

## Chapter 8.4

# **STRUPLO for Windows**

based on STRUVIR

(STRUPLO-91 to VRML)

beta-3 version September, 1996

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<b>1.1 HISTORY OF THIS VERSION.....</b>	<b>3</b>
<b>1.2 INTRODUCTION.....</b>	<b>3</b>
<b>1.3 OUTPUT FILES .....</b>	<b>3</b>
<b>1.4 COLOURS.....</b>	<b>4</b>
<b>1.5 POTENTIAL PROBLEMS.....</b>	<b>5</b>
1.51 CORRECTED BUGS : .....	5
1.52 WORK-AROUND ADVICE FOR SOME CURRENT BUGS : .....	6
<b>1.6 DETAILED INPUT DESCRIPTION.....</b>	<b>6</b>
1.61 - STRUPLO INSTRUCTIONS. ....	7
1.62 ATOM PARAMETERS.....	11
<b>1.7 APPENDIX.....</b>	<b>11</b>

## 1.1 History of this version

**STRUPLO for Windows** is an MS-Windows implementation of STRUVIR, with a GUI to enable much simpler input. The program will directly read a variety of crystallographic input files including SHELX, GX, CIF, LHPM, XYZ etc. It is based on the code supplied by A. Le Bail for STRUVIR (Beta-3 Release). The GUI basically creates STRUVIR input files, which are then drawn on the screen and may be optionally saved in a variety of formats.

An on-line tutorial for STRUVIR is at :

**<http://fluo.univ-lemans.fr:8001/vrml/struvir/tutorial/tutorial.html>**

STRUPLO is the R.X. Fischer free structure drawing program recognizing tetrahedra and octahedra [R.X. Fischer (1985) *J. Appl. Cryst.* **18**, 258-262]. Augmented by A. Le Lirzin, 1989 (COLO, PRES, BZRR) for the recognition of other polyhedra and by D. Kassner, 1990 (RES, NRES in PARA, incorporation of Burzlaff routine in SPGR, logic of VIEW and ROTA, addressing in SHAD, reorganization of COMMON-block structure).

- Received at MSU August 1992, via Tim McCarthy from Giaquinta at MIT.
- writeup by Donald L. Ward from the original by W. H. Baur.
- Received at Laboratoire des Fluorures March 1996, via D.L. Ward by A. Le Bail
- HPGL and VRML capabilities added.
- Version enhanced with output for POV-Ray by Mark Koennecke, July, 1996 (see his comments in the Appendix).

## 1.2 Introduction

STRUVIR is a converter of STRUPLO (R.X. Fischer) data files into VRML (Virtual Reality Modeling Language) .WRL files for 3D visualization. (Netscape+Live3D or VRweb, or any Internet browser equipped with a VRML plug-in, or any standalone VRML viewer enabling two-sided lighting of faces).

IMPORTANT: old datafiles for STRUPLO-91 ALSO work for STRUVIR too, there has been no change in input format. All the previous STRUPLO capabilities for preparing output files for structural drawings are available for HPGL and POSTSCRIPT. An output for POV-Ray (thanks to Mark Koennecke) differentiates this beta-3 version from beta-2.

STRUVIR is built from a STRUPLO basis modified without permission and following the academic tradition which allows for not reinventing the wheel each day. In this case, the wheels are the STRUPLO polyhedra recognition algorithm, thanks to R.X. Fischer and A. Le Lirzin, and VRML of course. The name derives from STRU for STRUCTURE in STRUPLO and VIR for VIRTUAL in VRML. The VRML part is working better than the PS/HPGL drawing part in most cases.

A number of STRUVIR data files are supplied with the release of **STRUPLO for Windows**. These have the .SPL extension. It is important to note that when reading a STRUVIR file, the facilities of the GUI are by-passed, since the file is directly interpreted by STRUVIR.

## 1.3 Output files

There are two directories which **STRUPLO for Windows** uses, the *working directory* where the structural data files are stored and the *home directory* where the executable and system files are stored.

In the *home directory* **STRUPLO for Windows** will create two files which are always overwritten. These are generally of not much interest, but may be useful for diagnostic purposes.

