

DRAWxtl V5.5

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

by

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This program reads a basic description of the crystal structure, which includes unit-cell parameters, space group, atomic coordinates, thermal parameters or a Fourier map, and outputs a geometry object that contains polyhedra, planes, lone-pair cones, spheres or ellipsoids, bonds, iso-surface Fourier contours and the unit-cell boundary. Unlike earlier versions, the program now contains a graphical-user interface (GUI) that renders the structure object using a series of OpenGL calls using the glut-programming interface, and provides the capability to adjust many of the parameters and see the effect on the drawing in real time. As before, scene description files for the popular POV ray-tracer program, or a Virtual Reality Modeling Language (VRML) file are produced. The POV scene file can be used as is, but it can also be edited to make use of the more sophisticated features of POV like transparency, backgrounds or light effects. The VRML version is suitable for use with WWW browsers such as FireFox, and can be used to make displays suitable for interactive examination by users. Source URL's for this and associated programs are given in Appendix A. The original version of this program was a module for the visualization software of Advanced Visual Systems, Inc.; however, that program has not been maintained for several years. That code was written by Larry (Larry.Finger@lwfinger.net), Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, DC 20015-1305. The original POV and VRML modifications were proposed and coded by Martin (martin@ruby.chemie.uni-freiburg.de), Institut für Anorganische und Analytische Chemie, Universität, Freiburg, Germany. Addition of the Fourier-contour code was accomplished by Brian (Brian.Toby@ANL.gov) Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439 USA

Program Features:

DRAWxtl can make ball-and-stick, polyhedral, or mixed diagrams, with atoms represented as spheres or thermal ellipsoids. For the latter type, anisotropic coefficients can be input as U_{ij} , B_{ij} , or \square_{ij} , depending upon what is available. Since V5.3, the program has the ability to plot modulated and composite crystals up to 3-D modulations. All of the standard modulation functions defined in the CIF definitions can be handled, except for the rigid-body terms. At present, modulated structures may only be input with a CIF description of the structure.

Polyhedral diagrams can be made with polyhedra of any desired shape, not just tetrahedra or octahedra. For zeolite drawings, it is also possible to make the 'polyhedron' of tetrahedral ions about the center of the cages.

The program can read structural input from CIF, CSD (the Cambridge Structure Database), GSAS, SCHAKAL, and SHELX formats, as well as its own native format. In this way, the crystallographic data for complicated structures do not have to be retyped. Fourier maps may be input in the 'grd' format from GSAS, the 'stf' format of JANA2000, the 'w2k' from WIEN2K, the 'vsp' format from VASP, or the 'flp' format of FullProf. Alternatively, if structure factors are available in CIF format, DRAWxtl will compute the Fourier map.

The program also outputs a table of bond distances from each of the atoms in the asymmetric unit to all other atoms. All symmetry operators are used in this calculation, with distances less than a specified limit (defaults to 3.5 Å) written to the listing file. This output can be used to check that input parameters are valid. For modulated structures, the minimum, maximum and average values for the bond length are calculated and listed. For anisotropic atoms, the eigenvalues (RMS amplitudes) and eigenvectors for the ellipsoids are computed and listed.

This program is written in highly portable C++ and will run on a wide variety of machines including 386- to Pentium-based PC's, Macintoshes, high-end workstations, and Linux systems. The only requirements are a graphical-windows based system, a floating-point coprocessor, a C++ compiler, and libraries for OpenGL, and FLTK (The Fast Light Tool Kit) V1.1.9. The developers use Microsoft Visual C 6.0 for Windows and gcc and g++ for Linux and OS X. The program requires a display with at least 800 × 600 resolution. N.B. For those people that do not wish to use a windowing system, we have an updated, non-GUI, version available. Please check <http://www.lwfinger.net/drawxtl> for details.

DRAWxtl is open-source software, and is free to anyone. We hold copyright on the code, and like any other piece of intellectual property, we ask that you respect our rights.

Program Operation:

As in previous versions that were written for command-line input, a text file of instructions controls the drawing produced. In this version, however, the structure file can be changed by the widgets of the main and secondary screens, and the effect of such changes shown immediately on the main screen of the program (Fig. 1). As in earlier versions, the program produces the POV and VRML output files, which are then read by the companion renderers/viewers to produce the hard copy output, or files suitable for viewing with a Web browser. Since V5.1, the program can go directly from the main screen to an Encapsulated Postscript (EPS) file; thereby bypassing the external hard-copy program step for users that do not have POV installed. Be aware that the resulting drawing will be at screen resolution, which may not be what is desired.

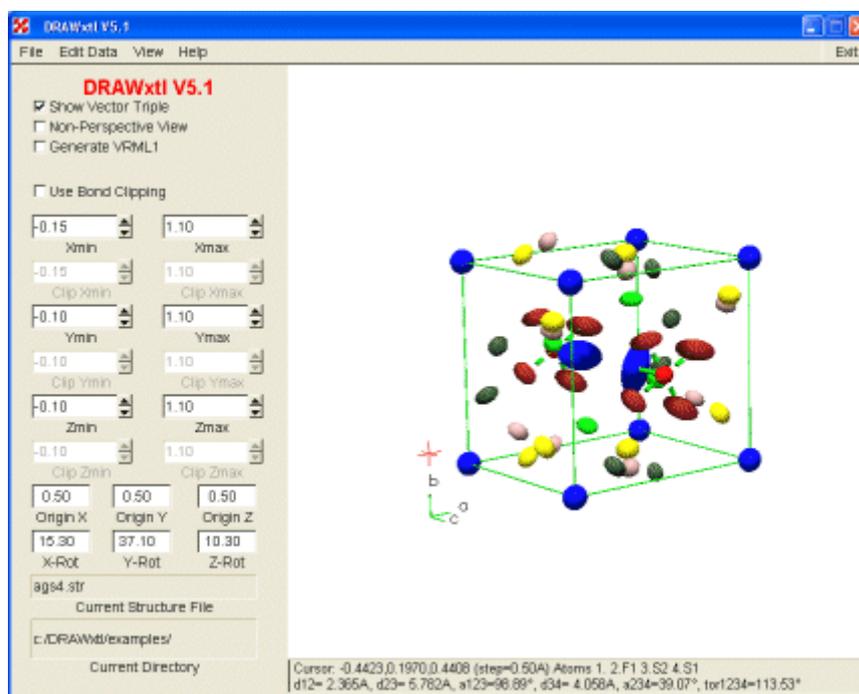


Fig. 1: Screenshot of main screen for **DRAWxtl**.

