pdb2pov v1.15

A program to convert PDB atomic structures to
`POV-Ray` v2.0 format scene files.
Edition 1.0, for pdb2pov Version One
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This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. Use at your own risk!

I consider this program to be `CharityWare`. If you like it, please consider sending a donation to the National SIDS foundation. You can read more about SIDS in the About.SIDS document included in this distribution.

1 Program Description

PDB2POV is a CLI program designed to convert Brookhaven format atomic structure files into POV-Ray Version 2.0 compatible scene files. The program has a large number of options to change the atomic rendering style for CPK, van der Waals, or covalent radii spheres. The user may also specify two ground styles (plain or checkerboard), area light sources, and a nice cloudy sky. Finally, the user may specify for X, Y, and Z axis rotations to orient the molecule.

The molecular format used is called `Protein Data Bank` (.pdb) format. This is one of the most prevalent formats used in modern chemistry. The entire Protein Data Bank consists of a few hundred protein and DNA molecular structures and can be obtained from the Brookhaven laboratories for a nominal fee (or from me if you know what you want).

This program was designed to be used with my molecular rendering program CPK v2.2, but may be used manually as well.

1.1 Distribution

In addition to the program, this distribution includes a number of atomic 'include' files to be used with the generated scene files.

You should have received:

- '`pdb2pov.000`' - 68000 (ieee math)
- '`pdb2pov.030`' - 68030+68881 optimized version
- '`pdb2pov.040`' - 68040+68882 optimized version
- '`Pdb2POV.doc`' - this file
- '`About.Sids`' - documentation about the SIDS foundation
- '`crambin.pdb`' - a small protein molecule
- '`crambin.pov`' - `POV-Ray` V2.0 scene file from crambin.pdb
- '`include/atoms2.inc`' - main atom include file (shiny plastic)
- '`include/atoms_covalent.inc`' - covalent atomic radii include file
- '`include/atoms_cpk.inc`' - CPK radii atomic include file
- '`include/atoms_vdw.inc`' - van der Waals radii atomic include file
- '`include/atoms_glass2.inc`' - atom definitions with 'glass' texture

1.2 Requirements for running pdb2pov

This program should run on any Amiga. There are no operating system specific calls, so I wouldn't be surprised if it runs under v1.3. I have not tested this, however. The program uses dynamic memory allocation to read the atomic structures, and should gracefully exit if it runs out of memory. I would recommend at least 1MB RAM memory in order to read relatively large structure files.

You will, of course, need a copy of POV-Ray version 2.0 or higher. This is an excellent public domain ray-tracer which may be found on a number of BBS and internet sites.

NOTE: I have customized POV-Ray to be slightly more compatible with this version of CPK. My version also has direct support for the Picasso II RTG 24 bit graphics board. This version is available on aminet and BIX. The name will be 'povami_picasso_xx.lha', where xx represents my internal version.

1.3 Installation

1. Drag the pdb2pov drawer to some appropriate location on your system.
2. Copy all files from the include directory to your normal POV-Ray include area.

1.4 Usage

If you just type the program name with no arguments you should see a USAGE message something like:

```
Program: $Id: pdb2pov.c,v 1.15 1993/11/09 15:29:07 eric Exp $
```

```
USAGE: pdb2pov InputFile OutputFile
        [-o object_only]
        [-t atm file format]
        [-s (writes cloudy sky)]
        [-g (writes plain ground)]
        [-h (writes checkered ground)]
        [-a (create area light)]
        [-v (do van der Waals radii)]
        [-c (do covalent radii)]
        [-b (do ball_and_stick)]
        [-d (bond cutoff threshold)]
        [-q (ball and stick + glass atoms)]
        [-x X-Axis rotation]
        [-y Y-Axis rotation]
        [-z Z-Axis rotation]

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```

The options are as follows:

- -o - Only write the object definition with no ground or sky
- -t - Read the input format in Tripos .atm format rather than the default Brookhaven pdb format
- -s - Generate statements for a nice cloudy sky background
- -g - Generate statements for a bumpy dark purple 'plain' ground
- -h - Generate statements for the classic checked ground
- -a - Generate statements for an `area light` light source. These produce soft shadows but can take a very long time to render.
- -v - Render the scene with van der Waals atomic radii
- -c - Render the scene with covalent atomic radii
- -b - Render the scene in ball and stick mode
- -d - Specify the distance (Angstroms) above which bonds will not be generated for ball and stick mode.
- -q - Generate a hybrid molecule with ball and stick atoms overlaid with glass spheres. This looks really good, but takes an extremely long time to render.
- -x - Specify an X-Axis rotation angle (degrees).
- -y - Specify a Y-Axis rotation angle (degrees).
- -z - Specify a Z-Axis rotation angle (degrees).

The *InputFile* and *OutputFile* parameters are assumed to have extensions of `.pdb` and `.pov`, respectively, so don't specify any extensions on the command line.

Here's an example:

```
pdb2pov.040 crambin crambin -s -h -x 90 -b -d 1.8
```

This would take '`crambin.pdb`' to '`crambin.pov`', generate sky and checkered ground, rotate the molecule 90 degress in the X axis, and generate ball and stick mode with a distance cutoff of 1.8 Angstroms.

The program tries to be intelligent about positioning the molecule so that the whole structure is within the field of view, but you're naturally free to adjust the position by hand for more aesthetic results if you wish.

You may also use the atomic radii flags (`-v -c`) to get different effects. By using the `-v` flag you'll get van der Waals radii spheres, and `-c` will use covalent radii. The default is to use approximate CPK radii.

Finally, a note about *ball and stick mode*. The program uses a bond distance cutoff of 2.0 angstroms for computing bonds. That is, any distance greater than this will not be considered a bond. If you find yourself getting lots of spurious bonds try decreasing this value. The default is generally reasonable for 'typical' atomic structures, though.

If the program can't recognize a specific atom type it will use the parameters for `carbon`. You may therefore need to edit the scene file or add to '`atoms2.inc`', '`atoms_glass2.inc`' and the radii files. If you update these files please send me a copy.

Appendix A Miscellaneous

A.1 The Brookhaven data bank

The Brookhaven data bank is one of the principal repositories for protein and nucleic acid crystallographic structures. The lab maintains an anonymous FTP site at: `pdb.pdb.bnl.gov`, (130.199.144.1). This site has the current structure database as well as a number of useful programs. Brookhaven also distributes a quarterly CD-ROM with the latest database. Send E-Mail to `pdb@chm.bnl.gov` for ordering information.

A.2 Program History

- V1.15 - First public release, December 1993

Concept Index

This section contains a list of general topics (or *concepts* in Texinfo parlance) derived from this document.

Table of Contents