1. **STRUPLOT.INS** This is the STRUVIR instruction file written by the GUI and interpreted by the STRUVIR code. A copy of this can be made by the menu item Save STRUPLO File.
2. **STRUPLOT.LST** This is an ASCII file containing some useful information like distances and angles. It may be necessary to open this file in order to verify if distances chosen for finding polyhedra are appropriate.

In the *working directory* the following graphics or scene-description files may be created, depending on the user requests. A new file with xxx running from 001 to 999 will be created and old files will not be overwritten.

1. **POLYxxx.WRL** The VRML file for polyhedra 3D view. Polyhedra having 3 to 12 vertices are recognised. Spheres may be obtained by the STRUVIR CIRC option. They are all drawn with a 0.5 Å radius.
2. **WIRExxx.WRL** The VRML file for wireframe 3D view.
3. **STRUPxxx.HPG** A 2D HPGL drawing that you may visualise with a HPGL viewer or insert into MS WORD 2 or 6 using the convenient image format (HPGL). From MS WORD, you may also export the drawing to the clipboard and get it with Paintbrush as a .bmp file, export to Lview31 and change to a .gif or a .jpg.... etc..
4. **STRUPxxx.PS** The PostScript file
5. **STRUPxxx.POV** The scene-description file for POV-Ray.

## 1.4 Colours

You may operate with colors at two independent levels, for the HPGL/PS outputs and for the VRML/POV-Ray outputs.

VRML/POV-Ray: Twenty colors are available. The choice is made by playing on the atom name order. The following example has 3 different kind of atoms CO (Co), S and O. They will be attributed colors number 1, 2 and 3 respectively. If polyhedra (octa or tetra) are recognized around CO, they will be drawn with color attributed to CO (not the color attributed to O). Changing colors is possible by changing the atoms order. This order can of course be modified by manual editing of the VRML/POV-Ray files.

```
TITL COSO4 H2O C2/C
CELL 6.963 7.580 7.470 90.116.30 90.
SPGR C 2/C
FORM 4
VIEW 0 1 0
XYZR -0.25 2.25 -0.25 2.25 -0.25 2.25
OCTA 90 20 2.05 0.25
TETR 109. 20. 1.5 0.2
PARA 1 1 1 1 1 1 1 2.6
END
CO 1      0.25      0.25      0.0          Color 1
S  1      0.0       0.093     0.25       Color 2
O  1      0.203    -0.017    0.362     Color 3
O  2      0.021    0.196    0.104     Color 3
O  3      0.0       0.615    0.25       Color 3
```

For instance if you want SO<sub>4</sub> tetrahedra drawn with color 4 and CoO<sub>6</sub> octahedra with color 5, this is possible by :

OA 1	0.203	-.017	0.362	Color 1
OB 2	0.021	0.196	0.104	Color 2
OC 3	0.0	0.615	0.25	Color 3
S 1	0.0	0.093	0.25	Color 4
CO 1	0.25	0.25	0.0	Color 5

Compare the results from files CSO4H.SPL and CSO4H2.SPL. It will be difficult, but not impossible to play with more than 5 colors with this example.

And the 20 colors (no more allowed !) are :

	R	G	B
1 Blue sky	0.0	1.0	1.0
2 Green light	0.5	1.5	0.0
3 Red pyrope	1.0	0.1	0.5
4 Yellow	1.0	1.0	0.0
5 Blue grey	0.6	0.6	1.0
6 Orange	1.0	0.6	0.0
7 Purple	0.5	0.0	0.5
8 Brown	0.5	0.3	0.0
9 Blue-green-dark	0.0	0.5	0.5
10 Red	1.0	0.0	0.0
11 Green	0.0	1.0	0.0
12 Blue	0.0	0.0	1.0
13 Pink	1.0	0.0	1.0
14 Red dark	0.5	0.0	0.0
15 Green dark	0.0	0.5	0.0
16 Blue night	0.0	0.0	0.5
17 Red wine	0.5	0.05	0.25
18 White	1.0	1.0	1.0
19 Grey	0.5	0.5	0.5
20 Black	0.	0.0	0.0

Colors for HPGL and PS output are those defined in the STRUPLO instructions below.

