Notes on OLEX2

Updated on 12 January 2018,at 09:05.

Ilia A. Guzei

2124 Chemistry Department, University of Wisconsin-Madison, 1101 University Ave, Madison, WI 53706 USA.

Table of Content

How to install OLEX2 under Windows

A: The program is available as a free download from http://www.olexsys.org, just follow the installation instructions from the web. OLEX2 must installed and <u>launched at least once</u> in the administrator mode in order for all features to work for all computer users. You will also likely need programs SHELXS and SHELXL (written by George Sheldrick) available free upon request from http://shelx.uni-ac.gwdg.de/SHELX/. SHELXS and SHELXL are necessary for structural solution and refinement, respectively. OLEX2 is smart and if you already SHELXS and SHELXL (or the entire SHELX suite) installed, OLEX2 is likely to find the programs on your computer. If it does not you ought to specify the path to the SHELXS and SHELXL files on your computer as follows.
Suppose your SHELXL package is in folder C:\SAXI\.
Under Windows 7 open the properties panel: Launch→right-click on Computer→Properties.
Under Advanced System Settings click on Environment Variables. Under System Variables select Path, and add to the (rather long) line the following:
;c:\saxi
Save and close. Now Olex will list the supported programs in its structure solution and structure refinement drop-down menus.

Q: What other programs do I need and how do I install them?
A: OLEX2 can work seamlessly with other programs such as SHELXL, PLATON, XP, superflip, and Pov-ray. The instructions below imply that you have licenses for the programs. The instructions are for Windows 7 and 8.
0. Close OLEX2.
1. Download SHELXL from http://shelx.uni-ac.gwdg.de/SHELX/ and install it in
`C:\SAXI\`
You may have to register – it is free.

2. Put XP.exe and superflip.exe in the same folder, `C:\SAXI\`.

3. Download the PLATON for Windows Taskbar and PLATON executable and check.def from http://www.chem.gla.ac.uk/~louis/software/platon/ and put them into
C:\PWT\
Make sure you put all PLATON-related files into this folder.

4. Some environment variables need to be set as follows. Go to Start→Control Panel→System and Security→System→Advanced system settings
and in the System Properties window click on the "Environment Variables…" button. It may look something like this:

OLEX2 Manual
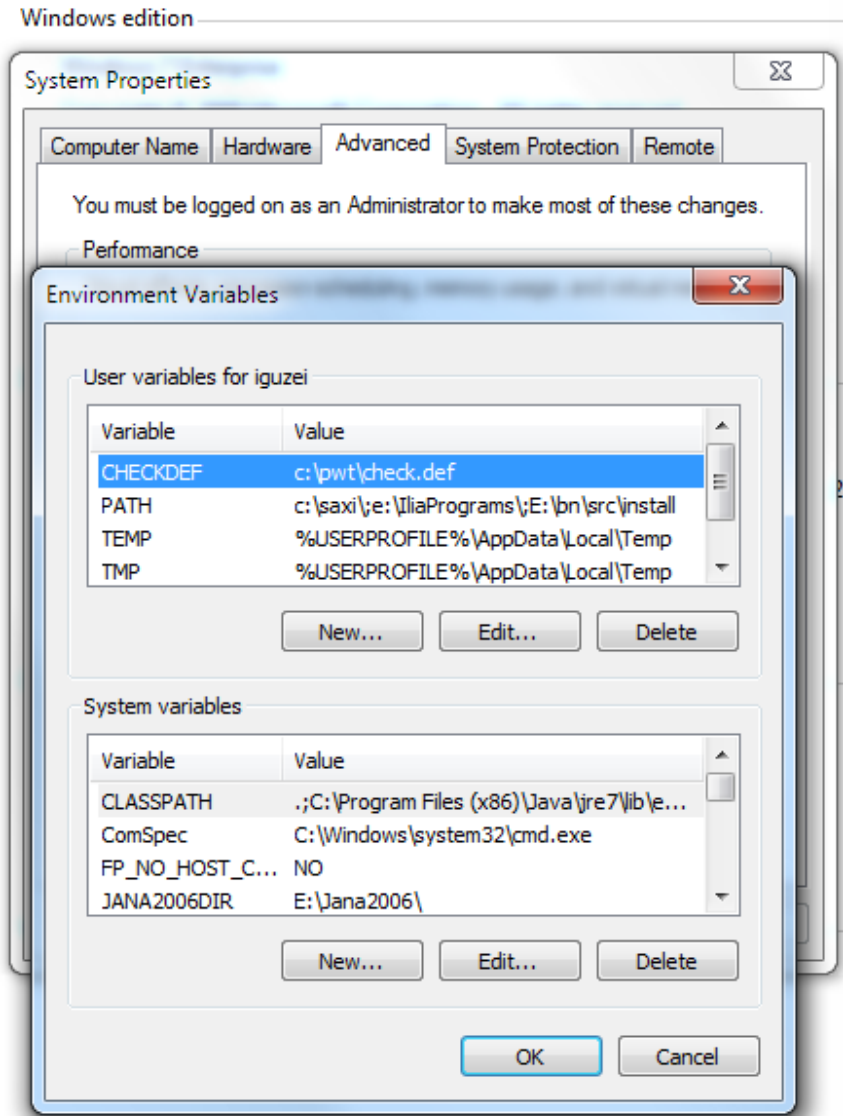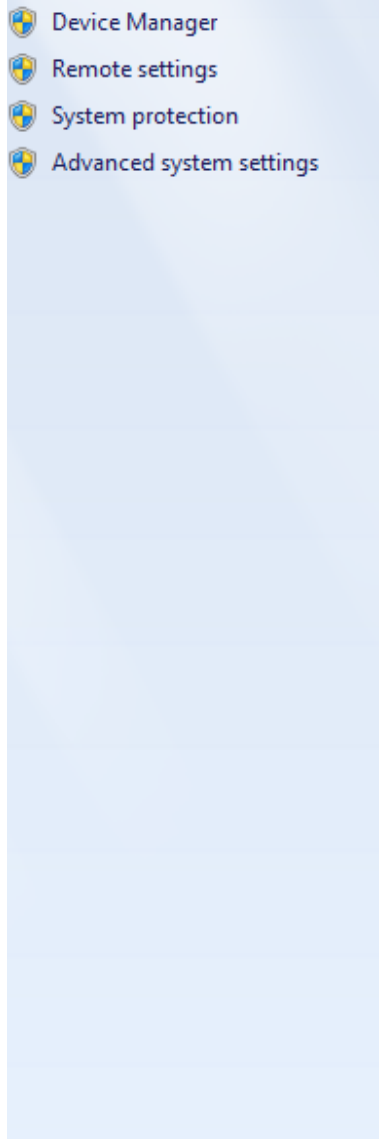
Under "User variables for username" click on "New…" and in the "Variable Name" type CHECKDEF and in the "Variable value" type c:\pwt\check.def as shown:
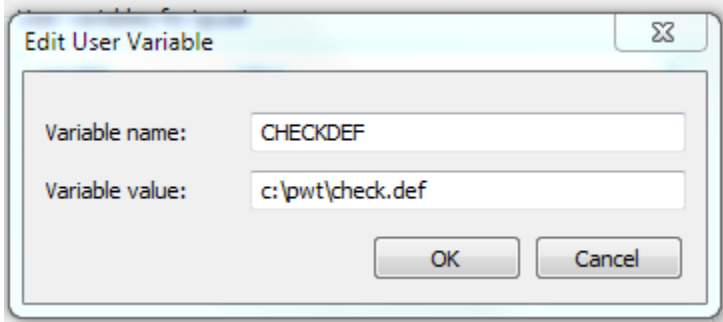
Click OK.

