SHORT REFERENCE MANUAL FOR the STRUCTURE VIEWER

XRSV

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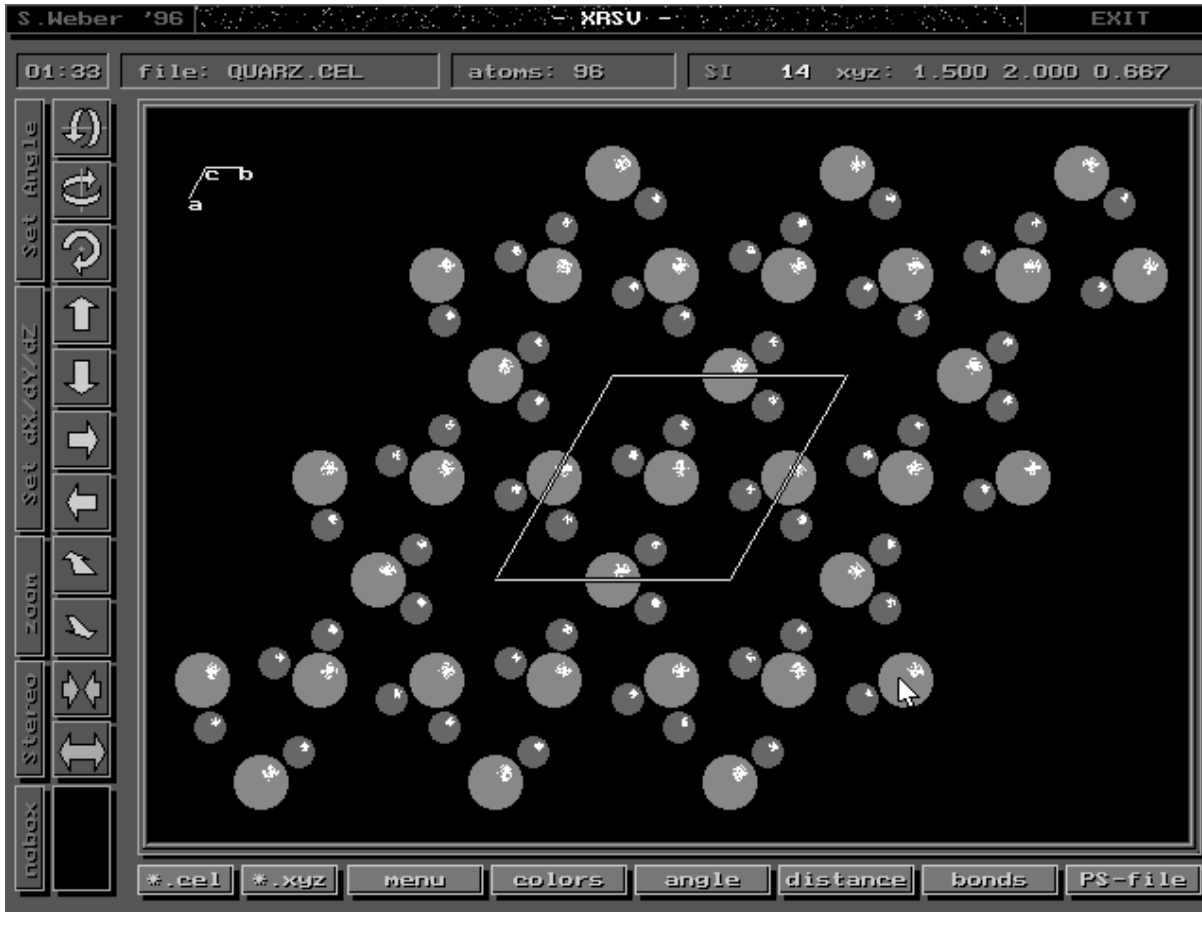
0. Introduction

XRSV is FREEWARE. XRSV originally is a modul of the software package XR95, which is still unfinished. It is therefore made available as a separate compilation. The executable XRSV.EXE is compiled for the Protected DOS mode (DPMI). This Structure Viewer allows simple ball-and-stick structure models to be displayed and printed as a PostScript file. The maximum number of displayable atoms is around 2000.

