

Chemistry 400 – Senior Seminar

Tutorial #4 – Creating Ray-Traced Molecular Images Using POV-Ray

Assignment:

- Use HyperChem, HyperChem Raytrace, and POV-Ray to **render** a picture of caffeine plus the molecule listed below. **Copy** and **paste** both pictures into a Microsoft Word file, **print** it out and give it to Dr. Johnston. Please **do not** e-mail the file to me (too big!).
- The files listed below should be located in the C:\hyper5\samples\ directory

Bill C. – organics\ampicill.hin

Amanda – aromatic\c60.hin

Bill M. – organics\chloroph.hin

Jeremy – organics\progeste.hin

Lora – organics\hemin.hin

Jadwiga – organics\riboflav.hin

Note: This tutorial *requires* both HyperChem and the POV-Ray software, both of which are installed on the computers in Science 117. POV-Ray may be downloaded free of charge from www.povray.org.

Background on the POV-Ray Software

The Persistence of Vision (POV) ray-tracing program is a program that creates photo-realistic images using a technique called *ray tracing*. Ray tracing is a mathematical algorithm that simulates the behavior of light rays, keeping track of the reflections, refractions, etc. for a collection of objects called a “scene”.

The program takes as its input a series of commands that together generate the scene. Components of a scene can include spheres, cylinders, arbitrary shapes, surfaces, pigments, textures, and a light source. The computer then *renders* the scene according to the instructions and generates the ray-traced image. Creating a scene by hand can be rather time consuming, but luckily HyperChem has a utility to create a POV-Ray scene for any molecule using either a ball and stick or spacefilling representation.

Loading a Structure into HyperChem

- Start the HyperChem program either from the **Start** menu or from the MSOffice shortcut bar (right side of the screen).
- Select **File/Open** and select the file **hyper5\samples\organics\caffeine.hin**. Click on **Open** to load the structure of caffeine into HyperChem.
- Use the **Rotate** tool to rotate the molecule until it is in the orientation you prefer.

Creating the POV-Ray Source File

- Start the **HyperChem Raytrace** program from the **Start** menu (**Start/Programs/HyperChem Raytrace**)
- Select **Options/Rendering...** and select **Ball & Stick** and make sure that **Show hydrogens** is selected.
- Select **File/Get HyperChem**. This reads the HyperChem structure into the HyperChem Raytrace program.

- Select **File/Save As...** and save the file **caffeine.pov** to your floppy or *Home* directory. (Please avoid saving the file to the hard drive when using the computers in Science 117 – someone has to clean up after you...!)

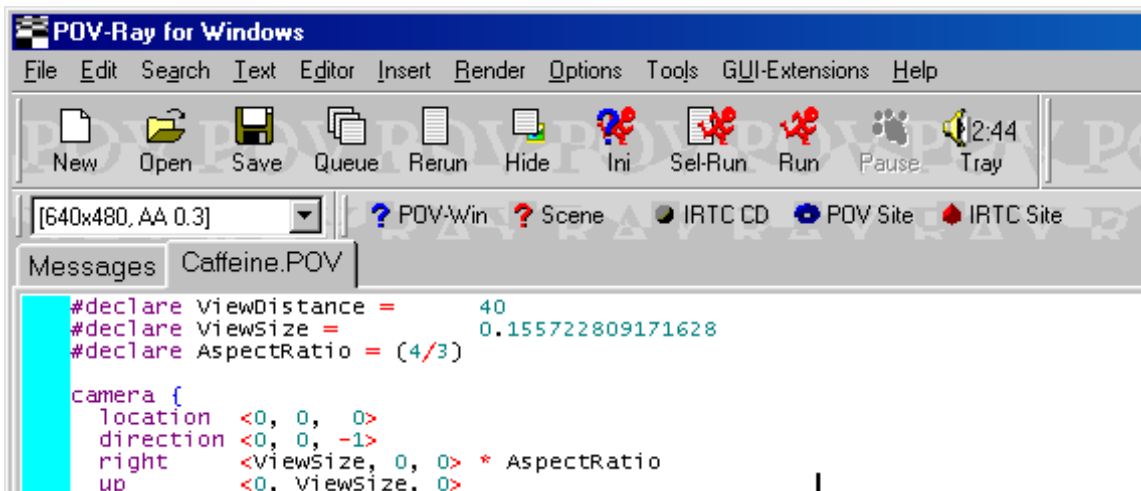
If you were to look at the first few lines of this file you would see...

```
#declare MolecularSystem = union {
sphere {
  <-1.964423,-0.3617501,6.520667E-06>, 0.48
  texture { Texture_C }
}
sphere {
  <-0.7665077,-0.928107,6.520667E-06>, 0.448
  texture { Texture_N }
}
```