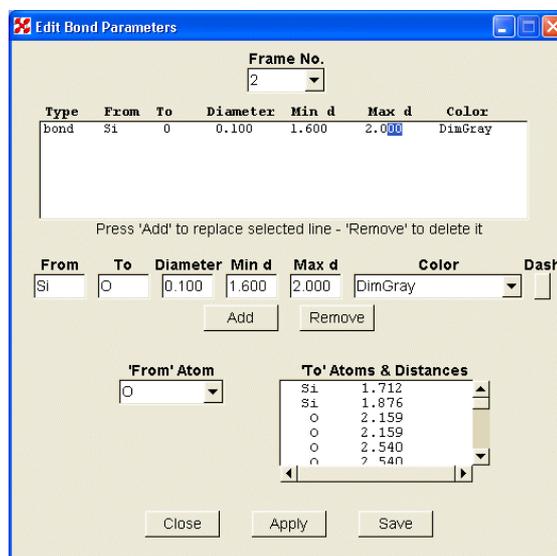
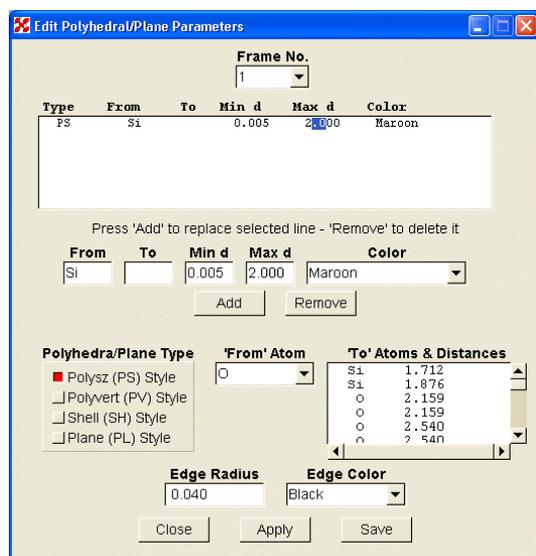
Another feature in V5.1 and later is the graphics cursor shown in the lower, left rear of the diagram above. Its position in fractional coordinates is shown on the line below the drawing. The various bond distances and angles and the torsion angle are shown for the last 4 selected atoms. To aid in atom selection, the following keyboard shortcuts have been implemented:

- 'C' or 'c' - turn the cursor on. Each successive press reduces the size of the steps. When the size is reduced below 0.01 Å, the cursor is turned off.
- 'x', 'y', 'z' - move the cursor in the positive direction parallel to the x-, y- or z-axis.
- 'X', 'Y', 'Z' - move the cursor in the negative direction parallel to the x-, y- or z-axis.
- 'P' or 'p' - place the graphics cursor on the atom nearest the mouse position.
- 'A' or 'a' - place the cursor at the position of the atom nearest the cursor.
- 'M' or 'm' - move the cursor to the min(M) or max(m) in the electron-density.
- 'L' or 'l' - label the atom at the cursor position.
- 'B' or 'b' - Place the bond distance between atoms 1 and 2 in the list.
- Hold left mouse and drag - rotate the graphics object using a virtual trackball.
- Hold right mouse and drag - zoom in/out on the object. On the Mac, hold down the command (Apple) key and drag the mouse.
- Hold middle mouse (both on 2-button mouse) and drag - pan motion. On the Mac, hold down the alt (option) key. The arrow keys may also be used to move the object.
- HOME key - remove all zoom and pan motions.
- Shift/leftclick - drag labels or the triple vector to a desired position. If the triple vector is dragged, all 3 of its labels will be moved with it.
- Ctrl/leftclick - remove the object at the location of the mouse cursor.

With the widgets located on the main screen, the user can select how much of the structure to portray, where to place the origin, and what orientation to view. Dragging the mouse in the graphics window can also change the latter parameters. With the menu items, the user may select the structure to be displayed, edit the various parameters, view the POV file or listing output, set some POV configuration parameters, or view the various help files. Fig. 2a shows the screen used to edit polyhedron or plane parameters and 2b shows the screen for bonds. Similar screens exist for ellipsoids, spheres, and general parameters. For those changes not addressed by these screens, the user also has the ability to edit the original or revised 'str' file.

Fig. 2a. Polyhedra/Planes edit screen

2b. Bond edit screen



The edit screens show the current object descriptions in the upper window, where the parameters can be modified, either by direct editing, or by double clicking on a line of the window. The data will be transferred to the boxes below, where changes may be made. When all boxes are filled, the 'Add' and/or 'Delete' buttons will be made active. New objects can be created using the lower part of the screen. After selecting the central atom with the 'From Atom' combo box and using the 'Polyhedra/Plane Type' radio buttons to select the type of object, the user highlights one or more characters in the line containing the coordinating distance to be selected. The parameters will be transferred to the middle row of boxes. After any necessary changes are made in that box, press the 'Add' button to create a new line. When either the 'Apply' or 'Save' button is pushed, the new parameters will be applied to the drawing. When the structure has multiple frames, the "Frame No," combo box is used to select the frame that is to be modified.

Input Instructions for DRAWxtl:

In this program, color is represented in symbolic form, and may be an RGB triple or one of the color names from POV's "colors.inc" file, which may be modified to define custom colors. The standard color names and associated RGB values are listed in Table I, and sorted by RGB values in Table II. Any of these colors may be made transparent by appending the phrase 'filter xx' after it, where 'xx' is a number from 0.0 to 1.0. The larger the value of 'xx', the more transparent will be the entity. Each line of the input file is preceded by a character sequence that describes the type of information, as follows:

aimsurf 'name' 'number' 'filename' 'style' 'color'

causes the program to read from the given file a precalculated surface mesh to display at the position of the specified atom. The file must be in the format used by the aim program (part of the WIEN2k program suite) for calculating Bader surfaces of atoms according to the AIM concept. (The calculated surface should cover the whole range of 0 to π in theta and 0 to 2π in phi, as no symmetry expansion is performed.) The rendering style can be 'dots', 'mesh' or 'solid'.

arrow 'xp' 'yp' 'zp' 'xc' 'yc' 'zc' 'length' 'diameter' 'color'

defines the position in fractional coordinates (xp, yp, zp) of the nuclear cell, the components (xc, yc, zc) of the spin vector, and the length, diameter, and color of the arrows. The reference direction for xc is parallel to direct space a, yc is parallel to $(a \times b) \times a$, and the reference direction for zc is perpendicular to $xc \times yc$. The only symmetry elements used in placing arrows are the translations described by the mag_trans command below.

