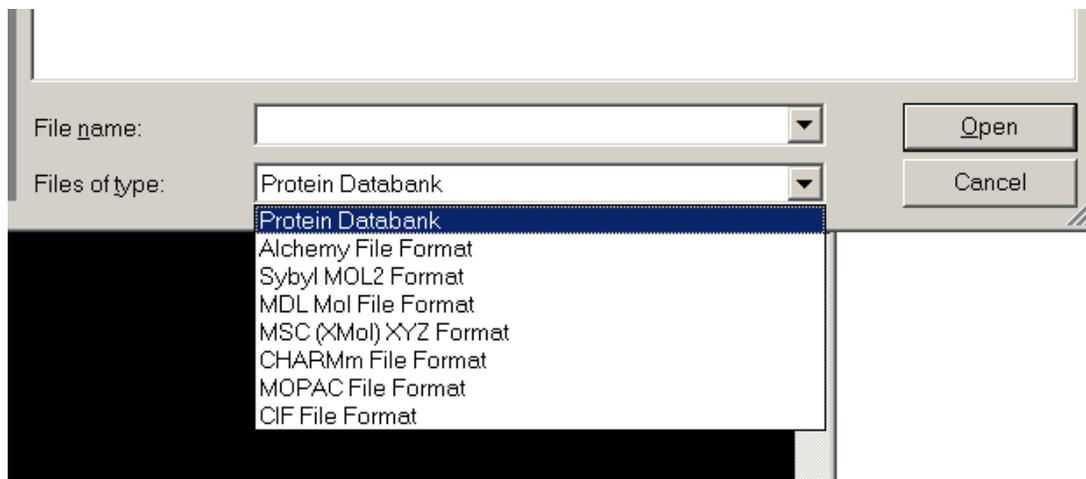


RasMol is molecular structure rendering freeware (To download: <http://www.bernstein-plus-sons.com/software/rasmol>). No installation is required since RasMol will run on a 3.5 inch disk (472 kB). Click on the icon as shown to the left to launch RasMol. The screen below should open up. Click on "File" and select "Open..." Browse to find the location of your structures files.



RasMol defaults to the Protein Databank files (pdb) as the "files of type:" (the most common file).

To view other file formats (mol, xyz) you must select the appropriate type from the list shown on the screen below. Once you select a file, the structure will appear in the window, displayed in the wireframe format.



To manipulate the structure, place the cursor (+) over the RasMol window, click and hold while moving the mouse. You can move the scroll bars at the right and bottom of the RasMol screen also. How to identify an atom is discussed later.

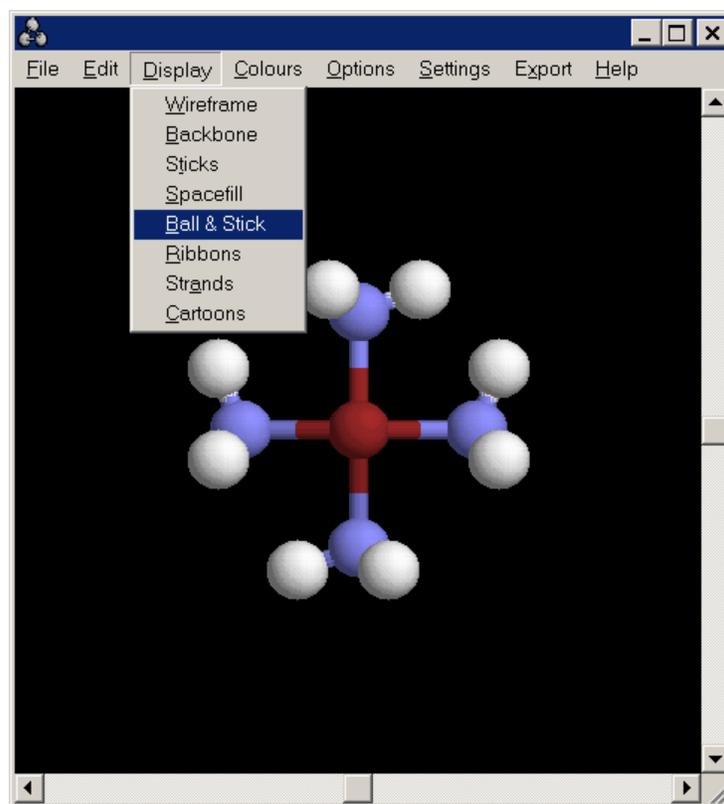
The CPK color scheme is used in most structure files. Common element colors include hydrogen (white), carbon (gray), oxygen (red), nitrogen (light blue), and chlorine (green).

The standard CPK colors for the most common elements are given below:

