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crystal

A program to make ball-and-stick, or polyhedral crystal structure drawings

This program reads a basic description of the crystal structure, which includes unit-cell parameters, space group and atomic coordinates, and outputs a geometry object that contains polyhedra, spheres, bonds, and the unit-cell boundary. This program exists in two versions: (1) an AVS module originally written by Dr. Larry Finger (finger@gl.ciw.edu) of the Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, DC 20015-1305, and (2) a modified version by Dr. Martin Kroeker (martin@oc2.oc.chemie.th-darmstadt.de), Institut für Organische Chemie, Technische Hochschule Darmstadt, D-64287 Darmstadt, Germany, which adds some view options and contains the output routines to generate a scene description file for the popular POV ray-tracer program. This scene file can be used as is, but it can also be edited to make use of the more sophisticated (or un-scientific) features of POV like transparency, backgrounds or light effects. The POV program is available from ftp.povray.org. Source code for 'crystal' is available at ftp://cryst.ciw.edu/anonymous/avs. The necessary files are crystal.c, symmtry.c, and makefile (the AVS version). Postscript and Word 6.0 versions of this writeup are also available as crystal.ps and crystal.doc, respectively. To compile the POV version, include a -D_POV_ switch on the compiler call.

Input Instructions for Crystal:

Both versions can read the same input file; however, the AVS version will ignore any color information that is presented - colors are set using the Geometry Viewer in AVS. In addition, the AVS version will ignore the **box**, **edges**, and **view** commands. Each line of the input file is preceded by a character sequence that describes the type of information, as follows:

titl

General description of the Structure

cell

unit-cell lengths and angles. If no angles are listed, they are assumed to be the fixed values for the symmetry class.

spgp (or **sgrp**)

Space Group name consisting of the Bravais lattice symbol followed by a space, the elements parallel to the first axis followed by a space, etc. Examples are I 41/a m d, P 21/n, I a 3 d, P b n m, etc. The generators will always select the origin choice with a center of symmetry at the origin. Furthermore, all monoclinic cells will have the unique axis parallel to the b axis.

sphere 'name' 'radius' 'color',

where 'name' is a one- or two-character symbol of the atom type, 'radius' is the radius of the sphere in Angstrom, and 'color' is one of the color names from POV's colors.inc file.

bond 'name1' 'name2' 'radius' 'min length' max length' 'color',

where 'name1' and 'name2' indicate the types of atoms to be connected by a bond, 'radius' is the radius of the resulting cylinder, and the minimum and maximum lengths are given in Angstrom.

polysz 'name' 'length' 'color'

defines a polyhedron, where 'name' is the name of an atom at the center of a polyhedron and 'length' is the maximum length of distances to atoms that are to be considered as the vertices of the polyhedron. No atoms that are mentioned in 'sphere' or 'polysz' commands will be considered as the vertices of a polyhedron. (but note that spheres on the vertices of polyhedra, as sometimes used to distinguish OH from O in phosphates, can be created by duplicating a position and using one of them as center of a sphere)

atom 'name' 'number' 'x' 'y' 'z'

defines the atoms. The 1- or 2-character name will be used on the commands that describe the objects to be created, the number is to keep track of the atom, and 'x' 'y' 'z' are the fractional coordinates in the unit cell.

box 'radius' 'color' (POV version only)

defines the radius and color of the cylinders that form the unit cell boundary.

edges 'radius' 'color' (POV version only)

defines the thickness and color of cylinders along the edges of polyhedra that may be used to emphasize the faces.

view 'xrot' 'yrot' 'zrot' (POV version only)

where 'xrot', 'yrot' and 'zrot' are view rotation angles in Cartesian space

end

The last line of a file.

Sample input file - set the origin at 0,0,0:

```
title Buckyball
cell 14.16 14.16 14.16
spgp F m 3
sphere c 0.4 Green
bond c c 0.1 1.2 1.5
atom c 1 0.04908 0.00000 0.24510
atom c 2 0.10028 0.08284 0.21346
atom c 3 0.18313 0.05120 0.16226
end
```

In the AVS version, the view limits are set by the use of slider widgets; whereas similar information is input via command line switches for the standalone POV version as follows:

-b xlim ylim zlim

defines X-, Y- and Z-limits of the view box in angstroms (defaults to -10..10 Angstroms around center)

-p xmin xmax ymin ymax zmin zmax

defines a-,b-,c- plotting range in fractions of the axes, similar to the Pluto (Motherwell & Clegg 1978) PACK RANGE command (this is especially useful for hexagonal cells, where the orthorhombic view box does not always give satisfactory results)

-h, -?

displays usage information

-n

suppresses plotting of unit cell 'box'

-o xcenter ycenter zcenter

defines center of view box in crystal coordinates (defaults to 0.5 0.5 0.5)

-v xangle yangle zangle

defines view rotation angles around the axes of the Cartesian view coordinate system (equivalent to the view keyword)