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

defines the atoms. The 1- to 4-character name will be used on the commands that describe the objects to be created, the number is to identify which atom of this type is referenced, and 'x' 'y' 'z' are the fractional coordinates in the unit cell. If the atom is located on a special position where the coordinate is given by a fraction such as $\frac{1}{4}$, the string '1/4' may be entered rather than 0.25.

average

causes the program to draw the average structure of an incommensurately modulated crystal even if information about positional or occupancy modulation is available in the CIF.

axislines 'width' 'color'

defines the width and color of the lines that depict the principal axes of ellipsoids. The color defaults to dark gray (Gray20). If this command is not given, any ellipsoids will be drawn with principal axes of 0.00015 times the overall scale factor, which should normally be appropriate.

background 'color'

sets the color of the background of the graphical views. The default color is white.

bestplane 'number' 'name1' 'name2' ... 'nameN' 'width' 'height' 'color'

causes the program to calculate the best fitting plane through a subset of atoms, where number is the number of unique atom names (name and number, e.g. C8) name1 to nameN that follow. The plane is drawn as a rectangle of dimensions width x height in the given color.

betaij 'name' 'number' ' β_{11} ' ' β_{22} ' ' β_{33} ' ' β_{12} ' ' β_{13} ' ' β_{23} ' 'color'

defines the anisotropic thermal coefficients for an atom and 'color' of the ellipsoid. The 'name' and 'number' should correspond to the atom input described above. For this form, the temperature factor is given by $T = \exp\{-\sum_j \sum_k h_j h_k \beta_{jk}\}$. In the POV version of the program, the principal ellipses are drawn in black. The ellipses will, of course, be invisible if the ellipsoid is also black.

bij or **Bij** 'name' ' B_{11} ' ' B_{22} ' ' B_{33} ' ' B_{12} ' ' B_{13} ' ' B_{23} ' 'color'

defines the anisotropic thermal coefficients for an atom and the color of the ellipsoid to be drawn. The 'name' and 'number' should correspond to the atom input described above. For this form, the temperature factor is given by $T = \exp\{-0.25 \sum_j \sum_k h_j h_k B_{jk} a_j^* a_k^*\}$, where a_j^* and a_k^* are reciprocal lattice constants.

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 the same units as the unit cell.

box 'radius' 'color'

defines the radius and color of the cylinders that form the unit cell boundary. If 'radius' is 0.0, plotting of the unit cell is suppressed. The radius of the cylinders will be scaled with the size of the drawing. The default size is 0.02.

cell 'a-length' 'b-length' 'c-length' 'alpha' 'beta' 'gamma'

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

clip 'xmin' 'xmax' 'ymin' 'ymax' 'zmin' 'zmax'

defines a-,b-,c- clipping range in fractions of the axes. Any bonds extending beyond these limits will be cut off at half-length. This command is to be used in conjunction with the pack keyword to produce 'dangling' bonds in the display of framework structures.

cutout 'color' (used only for POV and OpenGL)

sets the POV generation of thermal ellipsoids to have one octant removed, as in the program ORTEP. If this command is not given, all ellipsoids will be complete. The color is for the planes that describe the edges of the cutout

dash 'name1' 'name2' 'radius' 'min' 'max' 'color'

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

depthcue 'depth' (used only for POV)

defines the extent to which the size of polyhedral edges is increased as the edge is closer to the viewer.

edges 'radius' 'color'

defines the thickness and color of cylinders along the edges of polyhedra that may be used to emphasize the faces. The radius of these cylinders will also be scaled with the size of the drawing. By default, black edges of size 0.02 will be drawn.

ellipcolor 'name' 'number' 'color'

defines the color for ellipsoids when the thermal ellipsoid information has been read from a CIF, CSD, GSAS, SCHAKAL or SHELX import or inline file. The 'name' and 'number' must match the

identification information in the input file. The parameter 'number' may be an asterisk (*) to indicate all atoms with that name. In addition, these input lines must be after the **import** or **inline** command.

ellipsoids 'probability'

sets the size of the ellipsoid such that that fraction of the electron density is contained within the bounding surface. Use either 0.50 or 50 to get the standard (default) 50% ellipsoids.

finish 'ambient' 'diffuse' 'specular' 'roughness'

defines parameters for the POV lighting functions that are applied to all surfaces. Suggested values are 0.7 0.3 0.08 0.01 to reduce the harsh contrasts that can result from the default material properties in POV.

frame 'comment'

similar to 'end', marks the division between two sets of input that are to be superimposed in a single output file. Each frame must have a complete set of 'atom' lines, and lines describing the objects such as bonds, polyhedra, spheres, etc. to be created in this frame. Distinct packing ranges and space groups are optional. A prime example of this command would be to draw structures with adsorbed molecules with symmetry lower than the cage in which it resides. Another option is to draw ball-and-stick and polyhedral pictures in side-by-side unit cells. All other parameters are global and apply to all frames.

import 'file type' 'filename' 'phase number or data block (for GSAS, PCR, and CIF only)'

causes the program to read structural information from an external file. 'file type' defines the format of that file, and 'filename' is the name of the file. Import filters have been written for the CIF, DISCUS, FDAT (Cambridge Structure Database), GSAS, PCR (FullProf), SCHAKAL, SHELX, WIEN2K, and ELK (Exciting) formats. For GSAS and PCR formats, the number of the phase should also be given. For CIF, the number of the data block should be given. From these files, the atomic coordinates, thermal parameters, unit cell, and space group (CIF, FDAT, GSAS and SCHAKAL formats only) will be read. To set colors for the ellipsoids, use the **ellipcolor** command. You must also use the **ellipsoids** command to get ellipsoids displayed. In files that are imported, atom names of the form Si3A will have atom names of SiA with a number of 3.

inline 'file type'

is similar to **import**, except that the 'foreign' input information is included in the DRAWxtl input file. This form works for FDAT, SCHAKAL, SHELX, and Wien2K data. To set colors for the ellipsoids, use the **ellipcolor** command. You must also use the **ellipsoids** command to get ellipsoids displayed.

labelscale 'size'

changes the relative size of the **labeltext** entries. The default value is 1.0.

labeltext 'x' 'y' 'z' 'text string'

plots the given string at the specified position given in fractional coordinates.