If there is no PATH variable in the "User variable for username" section - click on the "New…" button again and in the "Variable name" type:
PATH
and for the "Variable value:" type
c:\saxi\;c:\pwt\
as shown below
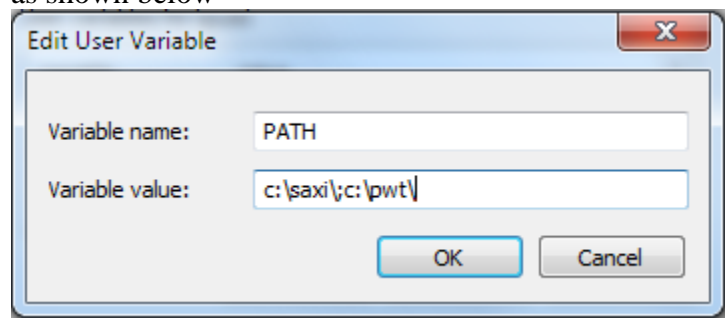
Click OK and close the windows you opened while navigating to the Advanced System Settings.
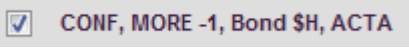
5. Start OLEX2. Let's check if the procedure worked. Open a structure. Go to Work→Refine and expand the Refinement Program dropdown menu. If you installed the programs correctly, you should see, at a minimum, SHELXL and olex2.refine there:
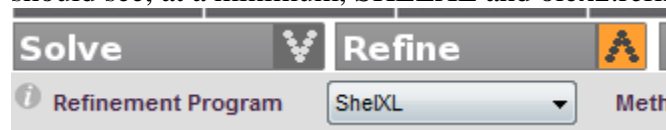
If you are not seeing SHELXL – go back to the Advanced System Settings and modify the PATH System variable (rather than User variable) to include `c:\saxi\`. To do so, highlight the PATH variable, click Edit, navigate to the end of this rather long line, and append `;c:\saxi\` to the end of the line. Note the leading semicolon – it is needed to separate the values on the line:
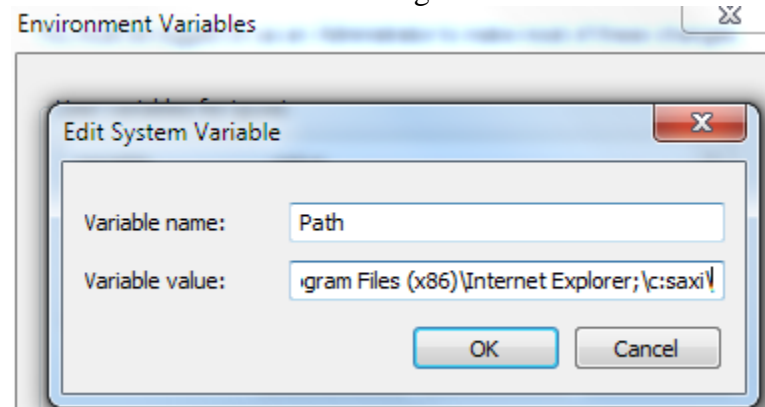
Olex2 should be restarted for the changes to take effect. If this does not work – move the `c:\saxi\;` part to the beginning of the "Variable value" line (note the semicolon). Olex2 should be restarted for the changes to take effect.

Once SHELXL is visible, select it in the dropdown menu, put a checkbox next to the "CONF, MORE -1, Bond $h, Acta" line: , and run a refinement.

Now click on the PLATON button located in the very top row

 .

PLATON should launch and you should see PLATON's interface with all the buttons.
If it does not work – modify the PATH environment variable for the System, similarly to the suggestions for the `c:\saxi` above.

Important: if you launched PLATON successfully, you need to close the PLATON interface and PLATON-generated windows before you can return to OLEX2, otherwise OLEX2 will hang and PLATON will run in the background (in which case it must be killed as a process in the Task Manager).

Optional: Another good structure solution program Superflip can be downloaded from http://superflip.fzu.cz/ and it too should be placed in C:\SAXI folder.

A computer restart may be necessary at this point.

How to install OLEX2 on a Mac

OLEX2, SHELX, and XPREP Installation Instructions for Mac
by Brian Dolinar, and from http://www.xrayforum.co.uk/viewtopic.php?t=1838.

In general, it is helpful to refer to a list of commands for the OSX terminal such as the one found here: http://ss64.com/osx/. The terminal will be used throughout the installation process.

OLEX2
> Download and install OLEX2 from http://www.olexsys.org/. You need OLEX2 version 1.2.6 or later.

SHELX
1. Register (free) as a new SHELX users at http://shelx.uni-ac.gwdg.de/SHELX/.
2. Once you have registered, a password will be emailed to you. Navigate to the Downloads tab. Click the link provided at the bottom of the page that says, "download the programs". When prompted, supply the username "shelx" and the password emailed to you.

3. You should now be looking at a file page that says "Index of /~gsheldr/bin". Click the Mac folder. Then download the .bz2 files you need. For Ilia's class, you will at least need shelxl and shelxs.
4. Navigate to your Downloads folder and double click on the bz2 files you downloaded. This will extract your SHELX executable files to your Downloads folder.
5. Open the application folder for OLEX2, but do not run the program. To open the folder, right click on the installed OLEX2 application icon (in the Applications folder) and select "Show package contents". Then in the window that appears open the sub-folders Contents and MacOS.
6. Place all the the SHELX executables you plan to use, plus SHREDCIF in this folder.
7. Open an OSX Terminal window to make sure these files are executable:
    type: cd /Applications/olex2.app/Contents/MacOS ["cd" stands for change directory]   this navigates to the place where you just put the SHELX executables

    type: chmod a+x shelx* shredcif
    If this fails because of permissions, repeat the instruction as
    sudo chmod a+x shelx* shredcif
    then give an administrator password

    this changes the permissions on all the SHELX programs and SHREDCIF to become executable files and gives all users permission to run them.
8. Run the OLEX2 application. Click the Work tab. Then click the drop down arrow for the Solve menu. Verify that both olex2.solve and SHELXS listed as solution programs.
9. Click the drop down arrow for the Refine menu. Verify that olex2.refine and SHELXL are listed as refinement programs.
10. If you have a structure loaded you can verify that SHELXS and SHELXL work by running them on that structure.

XPREP (This is for Chemical Crystallography at UW-Madison only. XPREP is not freeware)

1. Download XQuartz-2.7.7.dmg from http://xquartz.macosforge.org/landing/. This program contains certain libraries that allow XPREP to work correctly. Older computers may not need this, but newer ones do.
2. Open the .dmg file, then run the installer. The installation will take ~5 minutes. Be patient.
3. To obtain XPREP, download the program from the Box set up by Ilia. Select the mac version.
4. Once it is downloaded, rename xprepformac to xprep.
5. In the terminal, change the directory to your Downloads folder. Do this by typing the command "cd" and dragging the downloads folder into the terminal. Press enter. Your terminal should now be in the Downloads folder.
6. Type the following command into your terminal: "chmod +x xprep". This changes the mode on xprep to allow it to be executed by your computer. The icon should also change from a blank white icon to one that shows a black and green computer terminal.

7. Your terminal's directory should still be the folder that contains XPREP. Run XPREP by typing "./xprep" into your terminal. If it works, it will list some information about XPREP and prompt you for a reflection file.

8. To run XPREP on a structure, copy the executable into a folder with structurename.hkl and structurename.p4p files in it. Navigate the terminal to that folder. Type in the terminal

./xprep structurename
It should load the .hkl and .p4p files into xprep and show statistics about lattice centering.

Installing and using PLATON on a Mac

By Anthony Linden, Department of Chemistry, University of Zurich, Switzerland,
anthony.linden@chem.uzh.ch

Here is how to get PLATON running on a Mac. PLATON uses X11 for its GUI, so you need the X11 libraries and tools and you then need a fortran compiler. Ton Spek does not create compiled versions of PLATON with static libraries, hence you must compile it yourself and the need for all this.

The instructions below should work on OS 10.13, (High Sierra), 10.12 (Sierra) and 10.11 (El Capitan). The procedure sometimes changes a little for each new Mac OS version, mainly because X11 libraries sometimes change location and a PLATON executable compiled under one OS does not always work under another. Once you get this set up for one OS, it works from then on at least until the next OS is installed, so you usually only need to do the actual compile step when updating PLATON. It is advisable to update and recompile PLATON at least once a month, because it is constantly being improved.