Screen appearance



1. Menu bar on the lefthand side

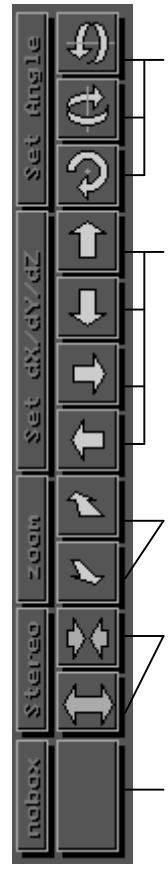
set **angle step** for rotation about the x,y,z-axes

set **xmin, xmax, ymin, ymax, zmin, zmax** for the range of data to be displayed. *e.g.:* three unit cells in x-direction, one in y-direction and 2.5 in z-direction starting from the origin "0 0 0" and "3 1 2.5".
The values have to separated by <SPACE>.

specify the **zoom factor** (*e.g.:* 1.5)

switch between **mono** and **stereo pair** display

switch ON/OFF the display of the **unit cell box**



left mouse click: **rotate about the x,y or z-axis** in positive direction

right mouseclick: in negative direction

translations **up, down, right, left** by 50 pixels

zoom out and **zoom in**

only for stereo mode: **decrease** or **increase distance** between left and right image

change on screen **background color**

2. Menu bar on the bottom

load *.cel file

envoke pop-up menu (also by right-mouse click)

click two atoms for measuring their distance

bond menu

import *.xyz file

show periodic table for colour editing

click three atoms for measuring their enclosed angle

PostScript menu

3. Pop-up menu

quit pop-up menu

display on screen **help file**

Input file editor/creator (*.cel files)

switch between **orthonormal** and **perspective projection**

clip mode: individual atoms are removed upon click and saved in the file *clip.xyz.* **Exit clip mode with <ESC> !!!**

click two atoms A-B and **connect** them with a definable color and linestyle (different line thicknesses only visible in the PS-output)

reset displayed unit cell (only for *.cel files)

display **unit cell data** (quit with right-mouse click)

fit size of displayed structure to window size

assign perspective factor

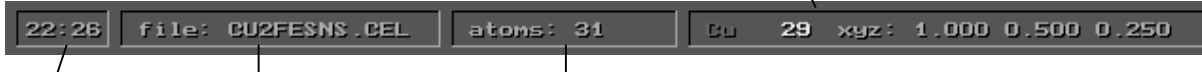
assign **additional radius factor**

the file *clip.xyz* will be **renamed** and placed in the directory **\XYZ** for future import.

erase all present connections

4.Info panel on top

element, atomic number, xyz-coordinates
(upon clicking an atom !)



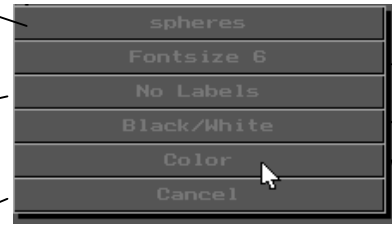
clock input filename number of displayed atoms

5. PostScript menu

draw **shaded spheres, empty circles** or **filled discs**

switch **atom labels** ON/OFF

quit menu without executing



set **fontsize** for atom labels as given in the input files (font: Times-Roman)

give filename and save as **black/white** graphics

give filename and save as **color** graphics

6. Bond menu

The possibility of drawing bonds will be improved in a future update of XRSV. At present XRSV distinguishes between ”bonds”(=connects atoms with same interatomic distance) and “connections“(=connects individual pairs of atoms)