list 'maxdist'

causes the program to list bond distances up to 'maxdist' in the preliminary scan. If this command is not given, 'maxdist' defaults to 3.5 Å

lonpair 'name' 'number' 'distance' 'radius1' 'radius2' 'color'

creates the specified number (either 1 or 2) of cones representing free electron pairs extending from atom 'name', where 'distance' is the length of the cone, 'radius1' is the size of the tip, and 'radius2' is the size of the spherical end cap.

lookat 'u1' 'u2' 'u3' 'v1' 'v2' 'v3'

causes the program to select an orientation such that vector **u** is towards the viewer, and the projection of vector **v** is vertical. This command overrides any **view** command, or the -v switch on the command line.

mag_trans 'Aa' 'Ab' 'Ac' 'Ba' 'Bb' 'Bc' 'Ca' 'Cb' 'Cc'

describes the relationship between the magnetic and nuclear unit cells. In this notation, the upper-case letter states which of the magnetic axes is being described, and the lower-case letter corresponds to the nuclear cell axis. This matrix defaults to the identity.

magnification 'factor'

sets the factor to modify the overall scaling in case the automatic value is not correct. This command matches the -m command line switch.

mapcalclimits 'xmin' 'xmax' 'ymin' 'ymax' 'zmin' 'zmax'

describes the region of direct space (in fractional coordinates) for which the map has been calculated. Map types that are self documenting such as FullProf and JANA2000 do not need this line. For other types, 0 to 1 in all three directions will be assumed.

mapcontour 'level' 'style' 'color'

defines a new contour at 'level'. The style can be either 'mesh' or 'solid', and the color is set by 'color'

mapcontour2d 'lower' 'step' 'upper' 'color'

defines a new set of 2d contours beginning at 'lower', with 'step' between contours. No contours beyond 'top' will be drawn. The color is set by 'color'. See the 'mapregion' command to see how to set 2d mode.

maplegend

draws a color ramp legend in the top left corner of the image

mapread 'maptype' 'filename' 'calctype' 'res'

reads a Fourier map of type 'maptype' from the file named 'filename'. At present, GSAS-style (maptype = grd), JANA2000-style (maptype = stf), WIEN2k (maptype = w2k), VASP (maptype = vsp), FullProf (GFOURIER output, maptype = flp), and O Format (maptype = dn6) electron density maps are read, as are electron density and ELF files from the FP-LAPW programs ELK and EXCITING (maptype=exc) and files in the quasi-standard XCrysDen format (maptype=xsf). If a SHELX/CIF-style Fo/Fc file (maptype = fcf) or a JANA-style M80 file (maptype = m80) is given, the electron density is calculated during the initial read, which may take a few seconds. Both A/B and Fo/phi data formats (Shelx commands LIST 3 and LIST 6) are supported. The calctype may be 'Fo', 'Fc', 'Fo-Fc', '2Fo-Fc', or Fo2 (i.e. Patterson) to indicate the type of map to calculate. If this parameter is not given, an 'Fo' map is calculated. Parameter 'res' indicates the resolution in steps per unit of the cell. If not given, it defaults to 4.

mapregion 'xmin' 'xmax' 'ymin' 'ymax' 'zmin' 'zmax'

describes the region of direct space (in fractional coordinates) that the map is to be displayed in the output. If not entered, these values default to the values given under 'mapcalclimits'. If the difference between the maximum and the minimum along one direction is zero, a 2d map will be plotted for the other two coordinates.

mapslice 'px' 'y' 'pz' 'nx' 'ny' 'nz' 'type'

describes a planar slice through a Fourier map at the location given by the coordinates 'px', 'py', 'pz' of a point in the plane and in the orientation determined by the plane normal 'nx', 'ny', 'nz'. Possible 'type' values are 1 (contoured slice), 2 (solid, color-coded blue to red) or 3 (solid, black to white).

molcomp 'dist'

causes any incomplete molecules in the display box to be completed. The value of 'dist' defines the maximum intramolecular distance. Caution: If this distance is greater than any intermolecular distance, or if the material is not molecular, the display list will overflow.

nolabels

removes all axis labels from the output diagrams.

noshadow

causes objects in the POV file not to cast shadows.

occupancy 'name' 'average' 'minimum'

defines the occupancy of the named site in the average structure of a modulated system, and the occupancy threshold for including individual copies in a plot of the modulated structure. Use a negative value for the sphere radius to scale atom sizes by their individual site occupancies.

origin 'xcenter' 'ycenter' 'zcenter'

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

orthographic

causes the camera to be changed from the normal perspective view to an orthographic view for VRML and removes all perspective from POV diagrams.

pack '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 highly oblique cells, where the orthorhombic view box does not always give satisfactory results).

phaseshift 'value1' 'value2' 'value3'

defines the initial phases t_n of the n'th modulation wave in a modulated structure.

phong 'value' 'size' (used only for POV)

defines the amount of Phong highlighting on spheres and ellipsoids. The 'value' ranges between 0.0 and 1.0, where 0.0 gives no highlight, and 1.0 causes complete saturation at the center of the highlight. The 'size' ranges from 1.0 (very dull) to 250 (highly polished). The default quantities are 0.1 and 1.0, which gives a large, dull highlight. If 'value' is 0.0, the image can be rendered much more quickly.

plane 'name' 'length' 'color'

defines the center of a plane group, such as CO₃, that is to be drawn in a structure, where 'name' is the name of the atom at the center and 'length' is the maximum distance to coordinating anions.

polyedge 'name' 'radius' 'color'

defines the thickness and color of cylinders used to emphasize the faces along the edges of polyhedra for atom 'name'. The radius of these cylinders will also be scaled with the size of the drawing.