C	H	O	N	P	S
Cl	Na	Br	Fe	Mg	UNK

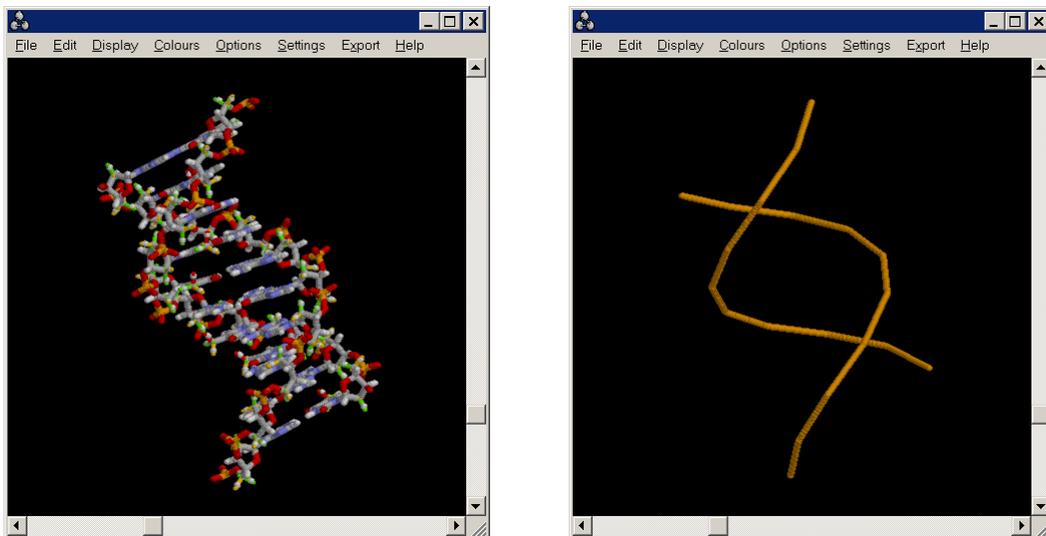
<http://info.bio.cmu.edu/Courses/BiochemMols/RasFrames/CPKCLRS.HTM>

To change the display type, click on "Display" to view the various choices. The spacefill display shows the realistic molecular shape and size. The other formats allow easier viewing into the structure. Crystalline solids will usually not display unless in the ball and stick format.

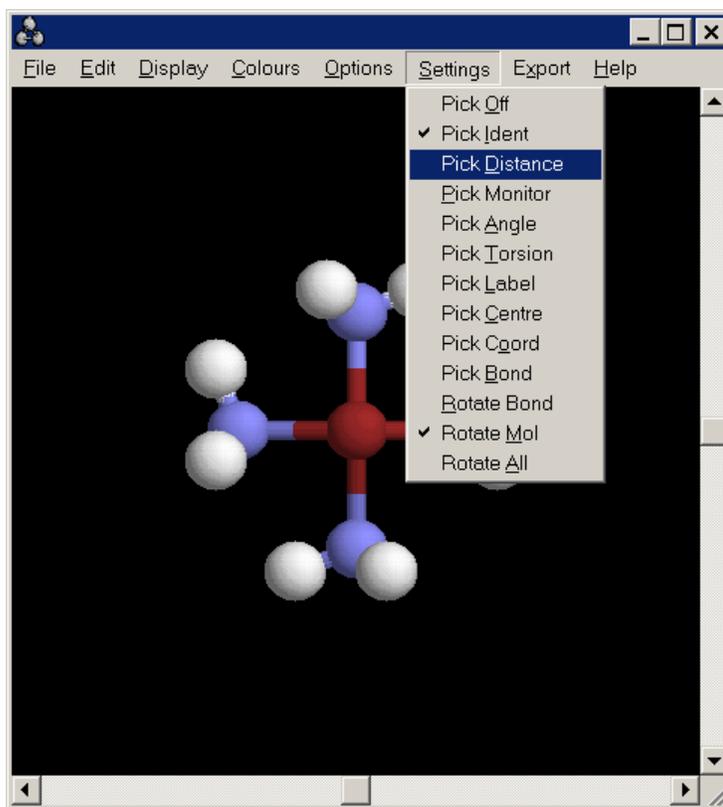


Under "Options" on the menu bar, you can add labels to identify all atoms in a structure (deselect to remove labels), turn hydrogen atoms off (helpful when many occur in structure), and view in stereo.

The ribbons and cartoons formats are very useful for proteins (recognize helices versus sheets) and backbone for nucleotides. Shown below are the stick form of DNA (left) and the backbone (right).



You can perform a number of measurements on the structure by selecting "Settings" and then the option you want as shown on the screen below. To identify

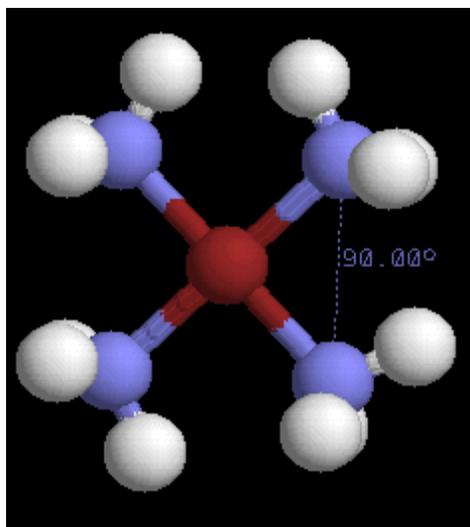


the atoms, select "Pick Label" and then click on an atom in the structure (an element symbol plus position number in the structure appears). To remove labels, close and then reopen the structure file.

Here are the explanations for three common measurements made on structures:

- ◆ To measure distance select "Pick Distance": click on any two atoms; for a bond distance, click on the two connected atoms
- ◆ To measure a bond angle select "Pick Angle": click on three consecutive connected atoms
- ◆ To measure a torsion angle select "Pick Torsion": click on four consecutive connected atoms

The results are displayed on the structure and are sometimes difficult to read! You may need to rotate the structure to view the result. Changing the display to the sticks format can help too. The image below illustrates the N-Cu-N bond angle in  $\text{Cu}(\text{NH}_3)_4^{+2}$  complex ion.



Distance units are given in angstroms. To convert to picometers (pm), multiply by 100.