If you are familiar with Unix/Linux, the following is probably clear to you. If not, please simply try to follow the instructions below exactly. Please read and type carefully, as there are important spaces and dashes within some commands. All commands typed in the XQuartz window are case sensitive. Unix commands usually do not give any feedback when they work correctly. Messages often mean something might not have worked.

This looks long, but is quite quick if all goes well. Don't be discouraged!

The following is based on Ton Spek's readme at http://www.platonsoft.nl/xraysoft/Mac-OSX/platon, but I have modified it a little to update the steps and remove the unnecessary installation of the full Xcode developer kit. Everything below is case sensitive. Any other instructions or even a compiled version you find on the PLATON web site might not be up to date.

1 - Download the latest XQuartz (2.7.11 or later) from http://xquartz.macosforge.org

2 - Install it and start it (located in Applications/Utilities). When the window opens, you are in the top level directory (folder) for your Mac user account. To return here at any time, type 'cd'. To find out which folder you are in at any time, type 'pwd'.

3 - Install Apple Command Line Tools. Type in the XQuartz window: xcode-select --install

4 - Download gcc and gfortran from http://hpc.sourceforge.net.
The binaries are near the top of the page; be sure to choose the version appropriate for your Mac OS version: e.g. gcc-7.1-bin.tar.gz (contains gcc and gfortran). It is recommended you use Safari for the

download to avoid the tar files being completely unpacked, after which the instructions below will not work (Firefox unfortunately unpacks the downloads).

5 - Move these two files to your Desktop (more convenient that way). Probably your Mac automatically uncompresses them, so the .gz is removed, but you still must have the single files with the .tar ending for the next step.

6 - In the XQuartz window, type the following lines Note that uppercase, spaces and dots are part of the command and must be typed exactly as given (add .gz to the file names if they are still present with that extension):
cd
cd Desktop
sudo tar -xvzf gcc-6.3-bin.tar -C /
sudo asks for your login password the first time, assuming you have administration rights. Otherwise the password for the admin account on your Mac.

7 - Create a folder named 'platon' at a convenient location. I use Desktop for now. Note that if you use uppercase letters for any part of the folder name, then you must type it exactly the same way from now on.

8 - Download the files: platon.f.gz, xdrvr.c.gz, check.def, sucrose.spf from:
http://www.platonsoft.nl/xraysoft/unix/platon and move them into that folder.

9 - In XQuartz, go to that folder. If already at Desktop from the above, then just type 'cd platon'. If lost, type:
cd
cd Desktop/platon

10 - gunzip the files platon.f.gz and xdrvr.c.gz (the Mac probably has done that automatically). If not:
gunzip platon.f.gz
gunzip xdrvr.c.gx

The file check.def might have acquired the .txt ending during the download, If so, type:
mv check.def.txt check.def

11 - Compile PLATON. This is the most critical and often troublesome step. Type carefully and exactly:
sudo gfortran -o platon platon.f xdrvr.c -I/opt/X11/include -L/opt/X11/lib -lX11

Note that in the above, the character after the dash in -I/opt is an uppercase i and the character after the dash in -lX11 is a lowercase L.

If nothing appears to be happening, just wait. The compiler takes a minute or two. If the command prompt reappears after a while without any messages, you have succeeded!

If this step fails with error messages after the long wait, either you did not type the above correctly, or the X11 libraries are not where they are expected to be, which might be the case if you are using an older Mac OS.

If you have an earlier version of the Mac OS, e.g. Yosemite or Mavericks, one of the following might work instead (these will certainly not work if you use El Capitan or later):
gfortran -o platon platon.f xdrvr.c -L/opt/X11/lib -lX11
gfortran -o platon platon.f xdrvr.c -L/usr/X11/lib -lX11

If this also fails, try to find the path to the /X11/lib folders and use that with the –L switch.

12 - Copy the newly created file 'platon' (the executable) and check.def to /usr/local/bin or any other location you like your executables, such as shelxl, etc., to be. I recommend not putting these in the /Applications folder. With El Capitan or later, if you do not already have the folder /usr/local/bin, you might not be allowed to create it. Simply use any convenient folder within your user account and use the path to it instead of /usr/local/bin in the following.

In the following, the dot at the end is important.
cp platon /usr/local/bin/.
cp check.def /usr/local/bin/.
chmod -R 755 /usr/local/bin/platon
chmod -R 755 /usr/local/bin/check.def

If these commands do not work, try prefixing them with 'sudo '.
sudo cp platon /usr/local/bin/.
sudo cp check.def /usr/local/bin/.
sudo chmod -R 755 /usr/local/bin/platon
sudo chmod -R 755 /usr/local/bin/check.def

Quit XQuartz and start it again so the system leans about the new program (or type 'hash -r' if in the default bash shell, 'rehash' if in tsch or csh). Only needed the first ever time you install PLATON.

13 - Set up an environment variable for the location of the check.def file to be used as part of CheckCIF validation. If this step is skipped, it is not important because PLATON will create a new check.def in your current working folder each time if it cannot find check.def otherwise.

If you wish to define the environment variable, it has to be done each time you start XQuartz, so for convenience it needs to be in the .bash file if you use the default bash shell in XQuartz, or in .cshrc if you change to csh or tcsh.
For bash: export CHECKDEF=<path>/check.def
For tcsh: setenv CHECKDEF <path>/check.def
Where '<path>/check.def' might be '/usr/local/bin/check.def' if you put check.def where I suggest above.

14 - Test: type 'platon sucrose.spf' in the XQuartz window (you have to be in the platon folder again if you moved away), click on ORTEP in the main PLATON menu for an ORTEP plot.

If all is well, you have a working version of PLATON that you can now use quite independently of any other program simply by using the command line in XQuartz, such as 'platon x.cif'. Similarly, if the shelx programs are on a known path, you can run them manually from there too. All you need to do is 'cd' to the folder with your current structure files in them.

To update PLATON at any time, you need to repeat steps 7-12. The availability of a new version is indicated on the PLATON opening window (red text starting with WEB:). The compilation and installation steps can be simplified by creating a makefile with the relevant instructions. See hints at http://www.cs.colby.edu/maxwell/courses/tutorials/maketutor/. A makefile for compiling PLATON is below. Remove the # from the first two lines if your Mac does not automatically unzip the downloads. <tab> means insert the tab character on those lines. Simply save this as a file called 'makefile' and run it in XQuartz with the command 'make' initially to compile and then, if no errors, 'make install' to move things to the right places.

platon:
#<tab>   gunzip -f platon.f.gz
#<tab>   gunzip -f xdrvr.c.gz
<tab>   gfortran -o platon platon.f xdrvr.c -I/usr/X11/include -L/opt/X11/lib -lX11

install:
<tab>   mv platon /usr/local/bin/.

`<tab>`	cp check.def /usr/local/bin/.
`<tab>`	chmod 755 /usr/local/bin/platon
`<tab>`	chmod 755 /usr/local/bin/check.def
`<tab>`	chmod 755 /usr/local/bin/check.def

How to get OLEX2 to use PLATON

By Anthony Linden, Department of Chemistry, University of Zurich, Switzerland, anthony.linden@chem.uzh.ch

On a Mac, to get Olex² to know that PLATON exists, and thus show the 'Pton' button at the top of the main GUI instruction panel, and to start PLATON, you need to do the steps below. This only works from version 1.2.8 of Olex² released in August 2016, or later versions. Earlier versions had bugs which made getting PLATON to work more complicated, although it can be done. Therefore, please ensure you have the latest version of Olex² installed.

1 - Install PLATON as described above. Make a note of the full path to where you put the PLATON executable. For example, /usr/local/bin if you put it there.

2 - Start Olex². In the main GUI instruction panel, select the Home panel and then click on the Settings tab. The second last item in the list that appears is "path:". Enter the full path to your PLATON executable here and then click out of the path definition box. Quit Olex² and restart it. Come back to the path definition box and ensure the path you typed is shown. If the box is empty try again.

3 - You are done! Platon should work now, but you have to have a refined structure with a CIF or .res file to test this, e.g. try the sucrose sample structure and refine it with SHELXL with the option ACTA activated.