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. The polyhedra can be of any desired complexity - more than tetrahedra or octahedra can be drawn. For polyhedra with both upper and lower limits (which might be desirable for intermetallic compounds), use the 'shell' command.

polytolerance 'length'

polylimit 'length'

polyfudge 'length'

modifies the internal limit for the deviation of vertices from the common plane. While the default value (0.1) will always generate correct drawings, it may sometimes be desirable to increase it to create idealized views of nearly symmetrical polyhedra that would otherwise show creased surfaces.

polyvert 'name1' 'name2' 'length' 'color'

defines polyhedra in the manner of the 'polysz' command, except that the polyhedron around the 'name1' atom will only include atoms of type 'name2'.

qvector 'value1' 'value2' 'value3'

defines the components of the wave vector \mathbf{q} for a modulated structure.

rem, REM

Any line preceded by this command is ignored.

shell 'name' 'length1' 'length2' 'color'

defines a polyhedral shell, where name is the name of an atom at the center of a polyhedron and length1 and length2 are the minimum and maximum lengths of distances to atoms that are to be considered as the vertices of the polyhedron. The polyhedra can be of any desired complexity, and can be stacked as desired.

slab 'a' 'b' 'c' 'alpha' 'beta' 'gamma' 'xoff' 'yoff' 'zoff' 'xrot' 'yrot' 'zrot' 'flag'

defines a (possibly oblique) cutout box of the specified axis lengths and angles that is offset by xoff,yoff zoff from the origin of the structure and rotated at angles xrot yrot zrot relative to it. If flag is set to 1, any part of the structure outside the box is deleted. If flag is 2, the outline of the box is overlaid on the unchanged image to allow accurate placement of the cutout box.

spgp, sgrp, or spgr 'symbol'

Space Group name consisting of the Bravais lattice symbol (must be upper case) 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, unless the full symbol is used, i.e. P 1 1 21/n describes a monoclinic cell with *c* as the unique axis. N.B. Rhombohedral space groups must be represented in the hexagonal form.

sphere 'name' 'radius' 'color'

sphere 'name' 'number' '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 the color of the sphere to be drawn. If the first form is used, all atoms with 'name' will be drawn. The second restricts the command to atoms with the name and number.

title, titl 'descriptive material'

General description of the structure - this line may appear anywhere in the file, but is generally first.

uij, Uij 'name' 'number' 'u₁₁' 'u₂₂' 'u₃₃' 'u₁₂' 'u₁₃' 'u₂₃' 'color'

defines the anisotropic thermal coefficients for an atom and color of the ellipsoid. The 'name' and 'number' should correspond to the atom input described above. For this form, the temperature factor is given by $T = \exp\{-2\pi^2\beta_j\beta_k h_j h_k b_{jk} a_j^* a_k^*\}$, where a_j^* and a_k^* are reciprocal lattice constants.

values 'name' * 'radius'

values 'name' 'number' 'radius'

defines additional atomic properties for the given element or individual atom. Currently the only supported property is the van der Waals radius to be used in cavity calculations (see the voids keyword).

vectors

turns on the orientation vector triple at a corner of the diagram.

view 'xrot' 'yrot' 'zrot')

where 'xrot', 'yrot' and 'zrot' are view rotation angles in Cartesian space. These values correspond to a rotation of 'xrot' about the *x* axis, followed by a rotation of 'yrot' about the **new** *y* axis, and, a rotation of 'zrot' about the **new** *z* axis.

voids 'method' 'probe_radius' 'gridx' 'gridy' 'gridz' 'color'

causes cavities in the structure to be determined using the given method and probe radius (e.g.1.4 for a water molecule). 'gridx', 'gridy' and 'gridz' determine the resolution of the grid used for subdividing the unit cell. Currently supported methods are 1 for a slow but reliable, sequential test at all gridpoints, 2 for using the MSMS program of Sanner, and 3 for a pseudorandom sampling of points. Methods 2 and 3 should be considered experimental.

vrml1 (used only for VRML)

causes the output VRML file to have the older, VRML1 syntax for compatibility with some older viewers that are not VRML97 compliant.

vrm12 or **vrm197** (used only for VRML)

These commands do nothing, but are kept for compatibility with old data files. VRML97 format is now the default. A description of some of the VRML97 features is given in Appendix B. Do NOT use this form unless your VRML viewer is VMRL97 compliant!

x3d (used only for VRML)

This command causes the output VRML file to have X3D 'Classic VRML' encoding and .x3dv extension.

xyzoff 'u1' 'u2' 'u3'

causes all atom coordinates to be shifted by **-u**. This command is used whenever the origin defined for a structure does not conform to the standard origin selected by the space-group generator.

end, END

is the last line of a file that is processed. Any information past this point will be ignored.

Appendix A: On-line sources for information and software.

- POV - Source code for the Persistence of Vision Ray Tracer (POV-Ray) software, user documentation and precompiled executables for several platforms are available through <http://www.povray.org>. Code is also available through <ftp.povray.org>, and a number of mirror sites listed on the web site. At the time of this writing, both version 3.6 of POV and a fully functional release candidate for 3.7.0 are available.
- VRML - Documentation and viewers for the Virtual Reality Modeling Language are available through <http://www.web3d.org>. These files are particularly suitable for viewing across the Internet, therefore, many of the viewers are in the form of plug-ins for popular web browsers. In addition, stand-alone viewers are available. The files produced by DRAWxtl adhere to the VRML V1.0 format, or the VRML97 (2.0) format. For browser plug-ins, we recommend the free product available at <http://www.parallelgraphics.com/products/cortona/>. It supports Internet Explorer, Netscape, Mozilla, and FireFox browsers. Another promising cross-platform viewer is view3dscene, available at <http://vrmlengine.sourceforge.net/view3dscene.php>.
- ASYMPTOTE, a powerful vector graphics framework for technical illustrations, is available at <http://asymptote.sourceforge.net>. Besides high-quality 2D images in a number of file formats it can also create PDF files with embedded, interactive 3D content.
- Source code, OS X and Windows executables for 'DRAWxtl' are available at: <http://www.lwfinger.net/drawxtl/>. Linux users may want to check the package repositories of their favorite distribution for rpm or deb packages – at the time of this writing, we are aware of at least Debian/Ubuntu and RedHat packages being available.

Appendix B: Adding life to VRML files

One of the major differences between VRML-1 and VRML97 (VRML-2) is the availability of functions that can be used to create dynamic effects such as motion and color changes. While their purpose is more obvious in macroscopic environments like rooms and buildings, these can also be a useful addition to the crystal structures generated with DRAWxtl, especially in an educational context.

As there does not appear to be a universally applicable set of functions, they are not automatically included in the files generated by DRAWxtl. This section provides only a short overview of the features we have found useful in our work.

A detailed description can be found in the VRML97 standard document (<http://www.web3d.org/x3d/specifications/vrml/ISO-IEC-14772-VRML97>) and in monographs like Carey & Bells 'The Annotated VRML 2.0 Reference Manual', which is also available online at <http://www.aw.com/devpress/titles/41974.html>.

1. Naming objects

Dynamic effects can be added to a static scene by adding a unique name to one of the positional or material declarations (Transform or Material nodes). Its subfields like translation, rotation or color can then be set by a function that is driven by an internal timer, the viewer clicking on an object, or a combination of both.