## 1.5 Potential problems

The .SPL data files delivered with the release of **STRUPLO for Windows** have been tested and visualized successfully with the VRweb and Live3D viewers. This is insufficient to claim a complete absence of bugs. Particularly, the coherency of shading according to light sources has not been checked : the drawing is sometimes 'bizarre' as stated by some pre-beta testers. Viewers like Cosmo Player from SGI and the Microsoft VRML Add-in will not give good results, essentially because the STRUVIR VRML output is not well optimized. Only those viewers enabling two-sided face lighting in VRML 1 should be used. You may also find that 'flat shading' renders better the VRML STRUVIR files than 'smooth shading'.

There are inbuilt limits to the size of structures which STRUVIR can handle : 1000 polyhedra, 6000 atoms, 20 colors, 150 atoms around one atom in distance calculation. Exceeding these limits may lead to a crash in some cases although the program should stop by itself with an explanation for the user.

### 1.51 Corrected bugs :

March, 01 1996 : it was previously not possible to obtain more spheres than atoms involved in polyhedra.

March, 27 1996 : Live3D under Windows 95 loaded the .WRL files then Netscape 2.0 crashed. This did not happen under Windows 3.11. Apparently a ",-1" was lacking somewhere.

July, 11 1996 : A. J. Holland during his work for including executables of STRUVIR for various platforms in the CCP14 suite found that some data files caused a crash on DEC ULTRIX, ALPHAVMS and VAX-VMS only. The 2002 FORMAT in the subroutine WRITE sometimes produced lines exceeding 132 characters.

July, 26 1996 : added one line in the documentation. ALL CHARACTERS IN UPPERCASE

### 1.52 Work-around advice for some current bugs :

1. With the option CIRC, use small sizes like CIRC 0.03 CS instead of CIRC 0.30 CS (the .HPG file will give the caesium atoms as points but the .WRL files will be OK) otherwise nothing may work because STRUPLO apparently has problems with superimposed circles.
2. Sometimes polyhedra may appear incomplete when the range selected by the XYZR option is small. There is a simple way to deal with this bug in VRML. The .WRL ASCII files may be edited and the incomplete polyhedron may be easily recognized and deleted. Data concerning each polyhedron in POLYxxx.WRL begin with a comment line like the following :

```
# POLYHEDRON 46 YB
Material{diffuseColor .000 1.000 1.000
  specularColor 0.5 0.5 0.5
  shininess 0.2 }
Coordinate3{point[
  -.101 5.419 2.710,
  1.762 4.065 4.133,
  .....etc
  2, 6,-1,
  1, 7,-1,
  4, 7,-1 ]}
# POLYHEDRON 228 YB
Material{diffuseColor .000 1.000 1.000
.....etc
# POLYHEDRON 39 YB
.....etc
```

So you have just to delete the undesired polyhedron. Numbers 46, 228, 39 etc are those easily found in the atom list in the output file STRUPLOT.LST

### 1.6 Detailed input description

The input of all data is in free format. numbers or symbols are separated by blanks, typed in any arbitrary column between columns 5 and 80. The first four columns of the instruction data are reserved for options specifying the type of instruction. Any text in the first four columns, other than the options listed here, will be ignored. Numbers can be given as integer, floating point, or floating comma numbers; all three types will be transformed to floating point numbers. Atom parameters may be given in free format or fixed format as described below.

All characters MUST be in uppercase (*e.g* TITL, CELL, SPGR, SYMM, PARA *etc*) including atom names (*e.g* H, LI, BE, AL, CO not h, Li, Be, Al, Co) and spacegroups (*e.g* P M M M, C 2/C, F D 3 M *etc*)

A typical example input file is:

```
TITL COSO4 H2O C2/C
CELL 6.963 7.580 7.470 90. 116.30 90.
SPGR C 2/C
```

```

FORM 4
VIEW 0 1 0
XYZR -0.25 2.25 -0.25 2.25 -0.25 2.25
OCTA 90 20 2.05 0.25
TETR 109. 20. 1.5 0.2
PARA 1 1 1 1 1 1 1 2.6
END
CO 1          0.25      0.25      0.0
S 1           0.0       0.093     0.25
O 1           0.203     -.017     0.362
O 2           0.021     0.196     0.104
O 3           0.0       0.615     0.25

```

### 1.61 - STRUPLO Instructions.

The sequence of instructions is arbitrary except that TITL and END must be the first and last options, respectively, followed by the atom parameters.