It is possible that PLATON still does not know where check.def is, but that is no longer a problem, because if PLATON cannot find check.def, it creates one each time in the current working directory and uses that.

Note that if the executables for all external programs like SHELXL, SHELXT, etc. are in the same location as PLATON, Olex² will have no trouble finding them and they do not then need to be placed in the Olex² application folder itself.

About program OLEX2

Q: How do I reference OLEX2?
A: O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann. "*OLEX2*: a complete structure solution, refinement and analysis program". *J. Appl. Cryst. 2009, 42, 339-341*.

Q: Do I have the latest version?
A: In the console type
echo GetCompilationInfo() [provides the compilation date]
Or check the About button.

Q: How do I get the latest release with the latest features?
A: Under Help→Update Options change the Repository URL to
`http://dimas.dur.ac.uk/olex-distro-test/update/`
Then restart OLEX2. Note that the new added functionality in the "test" version may not be very well documented, but you will have a more powerful program.
Alternatively, type
`update`
in the command line and watch the progress in percent right below in the status bar. Once the percentage reaches 100% restart OLEX2.

Keyboard shortcuts

F2 - toggles the solid background color.
F3 - toggles atom labels.
F4 - toggles the gradient background color.
F5 - activates the **work** tab.
F6 - activates the **view** tab.
F7 - activates the **tools** tab.
F8 - activates the **info** tab.
ESC - deselects selected atoms or quits the current MODE of operation (such as atom labeling).
`ctrl-A` - select everything.
`ctrl-G` - launch the *grow* mode.
`ctrl-H` - toggles the H atoms.
`ctrl-I` - inverts the selection. If nothing is selected works as ctrl-A.
`ctrl-O` – launches the Open File dialog.
`ctrl-Q` - cycles through "no Q peaks", "show isolated Q peaks", and "show connected Q peaks".
`ctrl-R` - runs a refinement.
`ctrl-T` - cycles through "hide molecule/show text", "hide text/show molecule", "show text and molecule".
`ctrl-Z` - undo the last action. It works whenever possible.
`TAB` - expands the command (when typing in OLEX's console).
`mode off` (not a shortcut, but a quick way to exit a current mode)
"↑" key brings the previously issued commands from the console.
`Page Up` and `Page Down` buttons will scroll the content of the command line window inside OLEX2.

Mouse traps

Left click rotates the model
Right click and hold - zooms the view

left and right buttons down – translates the molecule
CTRL + left click – rotates the model around the axis perpendicular to the screen
left and right buttons down – translates the molecule
ALT + left click – zooms the view
CTRL + SHIFT + left button down – translates the molecule

Left click on an atom – selects the atom
Double click on an atom – selects the molecule

right click on the background – opens the scene menu
right click on an atom – open the atom property menu

Alphabetical list of commands

The list is not exhaustive yet. I am listing the commands I know how to use.

addbond atom1 atom2
addbond (GUI-selected atoms)
Adds a bond between `atom1` and `atom2` unless a `CONN` command prevents it.
Selecting two atoms (such as C1 and C2) in the GUI and typing `addbond` is equivalent to typing
`addbond C1 C2`
Issuing an `addbond` command is equivalent to inserting the shelx BIND command in the instruction file and the bond is added to the connectivity table.

addins [text]
Inserts `text` into the ins file. Great for including additional commands. Synonym: "/ "
(forward slash with a space. For example, to add an extinction card EXTI to the INS file one can type either of the two:
`addins exti`
`/ exti`

asr
(Absolute Structure Refinement). Adds TWIN and BASF instructions to the INS file in the case of a non-centrosymmetric structure.

azoom percentage [atoms]
Scales the radii of the specified `atoms` according to the `percentage`. If no atoms are specified the change is applied to all atoms. Note that `azoom` will change the size of the thermal probability ellipsoids. The command also works for Q peaks, for example:
`azoom 10 $q`

will make all q peaks smaller.

basis
toggles the basis vectors.

brad [value]   [parameters]
short for Bond RADius. Adjusts the width of the selected bonds.
`value` is a scale factor (default is 1) for all bond radii. Here 1 unit is 0.1 Å.
Syntax:
When any bonds in a molecule displayed in the GUI are selected
`brad  value`
will adjust their radii by scaling the current radius by a factor of `value`.
`brad [value] [parameters]`
this notation allows one to set the bond radii without selecting the bonds in the GUI.
`[parameters]` are bonds (such as C-H, N-N) are case sensitive.

Examples:
Select a C–C bond in the GUI. Type
`brad 0.8`
All C–C bonds in the GUI have changed to a radius of 0.8. Of course, bonds of different types
can be selected simultaneously.
`brad 0.5 C-H`
changes all C–H bonds to have the radius of 1/2 of the default thickness. Note that the elements
in this notation are case sensitive.
`brad 3 hbonds`
sets all hydrogen bonding interactions displayed in the GUI to be three times as thick as their
default (note: the default for the hydrogen bonding interactions is unity, but this unity is 1/10 of
the value of a regular C–H bond). But at least one hbond should be selected.

calcpatt
calculates the Patterson map. The map's features can be adjusted in the typical manner with the
Level slider and Tools→Maps.

cell
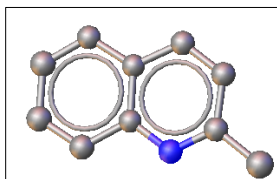toggles the view of the unit cell boundaries

center
centers the model in the GUI

chemdraw

inserts circles in six-membered rings:

The circles can be deleted by rotating the mouse wheel or typing undo or fuse.

close
Closes current structure.

compaq [switch]
Repositions atoms and/or fragments in the asymmetric unit as close to each other as possible.
possible switches: -a, -c, -m, -q.
compaq
All fragments are assembled around the largest one.
compaq -a
assembles together the incomplete fragments
compaq -c
similar to the default behavior, but takes into account the atom-to-atom distances and moves all atoms into the closest possible positions to the largest fragment in the structure
compaq -m
assembles non-metallic parts of the structure first, then moves atoms to the closest metal.
compaq -q
moves the electron density peaks closer to existing atoms.
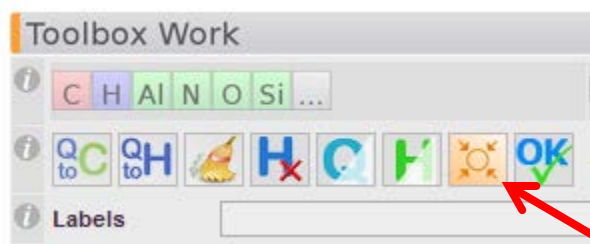
The compaq -c button in GUI

conn value1 [value2] atoms
Adjusts the number of atoms bonded to a selected atom(s)

conn value1 value2 atoms
if both values are supplies value1 is the maximum number of bonds (default = 12), value2 is bonding radius.
By default, two atoms are bonded when (the distance between the atoms is less than R1+R2+delta).
conn value1 atoms

If `value1` is an integer it specifies the number of bonds the atom(s) makes.
If `value1` is floating it specifies the bonding radius of the atoms in the `list`.
`atoms` designates specific atoms, not atom types. Use the $ sign to change the bonding radius for all atoms of a certain type.

To see the default bonding radius of your atom(s) type
`info   atomname`
the R-bond column will list the radius.

Examples:

`conn 3 2.4 Ti2`
Atoms Ti2 will make no more than three (shortest) bonds with the Ti2's bonding radius set to 2.4.
`conn 3 Ti2`
Atom Ti2 will make three shortest bonds with the default radius
`conn 2.4 Ti2`
Atom Ti2's bonding radius is set to 2.4 Å and all possible bonds are shown.
`conn 2.4 $ti`
The bonding radii of all Ti atoms are set to 2.4 Å.

Also possible:
1. Select the atom(s) for which you want to set a new radius with the mouse in the GUI
2. type
`conn value1`
the `value1` will be applied as a new radius to the selected atoms

Important: if `value1` is an integer it is interpreted as a number of bonds, if not – as a radius.
Thus if a radius of 3 Å is needed the `value1` should be entered as 3.0.

