

MolView Folklore and Tips:

I include this file since most Mac users do not read writeups (myself included)... Below are 'Kludge' ways to do some special things to get better diagrams and why they are that way. In a perfect world where I have loads of time, updates will be made in the pgm to do these things...

CPK MODELS:

As briefly discussed in the manual, whenever you have the CPK button turned on, the image and PICT files are bit imaged. I had to do this to keep the pgm fast and not make it more of a memory hog than it is now. This can be good in that the binary image may be smaller than the object oriented one, and can be bad in that the object oriented one can be bigger than the screen and higher resolution than the screen. This leads to several 'tricks'....

1) Convert drawing to a bitimage:

Say I just want a bit image of a complicated ribbon drawing, but I do not want CPK models. You might want this because some heavily smoothed ribbon drawings will make programs like MacDraw barf. To do this:

- a) Hit the CPK button on the Tool palette.
- b) Hit the 'Delete all Atoms' button in the dialog box.
- c) Hit the 'Done' button.

Now when you select the CPK button from the 'Object Window', the image will be bit-imaged without any CPK atoms. Again, this will create a fairly small PICT file that can be read into any pgm like MS Word, but you did lose some resolution.

2) Make a high resolution CPK or Bit-imaged file:

I am sorry, I have not yet finished this routine. Currently, the output image MUST be the same as the window size (unless you want a system crash). To 'kludge' your way around this...

- a) Get into the 'bit-image' mode (using a CPK model or the above example).
- b) Blow up the image.
- c) Translate your way around the object, Making a PICT file of each section until you have PICTs for the whole thing.
- d) Go to a program like MacDraw Pro and piece them together, group the pieces, and scale them down using the 'Page Setup' command in the 'File' menu.

Alternatively,

Get a BIG monitor like mine (24") and make a big PICT and use the printer driver to scale it down...

What you are doing is basically taking the image at the resolution that I am

limited to (72dpi) and effectively increasing the resolution for printing by scaling it down.

3) Make a high resolution drawing without being in the 'Bit-imaged' mode. Make the drawing bigger than the screen and make a PICT file. Use the other drawing programs to shrink it down. This is effectively what is done in postscript files.

4) PDB and 'O' Plot files:

a) PDB files: Be careful of Heme groups. They contain 'N A', 'N B', 'N C', and 'N D' groups. In the example Hb.pdb file, I just changed them the 'N_A', and etc. Since I read the files as free format, it confuses the program. Will fix this in the future.

b) 'O' plot files. When creating O plot files, do not include the menu. This creates a ton of useless 'objects' in the file that confuses and crashes the program. Prevent their creation by following the dialog in the 'plot_setup' command. Also, avoid labels at all cost.