#### **TITL** *text*

Default: TITL (blank)

Up to 40 characters can be plotted as a heading. TITL must be the first option, even if the text is left blank. Subsequent lines, starting with TITL, are without action and can be used as comments.

#### **MODI** *D PA1 PA2 AR1 AR2 OR1 OR2*

Default: MODI 1 0 0 28.8 21.6 0 0

D - selects the plotting device. D is not used in the STRUPLO version of June 86. This can be modified by the user in subroutine DRAW where D has the variable name ID.

PA1 PA2 - are length and width of the paper; these parameters are only needed for the PAGE call in the DISSPLA software.

AR1 AR2 - are length and width defining the plotting area. The plot will be scaled with regard to these parameters.

OR1 OR2 - are coordinates in cm (or inches) to translate the plot. This usually will cut off the plot, but might be desired in special cases. In most cases this option can be omitted; default values can be changed in BLOCK DATA if necessary. Only if the plot output will be sent to different devices (plotter, laser printer, etc.) will parameter D need to be given.

NOTE - In almost all cases with *STRUPLO for Windows* this command will not be required.

#### **PARA** *A B C D E F G H I J*

Default: PARA 1 1 1 1 1 1 1 3.2 0 0.01

Specification of plot parameters

A - Scale factor. The plot is scaled to the full width of the paper, leaving a margin for the heading. The width of the paper is defined in AR1 and AR2 in BLOCK DATA, or as specified with option MODI. Scale factors > 1 will cut off the drawing, but might be desired in special cases.

B - Index for center in origin. 0 = no center in the origin, 1 = centrosymmetric with center in the origin

C - Index for outlines of unit cell. 0 = no outlines, 1 = outlines are drawn. The present version of the program does not check overlaps in the outlines with polyhedra or spheres. It might be necessary to draw the outlines of the parallelepiped by hand if the view direction is not parallel to one of the crystallographic unit vectors.

D - Index for type of representation.

0 = skeleton model. This representation, often used for framework structures, shows only the connections between the centers of neighboring polyhedra.

1 = polyhedral representation. Tetrahedra and octahedra are sought by the program within the limits given in options TETR and OCTA. All polyhedra are hatched with equidistant lines parallel to that edge of the triangle which is opposite the vertex with the highest Z-coordinate. In this way the density of hatching illustrates the inclination of a polyhedral face.

E - Index for tetrahedra. 0 = no tetrahedra, 1 = tetrahedra are sought and drawn within the values given in option TETR. The default values correspond to average Si-O distances.

F - Index for octahedra. 0 = no octahedra. 1 = octahedra are sought and drawn within the values given in option OCTA. The default values correspond to average (Na,Ca)-O distances. If lines are drawn belonging neither to tetrahedra nor octahedra, the default parameters have to be changed in option TETR or OCTA.

G - Index for program execution. 0 = only tables with atomic coordinates and distances and angles are printed, no plot is produced. 1 = tables with atomic coordinates and distances and angles are printed and a projection of the crystal structure is drawn.

H - Maximum value for interatomic distances to be calculated. If more than 100 distances up to the value H are calculated, the execution of the program will be terminated. In this case the maximum distance should be given a lower value.

I - Retrace parameter NRES. Outlines of polyhedra and circles are plotted  $2 \cdot \text{NRES} + 1$  times with a distance given by RES (see J).

J - Retrace displacement RES. This value is multiplied by the scale factor.

#### **CELL** *a b c alpha beta gamma*

Default: CELL 10 10 10 90 90 90

The cell constants are expected in Angstroms and degrees.