Database for the CIF file

This is an advanced option as of August 14, 2014.
In OLEX2 under Report→Publicaton one can add authors and affiliations. However, I managed to enter my affiliation incorrectly and had difficulty correcting the entry. To get ultimate control over the database one should do the following (and it takes 3 minutes).
Download and install the SQliteBrowser database editor from
http://sourceforge.net/projects/sqlitebrowser/files/latest/download
Launch SQliteBrowser. Click on Open Database. Leave it as is for now.
Go to OLEX2 and type
shell datadir()/db
to see the database file. Copy the path to this folder. Go back to the Open Database dialog and paste the path in there. Open the olex2.sqlite file and edit your heart out.
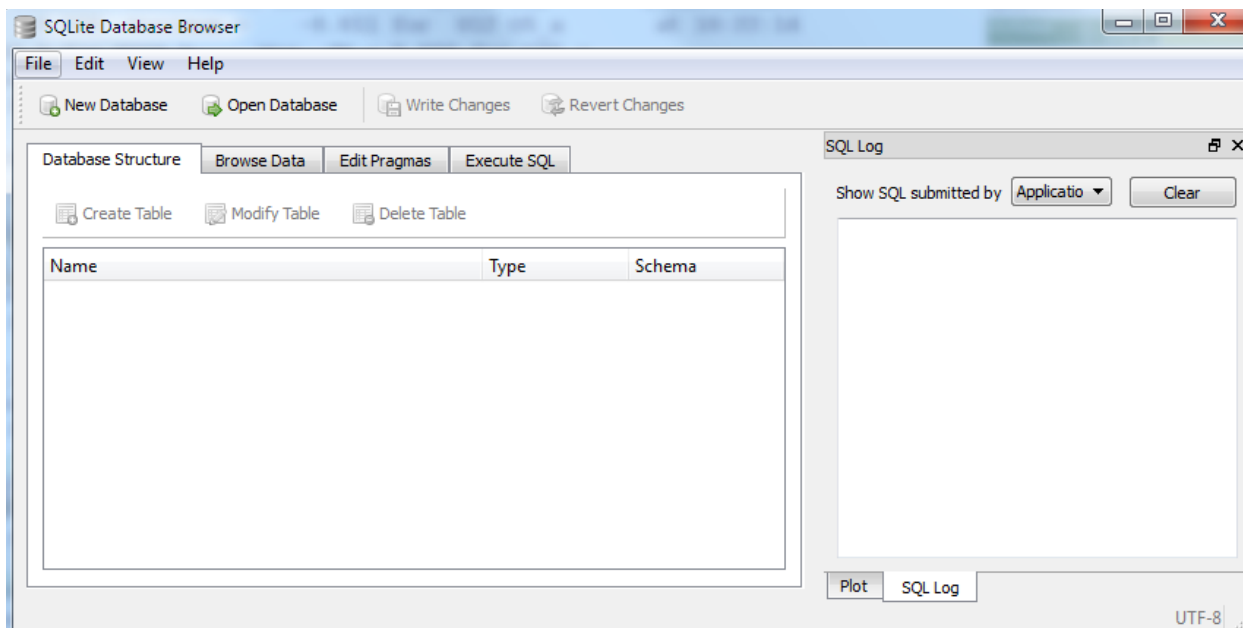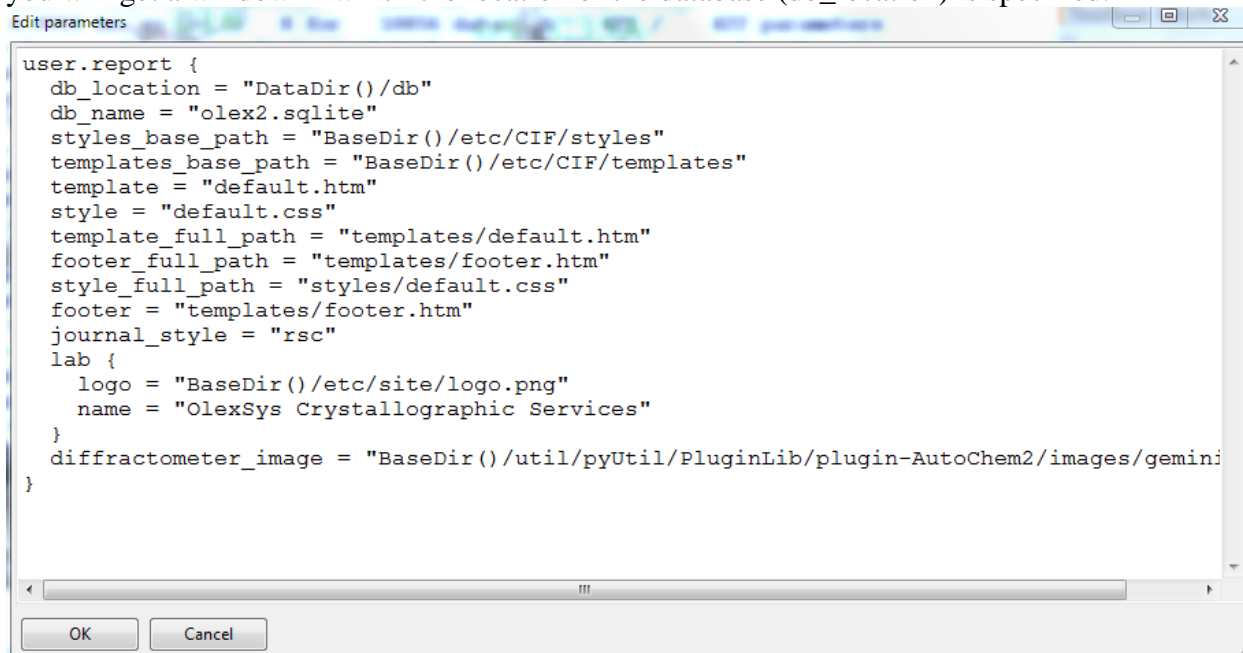
Restart OLEX2 for the changes to take effect.

Also, if you type
```
spy.editparam(user.report)
```
you will get a window in which the location of the database (db_location) is specified.


```
user.report {
   db_location = "DataDir()/db"
   db_name = "olex2.sqlite"
   styles_base_path = "BaseDir()/etc/CIF/styles"
   templates_base_path = "BaseDir()/etc/CIF/templates"
   template = "default.htm"
   style = "default.css"
   template_full_path = "templates/default.htm"
   footer_full_path = "templates/footer.htm"
   style_full_path = "styles/default.css"
   footer = "templates/footer.htm"
   journal_style = "rsc"
   lab {
      logo = "BaseDir()/etc/site/logo.png"
      name = "OlexSys Crystallographic Services"
   }
   diffractometer_image = "BaseDir()/util/pyUtil/PluginLib/plugin-AutoChem2/images/gemini
}
```

The location can be opened with
```
shell datadir()
```

default
restores all program defaults.

degen

prints the list of atoms on special positions

delbond atom1 atom2
delbond (selected atoms)

Removes the bond between `atom1` and `atom2`.
Selecting two atoms (such as C1 and C2) in the GUI and typing `delbond` is equivalent to typing
`delbond C1 C2`
Issuing a `delbond` command is equivalent to inserting a shelx `FREE` command in the instruction file.
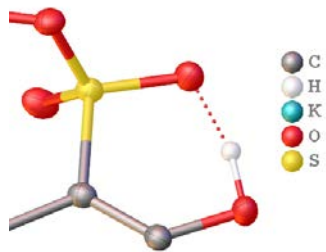
deltai [value]

specifies the connectivity delta for forming hydrogen bonds (and short interactions). `Value` is distance in Angstroms. For example, an undesirable hydrogen bonding interaction O-H...S shown below
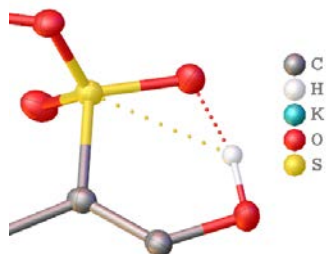
can be eliminated with
`deltai 1`
which reduces the default delta of 1.2 Å to 1 Å.