These are some of the commands used to generate the scene containing a representation of the caffeine molecule. If you are interested, more information about these commands is available in the help file for POV-Ray and on the POV-Ray web site (www.povray.org).

Rendering the POV-Ray Scene

- Start the **POV-Ray** program from the **Start** menu (**Start/Programs/POV-Ray for Windows v3.1/POV-Ray for Windows**) or the MSOffice shortcut bar.
- Select **File/Open File...**, select the file **caffeine.pov** and click on **Open**.
- The window you see will look something like the picture below.



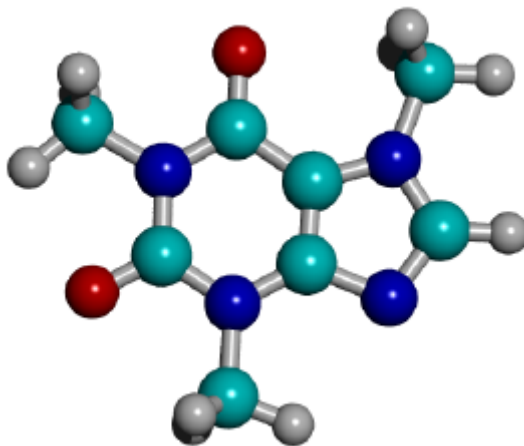
- Click on the drop-down menu just above the **Messages** tab and select **[640x480, AA 0.3]**. This controls the size and *anti-aliasing* of the final picture produced. Anti-aliasing is a technique to remove the jagged-ness typically found in computer graphics.
- Select the **Render/Start Rendering** menu. A window showing a rendering of your molecule should appear.

Modifying the POV-Ray Scene

For this example, I would rather render my molecule with a **white** background (especially for inclusion in this tutorial. This is quite simple to do by modification of the **caffeine.pov** file.

- Scroll down to the very bottom of the file using the scroll bar on the right. Find the line that says “background { Black }” and change it to “background { white }”
- Re-render the scene by selecting the **Render/Start Rendering** menu.

The newly output rendering is shown below.



For your information, pre-defined colors other than Black and White include Red, Green, Blue, Yellow, Cyan, Magenta, Clear (note that case is important). For even more color definitions, look at the **color.inc** file in the **POV-Ray for Windows v3.1\include** directory.

- At this point we are done with the **POV-Ray** program, so go ahead and select **File/Exit**.

Manipulating the Graphics Output

You may wonder what happens to the graphics created once you quit the program. There is a special directory on the hard drive of the computer called **C:\pov_images**. This directory will contain the last scene rendered for a particular input file as a bitmap (.bmp) file. Let's go ahead and find the image we generated for caffeine.

- Double-click on the **My Computer** icon on the desktop.
- Double-click on the **C:** icon in the My Computer window.
- Double-click on the **pov_images** folder.
- Double-click on the **caffeine.bmp** file. The file will open in an Microsoft Paint (an image-editing program).
- Select **Edit/Select All**. Then select **Edit/Copy**. Now you can **Paste** your picture into Microsoft Word, Microsoft PowerPoint, or most any other Windows program.