Thus, a fragment like

```
Transform {  
  translation -0.87100 -1.50862 -2.88  
  Shape {  
    geometry Sphere {radius .5}  
  }  
}
```

Which would place an atom of diameter 0.5 at -0.871 -1.50862 -2.88, could be turned into

```
DEF movingSphere Transform {
  Shape {
    geometry Sphere {radius .5}
  }
}
```

where some function would generate translations as desired.

2. Using the internal timer

All standard-conforming VRML97 browsers are expected to provide an internal clock called a TimeSensor. Its output - wallclock time in seconds - can be used as a trigger, and the fractional seconds form a sawtooth-like signal in the range from 0 to 1 that can drive periodic events.

This takes the form:

```
DEF Wallclock TimeSensor {
  loop TRUE
  stopTime -1
  cycleInterval 10
}
```

(where the speed can be regulated via the cycleInterval value). To continue our example, we could now use the output of this function to move our sphere. However, its 'heartbeat', the fractionChanged signal, is always between 0 and 1, so we need an auxiliary function to turn this into realistic coordinates.

3. Generating new coordinates or color codes

VRML97 provides a series of 'Interpolator' functions to turn a periodic signal into a smooth succession of coordinate or color values.

These take the form:

```
DEF Parabola PositionInterpolator {
  key [ 0 .25 .5 .75 1 ]
  keyValue [ -0.87100 -1.50862 -2.88,
    -0.87100 0.50862 -2.88,
    -0.87100 1.50862 -2.88,
    -0.87100 0.50862 -2.88,
    -0.87100 -1.50862 -2.88]
}
```

where the 'keyValues' provided for the set of 'keys' are used to compute the function that links input and output. The example above would make our atom oscillate along the y axis around its initial position.

Similar functions exist for rotations:

```
DEF turnZ OrientationInterpolator {
  key [ 0 .333 .666 1 ]
  keyValue [ 0 0 1 0,
    0 0 1 2.09,
    0 0 1 4.18,
    0 0 1 0.]
}
```

And for colors:

```
DEF atomcolor ColorInterpolator {
  key [ 0 .1 .2 .3 .4 .5 .6 .7 .8 .9 1. ]
  keyValue [1. 0.6 0.,
    1. 0.65 0.,
    1. 0.7 0.,
    1. 0.8 0.,
```

```

1. 0.9 0.,
1. 1. 0.
1. 0.9 0.,
1. 0.8 0.,
1. 0.7 0.,
1. 0.65 0.,
1. 0.6 0. ]
}

```

(which would make our atom turn orange, yellow, and orange again (which may even be useful if it belongs to different coordination polyhedra or unit cells at various stages of its movement)).

4. Connecting effects and objects

The values that are produced by Sensor or Interpolator functions have to be sent to the desired objects (or other functions) via specific routes. In our example, we must feed the output of our TimeSensor to our OrientationInterpolator, and the new coordinates that it generates must be routed to the Transform node around our atom.

Thus,

```
ROUTE Wallclock.fraction_changed TO Parabola.set_fraction
ROUTE Parabola.value_changed TO movingSphere.set_translation
```

And

```
ROUTE Wallclock.fraction_changed TO turnZ.set_fraction
ROUTE turnZ.value_changed TO movingSphere.set_rotation
```

Or

```
ROUTE Wallclock.fraction_changed TO atomcolor.set_fraction
ROUTE atomcolor.value_changed TO spherematerial.set_color
```

(for the other examples) is needed to put our atom in motion.

5. More general functions

Further (and more complex) dependencies between events and actions can be defined via small functions or programs written in JavaScript.

If, for instance, we wanted to turn the wallclock time itself into a signal that fits our purpose better than the sawtooth-like 'fraction_changed', we could pass it through this function:

```

DEF mytimer Script {
  eventIn SFloat division
  eventOut SFloat output
  url "vrmlscript:
  function division (input) {
    output = input / 3 - Math.floor (input/3);
  }
  "
}

```

and then

```

ROUTE Wallclock.time TO mytimer.division
ROUTE mytimer.output TO Parabola.set_fraction
ROUTE Parabola.value_changed TO movingSphere.set_translation

```

to move our atom.

6. Switching between alternate representations

It is sometimes useful to depict a structure in different representations, for instance as an ORTEP-style drawing of the individual atoms and reduced to the coordination polyhedra around the cation or the anion. With VRML97, these can be combined in a single file, where clicking on any part of the structure switches to another representation.

To achieve this, the different parts form the choices of a 'Switch' statement that is coupled to a TouchSensor:

```
DEF selectOne Switch {
  choice [
    View1{}
    View2{}
    View3{}
  ]
  whichChoice 0
}
DEF ClickMe TouchSensor{}
```

(where the different Views are either complete definitions or references to prototypes as explained below). The TouchSensor envelopes the object that is contained in the same Transform node (which is the complete structure in this case), it is triggered whenever the viewer moves the pointer over it and presses a button. Normally, only the first view (choice 0 of the switch) is visible.

If the output of the TouchSensor is connected to a Script that changes the choice counter:

```
DEF Trigger Script {
  eventIn SFBool doit
  eventOut SFInt32 set_hide
  url "javascript:
function doit(touched) {
  if (touched) {
    set_hide = set_hide +1 ;
    if (set_hide > 2) set_hide = 0;
  }
}
"
}

ROUTE Trigger.set_hide TO selectOne.set_whichChoice
ROUTE ClickMe.isActive TO Trigger.doit
```

the representation can be switched at any time by a simple mouse click, while the orientation is preserved.

7. Animating larger frameworks

Many dynamic effects can be used in the same scene file. Note, however, that the destinations of a ROUTE must have unique names and there must be individual ROUTEs leading from the transforming function to them. So, if you want several moving spheres in the example above, you must name them

```
DEF movingSphere1 {...}
DEF movingSphere2 {...}
```

and route the new coordinates with

```
ROUTE Parabola.value_changed TO movingSphere1.set_translation
ROUTE Parabola.value_changed TO movingSphere2.set_translation
```

If you want to modify groups of objects (several atoms or polyhedra) in the same way, it is probably best to add a Transform node that encompasses all of them, and then modify its properties. If you want to animate larger entities (polyhedral building blocks or layers) within a crystal structure, it may be

easier to have DRAWxtl generate the desired portions separately and then copy them into the final file than to identify and group them in the output of a single DRAWxtl run. To improve readability, you can also group these sections as PROTOtypes that can be referenced through their names. Thus, a combination of a ball-and-stick model and a polyhedral component could be grouped as:

```
PROTO BallAndStick [] {
  Transform {
  children [
  ... lots of Spheres and Cylinders here ...
  ]
  }
}
PROTO Polyhedra[] {
  Transform {
  children [
  ... lots of IndexedFaceSets ...
  ]
  ]
}
```

and finally called as:

```
BallAndStick{}
Polyhedra{}
```

which is especially attractive if this is part of a Switch node (as described above) or a layered structure where the layers are animated to visualize phase transitions.