Typing `deltai` with no parameters output the current value of the delta. Should you change the delta it may be a good idea to change it back to the default value after you are done with figures.

direction

Prints the current orientation (vector perpendicular to the screen) of the model in fractional coordinates. If the selected direction is close to a principle direction the program also prints the direction of the current projection.
Example:
select two atoms in the GUI and type
`direction`
produces the following output:
`Direction: (-1.000*A, 7.846*B, 9.246*C)`
`View along 000-011 (normalised deviation: 0.045A)`
`View along 100-111 (normalised deviation: 0.045A)`

The first line of the output prints the equation of the direction. The two "View" lines refer to the direction (projection) perpendicular to the screen; in this case the viewer is "almost" looking down the [011] direction. This is NOT the direction specified by the two selected atoms.

If you now type
`matr 011`
the view is adjusted to look down exactly along the [001] direction.

To determine what direction is specified by the two selected atoms do the following:
with the two atoms selected (I know it's a redundant statement but bear with me) type
`line -n`
`direction`
The program will print out the direction equation and, if it's close to a primary direction, the deviation from the primary direction.

Echoing
By default the successfully executed commands are not displayed on the console. To see the issued commands on the console type
`silent off`
to enable echoing.

edit [file extension]
Typing `edit` by default opens the INS file for editing.
`edit lst`
opens the name.lst file for editing,
`edit res`
opens the name.res file. Also works with cif, ins, etc.

file filename.oxm
saves the current view with whatever is showing in Olex2. Loading this file should re-create the exact same view you had when you saved it.

fit

see `mode fit`

fixhl

Re-labels the H atoms consistently with the atoms they are attached to.

fix occu [value]

fixes the occupancy of the selected atoms. To assign a 33% occupancy to the selected atoms type

```
fix occu 0.33
```

fixunit [Z']

updates the formula based on the content of the asymmetric unit. The Z' value is unity by default. If the symmetry independent unit contains a number of molecules different from unity the Z' should be specified. It will be updated on the ZERR line in the INS file.

The OK button works similarly.

Example: the asymmetric unit contains one half of a molecule. To update the formula with the correct Z on the ZERR line type

```
fixunit 0.5
```

fmol

Displays all fragments

fuse

Resets the view to the symmetry-independent unit and quits some of the MODEs.

fvar [variable] [value]

This is a convenient and powerful command. There are four ways to use it.

1. When typed by itself, `fvar` outputs the values of all free variables to the console.

2. To assign a value to a variable, for example, to assign free variable number 3 a value of 0.72, one types

```
fvar 3 0.72
```

3. To assign several atoms to a free variable (let's say free variable number 4) select the atoms and type

```
fvar 4
```

If you you also want to specify the value of the free variable number 4 to be 0.2 type

```
fvar 4 .2
```

4. This option allows one to assign a positive and negative free variable (such as 5 and -5) to a set of atoms. When an *even* number of atoms is selected and the command is issued simply as

```
fvar
```

OLEX2 Manual

the first half of the atoms is assigned the occupancy as the next free variable (as deduced from the fvar line in the INS file; let's say there are four entries on the fvar line already) multiplied by one, in this case `51.000`, and the second half of atoms is assigned an occupancy of `-51.000`. The H atoms riding on these atoms follow suit.

Whereas option #4 is convenient, the `part` command may be a good alternative because frequently part numbers should also be specified when free variables are used.

grad [switch]
allows customizing the GUI background.
`switch: -p` [removes or inserts a picture as the GUI background]

`grad`
invokes a menu in which you can select the four colors for the four corners of the GUI canvas and the background will be colored with the proper gradient transitions.

To set a picture as your background use the switch `-p` with the full path to the picture file:
`grad -p='c:\xray\mypicture.jpg'`
and now F4 will toggle this new background. If it does not - restart OLEX2 (I know, I know). To remove the picture and return to the default gradient background type
`grad -p`

Graphics command for displaying the molecule:
`telp  [value] [atoms]`– displays the thermal ellipsoids of the value probability for the selected atoms. The atoms can be mentioned explicitly or selected in the GUI before this command is executed.
Example:
`telp 40 $c`
will display all C atoms at the 40% probability level.
`telph`
works like telp, but also shows the H atoms with their proportional displacement coefficients rather than small spheres of an arbitrary radius.
`pers [atoms]`
displays selected atoms as ball and stick. When no selection is made the change is applied to all atoms.
`proj [atoms]`
changes the display of the selected atoms to a line drawing.
`tubes`
changes the display of the selected atoms to a thicker line drawing (called "pipes" in some other programs)
Example:
`tubes $n`
will change the diplay of all N atoms and bond to the N atoms to the pipes display style.
`poly [argument]`
shows polyhedral for qualifying atoms. poly reguires an argument, thus its typical use would be

21

```
poly auto
```

grow [atoms] [switch]
generates symmetry-equivalent atoms in moieties residing on special positions.
switches:
-w: repeats the previous **grow** command on moieties in the asymmetric unit not bonded to the atoms outside the asymmetric unit. This is convenient for solvents and other moieties.
-s: generates the first shell (generates only the symmetry equivalent atoms covalently bonded to atoms in the asymmetric unit).

Example. A tetranuclear metal complex co-crystallizes with two solvent molecules of dichloromethane. The complex resides on an inversion center, thus the asymmetric unit contains a half of the complex and one solvent molecule (figure A). To see the entire complex one types
```
grow
```
to generate the second half of the complex (figure B). Note that the second solvent molecule is not generated. To see the second solvent molecule in order to represent the composition correctly you now type
```
grow -w
```
to properly represent the stoichiometry of the complex (figure C). Note that to generate figure C one must issue two grow commands, grow and grow -w, not just grow -w.
Alternatively, if you just want to show the full coordination sphere of the metal atom closest to the special position, instead of the first grow command you would type
```
grow -s
```
to complete the coordination sphere of that metal (figure D).



| A | B | C | D |
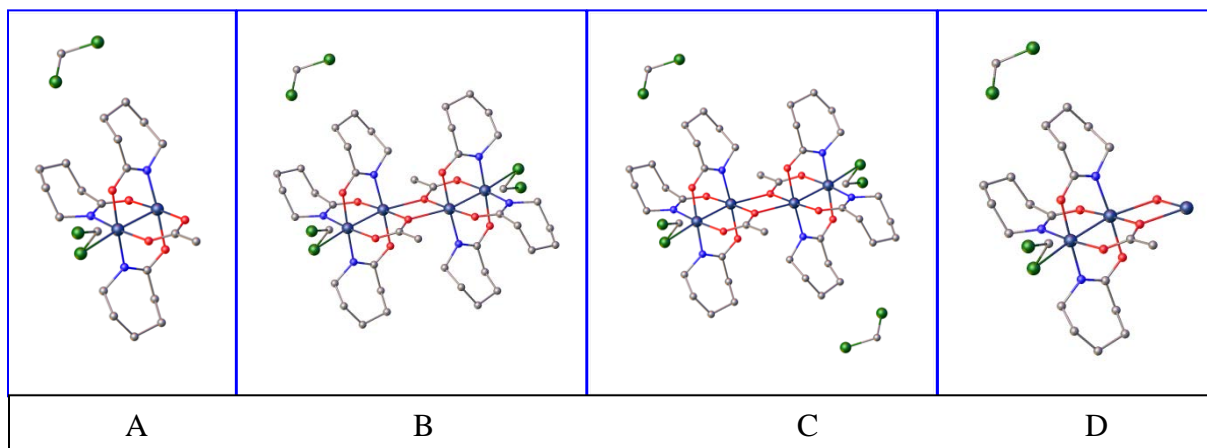
Also see mode grow.

**hide [atom list] [switch]**
hides atoms. Unfortunately, by design, if used without a switch it hides the selected atoms, not the bonds formed by them.
To hide all N atoms:
```
sel $n
hide
```

To hide all N atoms and the bonds formed by them:
```
sel $n
hide -b
```
Alternatively the atoms to be hidden can be selected in the GUI followed by
```
hide -b
```

## history

opens Notepad with 1000 last commands

## htab [dist] [angle] [switch]

analyzes the atomic connectivity list and inserts HTAB (and/or RTAB) and EQIV cards in the SHELXL instruction file in order to tabulate the hydrogen bonding interactions in the LST and CIF files with proper standard uncertainties. (Note that if the H atoms are in the idealized positions there will be no s.u.'s on the donor-H…acceptor angles.)

