

Guide to SHELXTL programs

1. Introduction:

SHELXTL is a suite of programs used to solve and refine single crystal x-ray diffraction data and incorporates a molecular graphics program called XP. Since most of the work you will be doing with SHELXTL involves creating graphics and measuring various metrical data, this guide will begin with a brief overview of XP commands. It is not meant to replace the in-depth instructions found in the BrukerAXS manual (on the shelves over the lab bench).

2. Necessary files:

Copy the following files to a directory under your "My Documents" folder:

```
from x####/solve/ -  
  x####.ins - instructions  
  x####.res - results  
  x####.lst - listing (output)  
  x####.hkl - hkl data  
  X####.cif - cif file
```

The only files you actually need to run XP is the .res file. If you have a .ins or a .cif file see me and I will show you how to convert these to .res files.

3. How to run the programs:

If you like command-line interfaces do this:

```
Open up a CMD window (run cmd.exe from the start menu)  
Change to the folder you just created (keep in mind this is a dos environment).  
To run any of the shelxtl programs type the following:  
'xp x####' - Molecular graphics  
'xl x####' - Refinement  
'xcif x####' - Table/Report making program
```

If you are a point-and-click GUI type do this:

```
Run the SHELXTL program from the start menu / desktop.  
Under 'File' set up a new project by filling in the file names/locations as prompted  
Run the various programs by choosing them at the top of the window (xl, xp, xshell, etc).
```

4. Instructions for XP

If opening XP from the command line type "xp x#####" The program does not need the file extension but reads the x####.res file.

This guide is organized into sections based on what you might want to do. And word in single-quotes is a command to be typed as-is. Some commands take arguments which are listed outside of the quotes and are then explained.

- Once XP is open:

'fmol' = reads in atom list (must do this to start)

'info' = lists all atoms in 'fmol' list

'reap x#####' = to start over from the original .res file

type 'reap x#####' followed by 'fmol' to rebuild the fmol list.

- Basic command syntax:

all commands are four-letter strings

'help' will give you a list of all available commands

'help' *command* will give you help for a specific command

all "residual" peaks are called "q"

some commands take arguments (such as atom names)

to refer to a single atom use its name (C1, Mn3, F105)

to refer to all atoms of a given element use \$ (\$h, \$c, \$q)

to refer to a range of atoms in the fmol list use > or 'to' (c1 to c15, n5 > c156)

to exclude atoms from a list or command use 'less' (proj less \$q, atyp -1 less \$h)

4a. Making pretty pictures in XP:

- Getting a good view:

'proj' = wireframe rotation gui

'pers' = static ball-and-stick view

'diag' = static, labeled wireframe view

'uniq' *atom(s)* = will display only 'molecules' containing listed atoms

'uniq cu1' will display the copper-containing moiety and leave out any solvent or other molecules. use fmol to restore the entire atom list.

'grow' = generates symmetry equivalent atoms *connected* to atoms already in the fmol list. This is useful for molecules sitting on symmetry centers so that only half of the molecule is unique. This will not draw in isolated solvent molecules.

'fuse' = undoes the grow command (reducing fmol list to asymmetric/unique unit only)

'sgen' *symcode atom(s)* = adds the symmetry-generated equivalents of the named atoms

sgen 1545 \$c adds all carbon atoms with symmetry code 1545

for a detailed explanation, see the manual.

'kill' *atom(s)* = deletes atom (permanently) from fmol list (e.g. *kill \$q* deletes all q peaks)

- Changing atom properties:

'atyp' #1 #2 atomname(s) = changes type of ball or ellipse and color of atoms listed
#1 = ball/ellipse type
#2 = color
e.g. *atyp -1 5 \$Mn* makes all Mn atoms purple ellipsoids
'help atyp' = list of ball/ellipse types
'help color' = list of colors

- Add/Delete bonds:

'join' #1 *atom1 atom2* to join two atoms and adds the bond to the connectivity list
#1 determines bond type, blank/default is solid bond.
'link' #1 *atom1 atom2* essentially the same as join.
'undo' *atom1 atom2* deletes bond between two atoms.
** using the *fmol* command at any time after join, link, or undo will reset the bonds to their original state.

- Changing label types (very handy for making pictures as default labels are awful)

'labl' #1 #2 = changes label size
#1 = label type (*help labl* for type codes)
#2 = label size (default is 600 – too big!)
e.g. *labl 1 300* is what I use (no hydrogens, no brackets, and relatively small)
** change label sizes before making a picture **

- Making a picture:

Once you get a view you like type 'save *filename*' This will create a file '*filename.sav*' which can be read in later with the 'next' command: 'next *filename*' This can be done without having read in the atom list with *fmol*.

'telp' #1 #2 #3 *commands* = to create ball-and-stick or ORTEP plot
#1 is stereo offset **always use 0 (zero)**.
#2 is atom radius percent
use -50 for 50% ellipsoids, 50 for sphere of arbitrary radius
#3 is bond radius, typically 0.03 - 0.05 larger number = larger bond
commands include 'cell' for unit cell box, 'less \$H' to hide hydrogens, etc.
e.g. *telp 0 -50 0.03 less \$h* thermal ellipsoid plot with thin bonds and no hydrogens
follow system prompts to label atoms
use mouse to move label box
space to add label
"enter" to skip label
"backspace" to go back through the labels
System prompts for filename, creates *filename.plt* (you can access this any time you open XP)

- Saving your picture to a readable file:

To write image to a readable file use 'draw *filename*' and follow system prompts

select "a" for Adobe Post Script or "h" for hpgl file to import directly into MS Word.

** These are the only functions that work. **

The system then prompts for

new filename (can be the same as *filename* above)

color or b&w (default is black and white, so be careful if you want color)

page type (for HPGL only, default is fine.)

There will be a pause while the program writes your file, eventually you'll get the prompt back.

4b. Metrical details in XP

- Calculating distances:

'envi# *atomnames*' = gives all atoms and their distances within the specified environmental radius to *atomnames* given. The includes symmetry equivalents not included in the current fmol list.

'envi' = first coordination sphere

'envi2' = second coord. sphere, etc.

e.g. *envi2 \$o* gives all atoms, bonds and angles to all oxygen atoms within the second coordination sphere

** the first number listed after the atom name is it's symmetry code. 1555 is the current fmol list, any other number indicates a symmetry equivalent atom not currently drawn. Use the sgen command (see above) to generate atoms using their symmetry codes.

'bang' *atom(s)* = give all bonds and angles in the current fmol list to *atom(s)* given.

- Calculating planes and lines and the angles between them:

'mpln' *atom(s)* = stores into memory the best-fit plane among *atoms* given. It lists deviations (in Å) of all atoms out of the plane. It will also re-orient your view to be perpendicular to the plane named.

additional 'mpln' commands will give the same as above plus the angle between all subsequent planes and lines (see below)

'mpln' followed by no atoms calculates the mean plane over the whole fmol list.

'line' *atom1 atom2* = stores into memory a line between two *atoms* (can be a bond or not). It will give angles between the line and all other lines and planes.