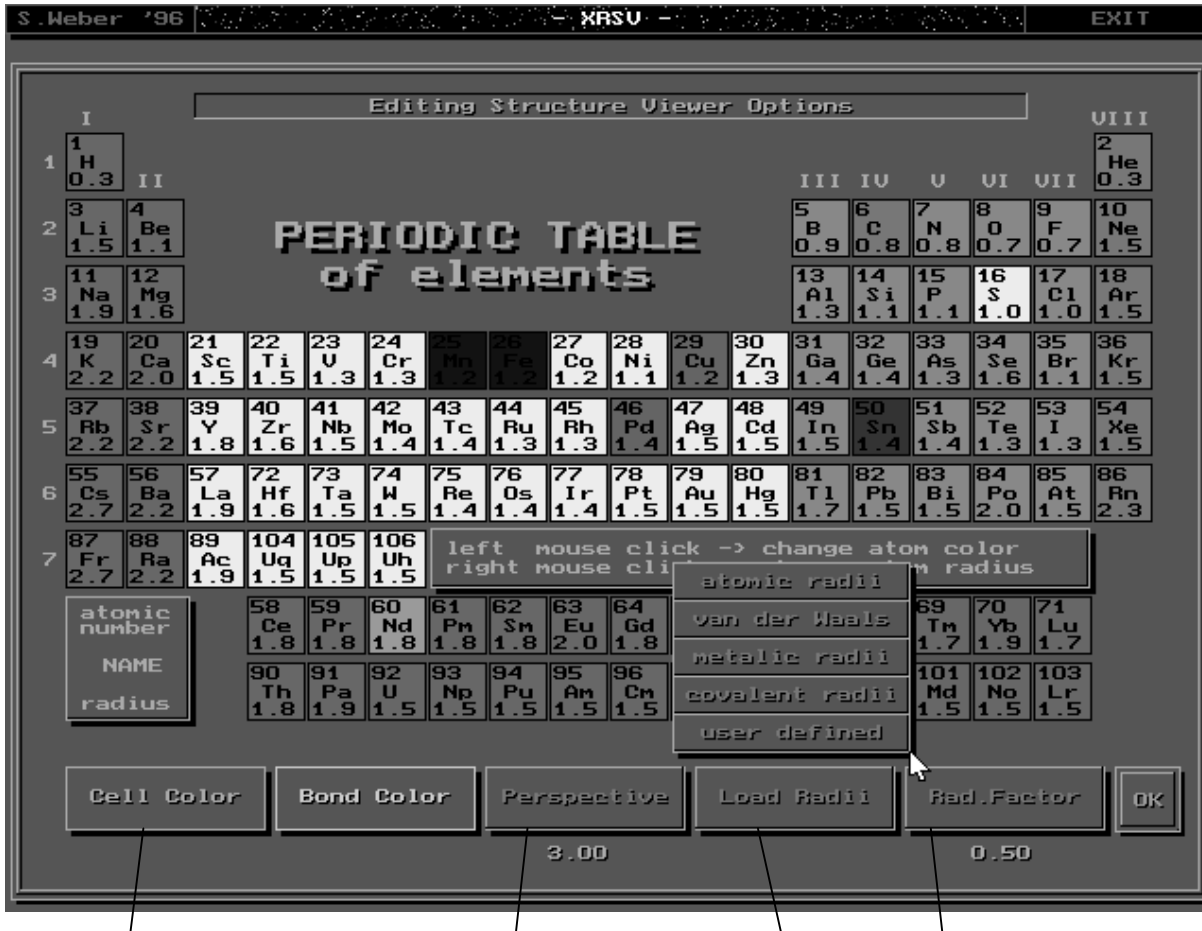
adding bonds: click two atoms to specify a bondlength and enter an allowed deviation. Then all pairs of atoms matching the given distance will be connected