Defaults for the distance and angle are 2.9 Å and 150° and the default elements for the H-bond detection are N,O,F,Cl,S.

```
switches:
```
`-t:` adds extra elements that should be comma-separated
`-g:` if any of the detected H–bonds are generated by symmetry transformations, the structure is grown using those symmetry operations

If the `htab` command is issued multiple times only unique results will be added to the INS file.

Examples:
```
htab
```
will insert HTAB cards (and the necessary EQIV cards) for the detected hydrogen bonds in the INS file.

To survey more interactions one may use
```
htab 3.2 120
```
where `3.2` is the donor…acceptor distance in Angstroms, `120` is the donor-H…acceptor angle in degrees.

`switch -t` allow the use of additional elements in the hydrogen bond searches:
```
htab 3.2 -t=Br,I
```
will ensure that in addition to the default donor/acceptor atoms all Br and I atoms will also be considered and all H-bonding interactions shorter than 3.2 Å will be listed.

```
htab -g
```
produces an expanded structure if any hydrogen bonds are generated with a symmetry operation.

If too many bonds are generated and inserted into the instruction file and a removal of some of them is desirable, the HTAB commands should be edited out manually from the INS file.

Sometimes hydrogen bonds are not displayed in the OLEX2 interface, for example when the donor–donor distance is too long, e.g. 3.08 Å. This can be resolved in at least two ways.
1. Execute
`htab 3.1 140`
`fuse`
The `fuse` command forces OLEX2 to recalculate the bonds. In general, all H-bonds listed in the RES file with HTAB commands should be displayed.
2. Alternative you can adjust the delta for interactions:
`deltai 1.3`

## info

provides information about the selected molecule, such as formula, electron count, and mass. Especially useful to troubleshoot uncooperative `match` procedure to detect the differences between would-be identical molecules.

## kill [object]

removes the specified `atoms` from the model.
To delete atoms C1 and C2 either type
`kill C1 C2`
or select C1 and C2 in the GUI and type
`kill`
or type
`sel C1 and C1`
`kill`

To kill all atoms of a certain type use $:
`kill $n`
removes all N atoms from the model.

If atom labels have been placed for diagrams, as in Tools→Images→Label selected atoms
`kill labels`
will remove them.  The labels can also be removed as described in Working with Molecular Graphics.

## label [atoms]

generates moveable atom labels for diagrams.

Examples:
`label o1 o2` [will create movable labels for atoms o1 and o2].
`label $o`    [will create movable labels for all oxygen atoms].

## labels [switches]

displays non-printable labels for the atoms according to the switch.  These options are also available under Work→Toolbox Work→Labels.

To display all non-H labels (equivalent to F3) either would work:
```
labels
labels -l
```

To display all H atoms labels as well:
```
labels -l -h
```

The Q peaks are treated as atoms as far as labeling is concerned except for one unique command
```
labels -qi
```
which displays the Q peak heights in e/$\text{Å}^3$.

The labels can be hidden by another
```
labels
```
command.

To display the afix code for the non-H  atoms :
```
labels -a
```
To display the afix code for H atoms:
```
labels -h -a
```

To display the actual occupancy of the non-H  atoms:
```
labels -ao
```
As an example this value might be 21 or -21 for disordered atoms or 10.5 if an atom lies on a special position.
To display the actual occupancy for H atoms:
```
labels -h -ao
```

To display the chemical occupancy for the non-H atoms:
```
labels -co
```
This would be the actual value of the free variable for disordered atoms.
To display the chemical occupancy for H atoms:
```
labels -h -co
```

To display the PART number for the non-H atoms:
```
labels -p
```
To display the PART number for H atoms:
```
labels -h -p
```

To display the Uiso multiplier for non-H atoms:
```
labels -r
```
To display the Uiso multiplier for H atoms:
```
labels -h -r
```

To display the Uiso for non-H atoms:

```
labels -u
```
To display the Uiso for H atoms:
```
labels -h -u
```

To display the free variable number for the occupancy of non-H atoms:
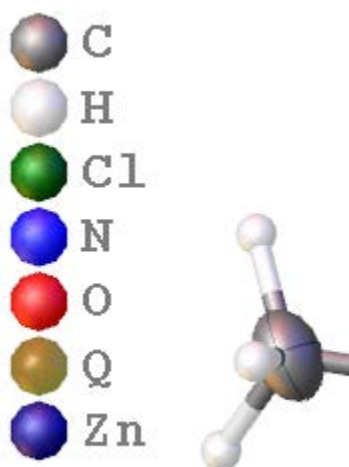```
labels -v
```
To display the free variable number for the occupancy of H atoms:
```
labels -h -v
```


legend

displays an insert showing atom types. Typing `legend` toggles the display of the insert. The insert can be moved within GUI by holding down the SHIFT key and dragging the left mouse button. As of April 29, 2016 this feature is only available in the DEV version of OLEX2.
```
Example:
```


line [-n] [atoms]   (note the command is singular)

Draws a least-squares fitted line for the atoms specified by the `atoms` and its length is displayed.   If only two atoms are specified a line is drawn between the atoms. The label can be hidden by right-clicking. In the case of more than two atoms the line length is determined by the atomic coordinates - a projection is taken and the max/min values are derived from the atomic coordinates.
If the -n switch is enabled no line is drawn and the molecular projection is reoriented to be viewed along the line determined by the `atoms`.
`Atoms` can be typed on the line or selected in the GUI.

Examples:
1. Select two atoms in the GUI and type
```
line
```
The atoms are connected with a line and its length is displayed.

OLEX2 Manual

2. Do not select atoms but type
line C1 C2
Atoms C1 and C2 will be connected with a line.

3. Select two atoms in the GUI, type
line -n
The molecular projection is shown along the line determined as described above, but the line itself is not drawn.

4. Do not select atoms but type
line -n C1 C2 C3
The molecular projection is now shown along the best-fitting line determined for atoms C1-C3.

Also see direction.

lines [value] (note the command is plural)
Displays the specified number of lines in the GUI. To display 40 lines type
lines 40
Note that you can cycle through the structure and text with CTRL-T that has three settings.
lines -1
displays all lines.

log
displays the content of the log file that contains all information about the OLEX2 run.

match [switch] [selection]
allows superposition of two or more molecule. The molecules must have the same composition and connectivity. By default, the program matches all atoms, thus if you do not want to see the H atoms they should be killed explicitly. A typical procedure involves three commands:
kill $h $q [to kill all the h and q peaks]
fuse [ensures the correct connectivity after atom elimination – very important command!]
match [will superimpose the molecules with all atoms used for matching].
or
match -i [will try to superimpose the molecules with and without inverting one of the molecules first]

To see how well the molecules fit on the right-hand panel select Tools→Overlay to see the RMS table. The table will refer to individual molecules as A, B, C…, which do not reflect the way your molecules are labeled.
To un-match the molecules type
fuse

A fragment can be inverted individually, by typing