#### **SPGR** *space group symbol*

Default: SPGR P1-

This is interpreted by Burzlaff's (Erlangen) symmetry interpretation routine. The centricity parameter B of PARA is overridden. The generated symmetry operations and Bravais translations can be found in the output file. WARNING: Any SYMM input, that is input after this, is added to the generated symmetry operations.

#### **SYMM** *symmetry operators*

Default: SYMM X,Y,Z

To be used only if the choice of origin is different from the one generated by the Burzlaff routine. Each line beginning with SYMM contains several operators separated from each other by a semicolon. The last symbol in a line must not be a semicolon. Translations are given as fractions (1/2, 2/3 ...). The identity operator x,y,z and centrosymmetric counterparts are not required. The syntax is consistent with the syntax in International Tables for Crystallography.

#### **FORM** *A*

Default: FORM 4

A format index; note that in all cases the atom name is read in A2,I2.

1 = read a SHELX parameter file (not instructions) including FVAR and interprets constraints. This part of the program has been taken from the 1983 version of STRUPLO and could not be tested in the current form. Check carefully for possible errors!



2 = Format (2A1,I2,26X,3F10.6), corresponding to the input format of the atomic parameters in the least-squares program ORFLS.

3 = Format (2A1,I2,3F10.6)

4 = Free format. An atom name consisting of two letters is expected in the first two columns, followed by a sequence number and the X,Y,Z-coordinates.

**VIEW X1 X2 X3 Y1 Y2 Y3**

Default: VIEW 0 0 1 0 0 0

VIEW can be used to specify a view direction. X and Y are coordinate triples, where the vector defining the view direction is given by the difference X-Y: it points from Y to X. If Y is not given, the zero vector 0,0,0 is assumed. The space diagonal of a unit cell, for instance, would be defined by VIEW 1 1 1. VIEW automatically performs a rotation around the view direction (Z-axis, see ROTA), that brings the longest projection of the edges of the view range (given by CELL and XYZR) parallel to the X-axis, thus resulting in a landscape format picture.

**ROTA A B C**

Default: ROTA 0 0 0

A,B,C are rotation angles around the orthogonal axes X,Y,Z, with the origin in the lower left corner, X pointing right, Y pointing up, and Z sticking out. The sense of rotation is righthanded for X and Z and lefthanded for Y as shown in the following graph. Initially Z is parallel to the crystallographic c-axis, Y is the trace of the crystallographic b-axis in the plane perpendicular to Z and X is parallel to  $Y \times Z$ , but this is changed by VIEW and ROTA. Multiple ROTA commands are cumulative. This means each ROTA command is applied to the view of the structure, as it exists at this stage. If a VIEW instruction is given, rotations start from the directions given by that instruction. VIEW always takes precedence over ROTA, this being true even if ROTA commands physically precede the VIEW command.

**XYZR A1 A2 B1 B2 C1 C2 D1 D2 E1 E2 F1 F2**

Default: XYZR calculated by program.

All data given here refer to the unit vectors of the unit cell. A1 A2, B1 B2, C1 C2 are minimum and maximum range (X,Y,Z) for polyhedra, D1 D2, E1 E2, F1 F2 are the X,Y,Z components for the range in which circles are to be drawn defined in CIRC. The range for the circles must lie within the range for the polyhedra. If only the range for the polyhedra is given, this range will be taken also for the circles.

**CIRC R N1 N2 N3 . . .**

Default: no circles

R = Radius (Å)

N1 - Atom names consisting of two letters corresponding to the names of the atomic parameters.

'CIRC 0.8 NA CA' draws sodium and calcium atoms as circles with radius 0.8 Å. The symbols listed in one line refer only to one radius which is always the first number in option CIRC. Up to 10 different radii (= 10 options CIRC) are accepted. If circles appear not to be drawn completely, change RES and NRES in PARA.

**TETR A B C D**

Default: TETR 109 20 1.62 0.2

A = tetrahedral angle, B = angle tolerance, C = mean distance from central atom to coordinated atoms, D = tolerance for C

Tetrahedra are sought and drawn with distances between central atom and vertices of C+-D [A] and angles between central atom and two vertices of A+-B [deg].