delete all bonds

switch between **hide/show** bonds

7. Color settings

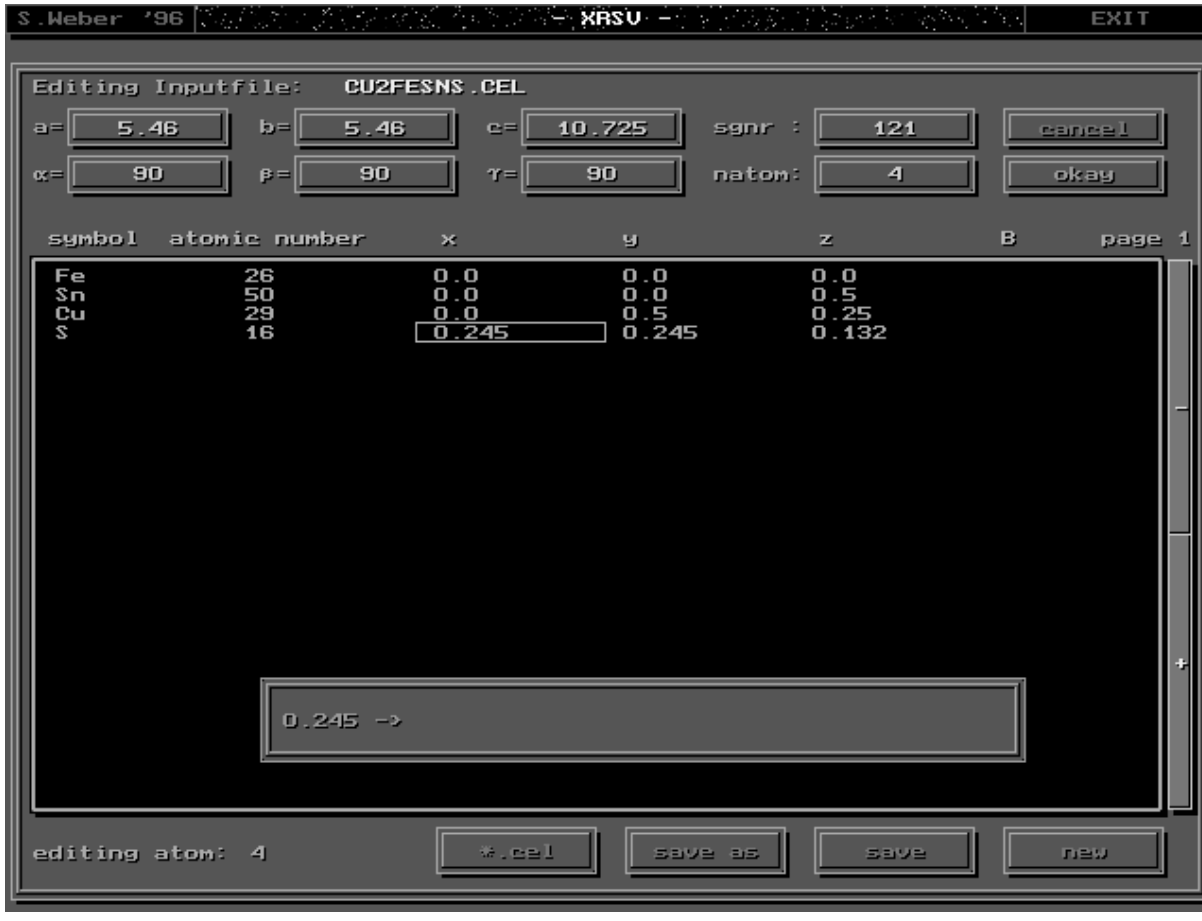
left mouse click : change atom color
right mouse click : change individual atom radius



unit cell box color perspective factor radii menu radius factor

(the perspective and radius factor are the same as in the pop-up menu)

8. Inputfile Editor/Creator



Click the right-mouse key, in order to switch to editing the **symbol, atomic number** and **xyz-coordinates** within the big window and to exit the window again. The column for the temperature factor **B** is redundant in the release as a stand-alone program. Dont leave empty lines in-between, even if the program would kill them automatically. Make sure the number of atoms **natom** matches the number of actual entries. The number of the spacegroup **sgnr** (if unknown) may be looked up in the end of the data file SYSTEM\XR.SGR .

9. Listing of the on screen help file

XRSV-Structure Viewer help-file (version: June 1996)

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Introduction

This program is FREEWARE. It was created, because there is a lack of structure displaying software for IBM PC-AT. The code is written in Borland Pascal 7.0. (more than 4000 lines) It is compiled for the Protected DOS mode.