```
inv
```

It is possible to match only selected atoms in two or more molecules. Select four or more atoms in one molecule, then four or more atoms (in the matching sequence) in another molecule (and other molecules if necessary) and type
```
match sel
```
Or
```
match -i sel
```

A convenient way to show the superimposed molecules is with the "stick" drawing style (achieved by typing `tubes` in the console) and different colors.

To color one of the superimposed molecules
right-click on the molecule→Fragment→Show this only [to display the molecules by itself]
ctrl-a [to select the molecule, both atoms and bonds]
right-click on the molecule→Selection→Group [to group atoms and bonds]
right-click on the molecule→Draw style [to display the Material Parameters palette]
In the Material Parameters palette double click on the color rectangle corresponding to Ambient Front and select the color of your choice followed by OK.
`fmol` [to bring back all the molecules on the screen]

Repeat as necessary for other molecules.
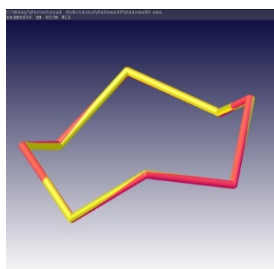
Example of two superimposed S_8 molecules, one red and one yellow.

For an additional example see section Structure Matching.

`matr [parameters]`
Orients the molecular projection according to the `parameters`.
`Parameters` can be supplied as
1. a [uvw] lattice line from the origin
2. a lattice line from lattice point u1v1w1 to lattice point u2v2w2
3. a full Cartesian matrix
the uvw values should be either space-separated or have the same number of digits.
Examples:
1. To orient the view along the crystallographic *a* axis any of the following will work:
`matr 1`
`matr 100`
`matr 1 0 0`
To orient the view along [5,12,1] the following would work (note that if the values have different numbers of digits either spaces or preceding zeros are necessary to ensure that each value has the same number of characters):
`matr 5121`   / would not work
`matr 5 12 1`
`matr 051201`
To orient the view along [0-12] it is necessary to either use spaces or supply the signs for each value or or supply preceding zeros to ensure that each index has the same number of characters. Either of the following three would work.
`matr 0 -1 2`
`matr 00-1+2`
`matr 00-102`
2. To orient the view along the vector from 010 to 12,2,4 use two numbers without spaces between indices (note the use of preceding zeros):
`matr 010 120204`
`matr 010 12 2 4`   /would not work

The current projection can be saved with a `save view` command:
`save view filename`
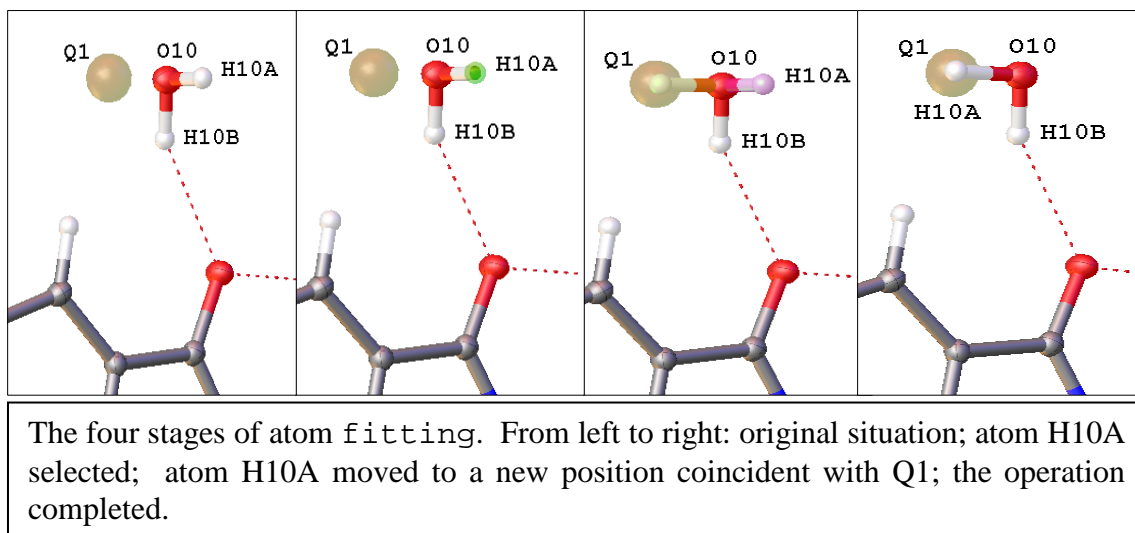and loaded later with
`load view filename`

OLEX2 Manual

mode fit [switch]
allows one to (1) move an atom or a group of atoms, (2) rotate a group of atoms, (3) split a group
of atoms.
switch can be –s followed by the number of atoms to not be displaced as in
mode fit –s=1 (see part (3) of this section).
1) If you want to move an atom to a new position in the GUI follow these steps.
   a) Select an atom.
   b) type mode fit on the console. The selected atom will acquire a greenish tint.
   c) Press the SHIFT button and use the left mouse button to move the atom in question to a
       new position. While you are dragging the atom the old atom position is also displayed
       and both the old and the new positions are connected with a bond.
   d) When you are satisfied with a new location for the atom press the ESC key. The atom will
       remain situated at the new position, the old one will disappear, and you will have quit the
       fit mode.

   Example: The program incorrectly assigns one of the water molecule's H atoms to atom
   O10, diagram below. Atom H10B is placed correctly, whereas atom H10A needs to be
   moved to coincide with Q1. The four steps are outlined in the diagram.

The four stages of atom fitting. From left to right: original situation; atom H10A
selected; atom H10A moved to a new position coincident with Q1; the operation
completed.

30

(2)   A group of atoms can be rotated about a bond. This is handy, for example, for –CF$_3$ groups and H atoms.
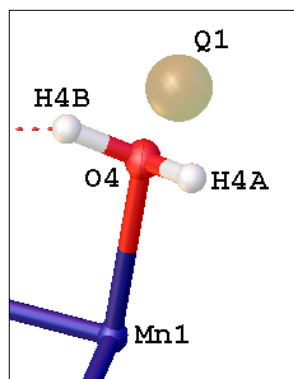
Example with a water molecule. A refinement program was asked to assign water molecule H atoms to atom O4 (see figure on the left), but a subsequent refinement revealed that one of the H atoms was not placed correctly, as demonstrated by the electron density peak Q1.

The goal is to rotate the water molecule about the Zn1–O4 bond to bring the H atoms into correct positions. Importantly, this rotation operation will not destroy any AFIX commands imposed on the geometry of the water molecule.

The first step is to decide which of the H atoms is in a wrong location. To figure it out display the Fourier difference map by Work→Toolbox Work→Electron density map:
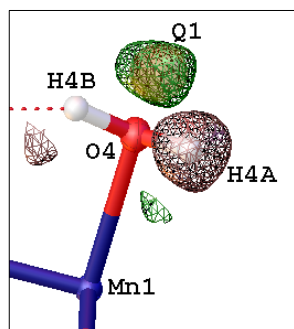
The green color shows areas with excess of electron density (it overlaps with Q1) whereas the brown-purple meshwork indicates holes. Atom H4a is in an incorrect position.

We will rotate the water molecule about the Mn1–O4 vector so that H4a will move to the position of H4b, and H4b will take the position of Q1.
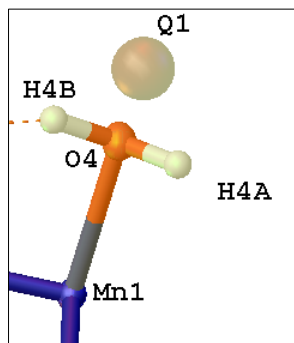
Hide the map by clicking on Work→Toolbox Work→Electron density map.

Select atoms O4, H4a, H4b in that order. The first selected atom will be on the axis of rotation.
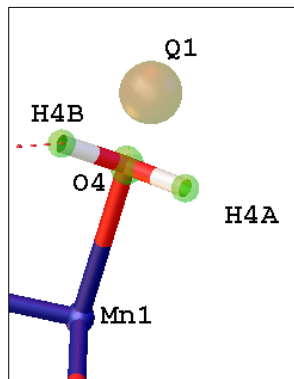
In the console type `mode fit.` Alernatively, select "fit" from the dropdown menu under Work→Toolbox Work→Select group of atom(s) and then
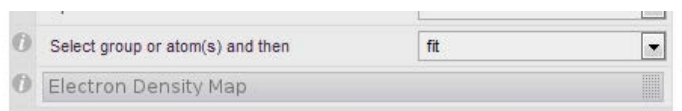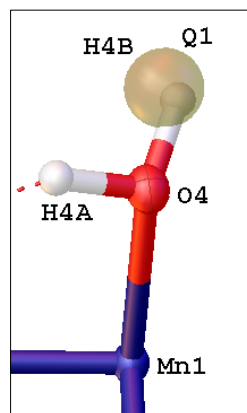
The selection will change the colors. