

Changing your molecule's appearance

The Render Control panel contains several sliders and selectors for changing how the molecule appears. Two renderman light sources are provided: ambient, and distant. There are sliders for changing the intensity of both sources, and the angle of the distant source. Changing the light sources will have no effect in "quick" rendering mode.

The Molecule Style selector allows you to choose between a stick model, Ball and Stick model, and a Space Filling model. The ball and stick model is only partially implimented at the moment. It won't work with the Quick renderer, and the sticks won't appear in any RIB files you create.

WARNING : There is a serious bug in the quick renderman renderer. If too many shapes are displayed it runs into memory problems and can crash the program, and sometimes the entire window server (ie - it can can cause you to be suddenly logged out). This is a bug in v3.0 of the NeXT operating system, and there is nothing I can do

about it. If you use more than ~150 atoms in the Ball and Stick or Space Filling mode, or more than ~500 atoms in the Lines mode, this problem may crop up. Using the "Quick" renderer will prevent this from happening, but it has its limitations.

The Render selector allows you to choose the rendering model to be used. Points will display dots wherever a shape would be rendered (not very useful). Lines will display lines only. If you use the Space Filling style with Lines, you will see outlines of all of the spheres in your molecule. Planes does hidden surface removal, but the spheres are made of several planes rather than appearing "smooth". Smooth is, like it sounds, for rendering smooth looking spheres. The spheres are still approximated as a group of planes, but the appearance is better, at least. This occurs only with the QRM renderers. If you save a RIB file, then use prman to render the molecule, or print a molecule, it will not appear blocky like this.

The final option, "Quick", is my workaround for the bug mentioned above. This option turns off the quick renderman renderer, and uses my

own 3d graphics routines. In the Lines style it is roughly the same speed as renderman, but it won't crash. In the Space Filling style, it will be MUCH faster than renderman as long as the color flag is off. If color is on, it will be about the same speed as renderman. In the Space Filling style, only the following atoms are currently supported : H,C,N,O,P,S. Any other atoms present in the molecule will simply not appear.

The "Use Color" switch is for use on color machines. Since I only have access to a monochrome NeXT-Station, I have not been able to test any of the color abilities of this program. Let me know if there is a problem. To use the color flag, you must select Use Color, THEN select a renderer to make it take effect. The Planes and Smooth renderers will use color regardless of this flag.

There are also 4 buttons provided to resize the Molecule View to a few preset sizes. These sizes are convient when you need to transfer the rendered image to another machine. The "unusual" sizes are used to correct aspect ratio problems.