**OCTA A B C D**

Default: OCTA 90 20 1.97 0.4

A = octahedral angle, B = angle tolerance, C = mean distance from central atom to coordinated atoms, D = tolerance for C

Octahedra are sought and drawn with distances between central atom and vertices of C+-D [A] and angles between central atom and two vertices of A+-B [deg].

**OMIT A B C D ...**

Default: OMIT no atoms are excluded

A B C D ... refer to the numbers in parentheses in the output list on unit 6. If the numbers follow each other in direct sequence they may be given as A -B, where A and B are the first and last numbers in this sequence. With instruction 'OMIT 9 15 -18 23 26' atoms with sequence numbers 9, 15, 16, 17, 18, 23 and 26 are excluded from the parameter list and will not be drawn. If an excluded atom belongs to a polyhedron the whole polyhedron will be omitted.

**SHAD NL N1 N2 N3 ...**

Default: SHAD 9 1 -H(8)

With this option the number of lines NL for the hatching of a polyhedral face can be chosen. If NL is negative, all polyhedra are left blank. NL from 0 to 20 gives the number of lines per face of the polyhedra N1 N2 N3 ... These numbers refer to the numbers of the central atoms. For explanation of the syntax, see **OMIT**

**COLO N1 C1 N2 C2 N3 C3 ...**

Default: COLO pen 1 (normally black)

N1 = Atom name consisting of two letters corresponding to the name of the atomic parameters. C1 = Pen number corresponding to atom name N1.

"Pen" colors used by PSPLOT are: 1=black, 2=grey, 3=red, 4=green, 5=blue, 6=magenta, 7=yellow, and 8=orange.

**PERS**

Default: PERS infinite distance (parallel projection) D

D - distance from the origin to the observer's eye (Å)

**BZRR R N**

Default: BZRR no such polyhedra

R = radius of sphere within which neighboring atoms are searched. N = atom name consisting of two letters corresponding to the names of the atomic parameters. A maximum of 5 BZRR instructions is allowed

**END**

No default option

## 1.62 Atom parameters

STRUPLO expects 5 values per atom

a) atom name (one or two letters in UPPERCASE : CO for Cobalt, not Co)

b) atom label (any number < 100)

c) fractional coordinates (X, Y, Z)

Only the atoms in the asymmetric unit are required. The format for the atom parameters is specified by the FORM option. The default is "free format".

## 1.7 APPENDIX

### Comments from Mark Koennecke about his implementation of POV-Ray in Struvir.

I have added output for the POV-Ray raytracer to STRUVIR. If the menu item Write POV-Ray file is selected, will be a file called STRUPxxx.POV in your working directory which contains your crystal structure ready to be rendered with POV-Ray. Please understand the limitations: STRUVIR can provide you with a convenient way to get crystal structures into POV-Ray, but cannot make a art of it. Creating artwork from STRUVIR's output is up to you !

The file you will get contains a set of declare statements, one for any of the 20 STRUVIR colors each. Polyhedra use these declares as their texture information. The distribution of the textures on the polyhedra follows the same rules as colours in STRUVIR. That is: if a polyhedron has color 1 in struvir it has texture declare one in the file etc. This way you can modify the texture information of whole groups of polyhedra by just modifying those declare statements. Please note that POV-Ray seems to be unable to cope with mutiple levels of declare, *i.e.* if you want to use one of POV-Ray's predefined textures you'd better copy the definition text from the include file into the declare statement.

After this you'll find a default light source and a default camera, looking down z, some distance from the crystal. Following this, the polyhedra are given. Each one as a union consisting of several triangles. At the end of the file all the spheres are given. Just a tip: if you want to move or scale your complete crystal structure in you scene enclose the whole polyhedron and spheres bit with a union and specify the necessary transforms at the end.

POV-Ray output is for POV-Ray-2.2 as at the time of writing POV-Ray-3.0 is not yet available on a unix. I tested the POV-Ray stuff with most of the example .dat files provided by Armel and got reasonable pictures. However as usual:

NO WARRANTIES OF ANY KIND ARE GIVEN. YOU ARE ON YOUR OWN WITH THIS.

Warning: Neither STRUVIR, nor POV-Ray are programs for the either crystallographically or computationally challenged!

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