XRSV is available as a separate compilation or integrated as a modul in XR95. It is a Structure Viewer allowing simple ball-and-stick structure models to be displayed and printed as a PostScript file. The maximum number of displayable atoms is around 2000 depending on the released version.

New features:
- new interface
- connections
- four linestyles
- clip-file -> *.xyz file conversion
- pop-up menu envoked by RIGHT MOUSE CLICK
- option: fit to window
- alphabeting order of inputfile listing
- clock

NOTE: XRSV can be started with a *.cel file as parameter. Then you dont have to select a file. (eg. XRSV.EXE NACL)
(Do not use *.xyz files as parameter!)

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Configuration file

The configuration file is:

SYSTEM\XRSTRC.CFG

If you should ever get a crash so that the Periodic Table displays only black boxes then the configuration file was damaged. Delete it and restart the program. A new one will be generated then!

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Radii file
All data for the radii are read from the file SYSTEM\IONRADII.DAT .
Read the notes in the end of it. This file was provided by the authors of
POWDERCELL. You may edit the 5th column for USERDEFINED radii.
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Format of the *.cel files

CELL : a b c alpha beta gamma
NATOM : number of atoms in assymetric unit
label(max. 4 characters), atomic number, x, y, z, temperature factor
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.
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natom times repeated
RGNR : spacegroup number (also "SGNR" allowed)

you may also use lower case letters (cell, natom, rgrnr)
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Inputfile Editor
Editor for *.cel input files. Click RIGHT MOUSE key to have access to
the data in the data window and to exit it again.
Within the data window you can set the labels, atomic numbers, x y z
coordinates and temperature factor B.
The latter is not needed for XRSV as a stand-alone program. But when
integrated in XR95, the temperature factors are needed for the
calculation of the diffraction intensities.
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Bonds and connections
XRSV distinguishes between BONDS and CONNECTIONS. Bonds have a fixed
length and are all drawn with the same color and for all interatomic
distances that are equal to that length within the specified
deviation. This is not yet a very convenient way for displaying bonds,
but the program is still under development.
Connections can be specified individually between any two atoms,
whereby a linestyle and the color can be chosen for each connection.

This feature might sometimes be more useful than the display of the bonds.

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Linestyles

For the bonds only solid lines are used with the specified bond_color.
For the connections you may choose individual colors and four different styles and thicknesses.

NOTE: the thicknesses are only applied in the PostScript output !

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Atom styles

For the PostScript output you can choose from three types of displaying the atoms.

1. shaded atoms (spheres)
2. filled circles
3. empty circles

The shading routines I wrote myself and they are also used by the authors of POWDERCELL for their PS-structure output.
If you want to print the structure with atom labels then you should choose empty circles because the readability is better then.
The option FONTSIZE refers to the fontsize of those atom labels, which are given in the first column of the input file (max. 4 characters).

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Import of *.xyz files

For my own need of displaying sections of quasiperiodic structures, for which no unit cell exists I included the feature of importing XYZ-coordinate data.

NOTE: the format of the *.xyz files is changed compared to earlier releases of XRSV. Now you have to specify the box dimensons in the last line. (see examples)

Such files can also be created if you clip some atoms from som unit cell.

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Atom clipping
I included this feature in order to be able to cut individual columnar
atom clusters out of some quasicrystal structure.
The clipped atoms are saved in a file named clip.xyz .
It is possible to rename this clip-file, whereby it will transformed
to a real *.xyz file and placed in the directory XYZ\...
It is thus immediately accessible for importing.

NOTE: Quit the clipping mode with <ESC> !!!
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Multiple unit cells

Choose option SET DX/DY/DZ. You can then give the lower and upper limits
of coordinates, within which atoms shall be generated.
Also fractional values are allowed (separated by SPACE).

e.g.:
xmin ymin zmin : -1 0 -1.5
xmax ymax zmax :   1 2 2.2

Existing bonds will be killed when drawing multiple unitcells and
have to specified anew. (will be improved in future)
Sometimes the program might crash ... I have to debug that.
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Atom data

If you click directly on the displayed atoms, then on the top-right
info box you will get information on:

label atomic number xyz-coordinates

---------- end of file ----------