File 'vrm12.wrl' in the distribution set demonstrates a self-rotating fragment of the faujasite structure.

Table I. Color Names and Associated RGB Values.

<u>Color Name</u>	<u>R</u>	<u>G</u>	<u>B</u>	<u>Color Name</u>	<u>R</u>	<u>G</u>	<u>B</u>
Aquamarine	0.439216	0.858824	0.576471	IndianRed	0.309804	0.184314	0.184314
BakersChoc	0.36	0.2	0.09	Khaki	0.623529	0.623529	0.372549
Black	0	0	0	LightBlue	0.74902	0.847059	0.847059
Blue	0	0	1	LightGray	0.658824	0.658824	0.658824
BlueViolet	0.62352	0.372549	0.623529	LightGrey	0.658824	0.658824	0.658824
Brass	0.71	0.65	0.26	LightSteelBlue	0.560784	0.560784	0.737255
BrightGold	0.85	0.85	0.1	LightWood	0.91	0.76	0.65
Bronze	0.55	0.47	0.14	LimeGreen	0.196078	0.8	0.196078
Bronze2	0.65	0.49	0.24	Magenta	1	0	1
Brown	0.647059	0.164706	0.164706	MandarinOrange	0.89	0.47	0.2
CadetBlue	0.372549	0.623529	0.623529	Maroon	0.556863	0.137255	0.419608
Clear	1	1	1	MediumAquamarine	0.196078	0.8	0.6
CoolCopper	0.85	0.53	0.1	MediumBlue	0.196078	0.196078	0.8
Copper	0.72	0.45	0.2	MediumForestGreen	0.419608	0.556863	0.137255
Coral	1	0.498039	0	MediumGoldenrod	0.917647	0.917647	0.678431
CornflowerBlue	0.258824	0.258824	0.435294	MediumOrchid	0.576471	0.439216	0.858824
Cyan	0	1	1	MediumSeaGreen	0.258824	0.435294	0.258824
DarkBrown	0.36	0.25	0.2	MediumSlateBlue	0.498039	1	
DarkGreen	0.184314	0.309804	0.184314	MediumSpringGreen	0.498039	1	
DarkOliveGreen	0.309804	0.309804	0.184314	MediumTurquoise	0.439216	0.858824	0.858824
DarkOrchid	0.6	0.196078	0.8	MediumVioletRed	0.858824	0.439216	0.576471
DarkPurple	0.53	0.12	0.47	MediumWood	0.65	0.5	0.39
DarkSlateBlue	0.419608	0.137255	0.556863	Mica	0	0	0
DarkSlateGray	0.184314	0.309804	0.309804	MidnightBlue	0.184314	0.184314	0.309804
DarkSlateGrey	0.184314	0.309804	0.309804	Navy	0.137255	0.137255	0.556863

DarkTan	0.59	0.41	0.31	NavyBlue	0.137255	0.137255	0.556863
DarkTurquoise	0.439216	0.576471	0.858824	NeonBlue	0.3	0.3	1
DarkWood	0.52	0.37	0.26	NeonPink	1	0.43	0.78
DimGray	0.329412	0.329412	0.329412	NewMidnightBlue	0	0	0.61
DimGrey	0.329412	0.329412	0.329412	NewTan	0.92	0.78	0.62
DkGreenCopper	0.29	0.46	0.43	OldGold	0.81	0.71	0.23
DustyRose	0.52	0.39	0.39	Orange	1	0.5	0
Feldspar	0.82	0.57	0.46	OrangeRed	1	0.498039	0
Firebrick	0.556863	0.137255	0.137255	Orchid	0.858824	0.439216	0.858824
Flesh	0.96	0.8	0.69	PaleGreen	0.560784	0.737255	0.560784
ForestGreen	0.137255	0.556863	0.137255	Pink	0.737255	0.560784	0.560784
Gold	0.8	0.498039	0.196078	Plum	0.917647	0.678431	0.917647
Goldenrod	0.858824	0.858824	0.439216	Quartz	0.85	0.85	0.95
Gray	0.752941	0.752941	0.752941	Red	1	0	0
Gray05	0.05	0.05	0.05	RichBlue	0.35	0.35	0.67
Gray10	0.1	0.1	0.1	Salmon	0.435294	0.258824	0.258824
Gray15	0.15	0.15	0.15	Scarlet	0.55	0.09	0.09
Gray20	0.2	0.2	0.2	SeaGreen	0.137255	0.556863	0.419608
Gray25	0.25	0.25	0.25	SemiSweetChoc	0.42	0.26	0.15
Gray30	0.3	0.3	0.3	Sienna	0.556863	0.419608	0.137255
Gray35	0.35	0.35	0.35	Silver	0.9	0.91	0.98
Gray40	0.4	0.4	0.4	SkyBlue	0.196078	0.6	0.8
Gray45	0.45	0.45	0.45	SlateBlue	0	0.498039	1
Gray50	0.5	0.5	0.5	SpicyPink	1	0.11	0.68
Gray55	0.55	0.55	0.55	SpringGreen	0	1	0.498039
Gray60	0.6	0.6	0.6	SteelBlue	0.137255	0.419608	0.556863
Gray65	0.65	0.65	0.65	SummerSky	0.22	0.69	0.87

Gray70	0.7	0.7	0.7	Tan	0.858824	0.576471	0.439216
Gray75	0.75	0.75	0.75	Thistle	0.847059	0.74902	0.847059
Gray80	0.8	0.8	0.8	Turquoise	0.678431	0.917647	0.917647
Gray85	0.85	0.85	0.85	VeryDarkBrown	0.35	0.16	0.14
Gray90	0.9	0.9	0.9	Violet	0.309804	0.184314	0.309804
Gray95	0.95	0.95	0.95	VioletRed	0.8	0.196078	0.6
Green	0	1	0	VLightGrey	0.8	0.8	0.8
GreenCopper	0.32	0.49	0.46	Wheat	0.847059	0.847059	0.74902
GreenYellow	0.576471	0.858824	0.439216	White	1	1	1
Grey	0.752941	0.752941	0.752941	Yellow	1	1	0
<u>HuntersGreen</u>	0.13	0.37	0.31	<u>YellowGreen</u>	0.6	0.8	0.196078

Table II. Color Names Sorted by RGB Values.

<u>Color Name</u>	<u>R</u>	<u>G</u>	<u>B</u>	<u>Color Name</u>	<u>R</u>	<u>G</u>	<u>B</u>
Black	0	0	0	Firebrick	0.556863	0.137255	0.137255
Mica	0	0	0	Maroon	0.556863	0.137255	0.419608
NewMidnightBlue	0	0	0.61	Sienna	0.556863	0.419608	0.137255
Blue	0	0	1	LightSteelBlue	0.560784	0.560784	0.737255
SlateBlue	0	0.498039	1	PaleGreen	0.560784	0.737255	0.560784
Green	0	1	0	MediumOrchid	0.576471	0.439216	0.858824
SpringGreen	0	1	0.498039	GreenYellow	0.576471	0.858824	0.439216
Cyan	0	1	1	DarkTan	0.59	0.41	0.31
Gray05	0.05	0.05	0.05	DarkOrchid	0.6	0.196078	0.8
Gray10	0.1	0.1	0.1	Gray60	0.6	0.6	0.6
HuntersGreen	0.13	0.37	0.31	YellowGreen	0.6	0.8	0.196078
Navy	0.137255	0.137255	0.556863	BlueViolet	0.62352	0.372549	0.623529
NavyBlue	0.137255	0.137255	0.556863	Khaki	0.623529	0.623529	0.372549
SteelBlue	0.137255	0.419608	0.556863	Brown	0.647059	0.164706	0.164706
ForestGreen	0.137255	0.556863	0.137255	Bronze2	0.65	0.49	0.24
SeaGreen	0.137255	0.556863	0.419608	MediumWood	0.65	0.5	0.39
Gray15	0.15	0.15	0.15	Gray65	0.65	0.65	0.65
MidnightBlue	0.184314	0.184314	0.309804	LightGray	0.658824	0.658824	0.658824
DarkGreen	0.184314	0.309804	0.184314	LightGrey	0.658824	0.658824	0.658824
DarkSlateGray	0.184314	0.309804	0.309804	Turquoise	0.678431	0.917647	0.917647
DarkSlateGrey	0.184314	0.309804	0.309804	Gray70	0.7	0.7	0.7
MediumBlue	0.196078	0.196078	0.8	Brass	0.71	0.65	0.26
SkyBlue	0.196078	0.6	0.8	Copper	0.72	0.45	0.2
LimeGreen	0.196078	0.8	0.196078	Pink	0.737255	0.560784	0.560784
MediumAquamarine	0.196078	0.8	0.6	LightBlue	0.74902	0.847059	0.847059

Gray20	0.2	0.2	0.2	Gray75	0.75	0.75	0.75
SummerSky	0.22	0.69	0.87	Gray	0.752941	0.752941	0.752941
Gray25	0.25	0.25	0.25	Grey	0.752941	0.752941	0.752941
CornflowerBlue	0.258824	0.258824	0.435294	VioletRed	0.8	0.196078	0.6
MediumSeaGreen	0.258824	0.435294	0.258824	Gold	0.8	0.498039	0.196078
DkGreenCopper	0.29	0.46	0.43	Gray80	0.8	0.8	0.8
Gray30	0.3	0.3	0.3	VLightGrey	0.8	0.8	0.8
NeonBlue	0.3	0.3	1	OldGold	0.81	0.71	0.23
IndianRed	0.309804	0.184314	0.184314	Feldspar	0.82	0.57	0.46
Violet	0.309804	0.184314	0.309804	Thistle	0.847059	0.74902	0.847059
DarkOliveGreen	0.309804	0.309804	0.184314	Wheat	0.847059	0.847059	0.74902
GreenCopper	0.32	0.49	0.46	CoolCopper	0.85	0.53	0.1
DimGray	0.329412	0.329412	0.329412	BrightGold	0.85	0.85	0.1
DimGrey	0.329412	0.329412	0.329412	Gray85	0.85	0.85	0.85
VeryDarkBrown	0.35	0.16	0.14	Quartz	0.85	0.85	0.95
Gray35	0.35	0.35	0.35	MediumVioletRed	0.858824	0.439216	0.576471
RichBlue	0.35	0.35	0.67	Orchid	0.858824	0.439216	0.858824
BakersChoc	0.36	0.2	0.09	Tan	0.858824	0.576471	0.439216
DarkBrown	0.36	0.25	0.2	Goldenrod	0.858824	0.858824	0.439216
CadetBlue	0.372549	0.623529	0.623529	MandarinOrange	0.89	0.47	0.2
Gray40	0.4	0.4	0.4	Gray90	0.9	0.9	0.9
DarkSlateBlue	0.419608	0.137255	0.556863	Silver	0.9	0.91	0.98
MediumForestGreen	0.419608	0.556863	0.137255	LightWood	0.91	0.76	0.65
SemiSweetChoc	0.42	0.26	0.15	Plum	0.917647	0.678431	0.917647
Salmon	0.435294	0.258824	0.258824	MediumGoldenrod	0.917647	0.917647	0.678431
DarkTurquoise	0.439216	0.576471	0.858824	NewTan	0.92	0.78	0.62
Aquamarine	0.439216	0.858824	0.576471	Gray95	0.95	0.95	0.95

MediumTurquoise	0.439216	0.858824	0.858824	Flesh	0.96	0.8	0.69
Gray45	0.45	0.45	0.45	Red	1	0	0
MediumSlateBlue	0.498039	1		Magenta	1	0	1
MediumSpringGreen	0.498039	1		SpicyPink	1	0.11	0.68
Gray50	0.5	0.5	0.5	NeonPink	1	0.43	0.78
DarkWood	0.52	0.37	0.26	Coral	1	0.498039	0
DustyRose	0.52	0.39	0.39	OrangeRed	1	0.498039	0
DarkPurple	0.53	0.12	0.47	Orange	1	0.5	0
Scarlet	0.55	0.09	0.09	Yellow	1	1	0
Bronze	0.55	0.47	0.14	Clear	1	1	1
<u>Gray55</u>	0.55	0.55	0.55	<u>White</u>	1	1	1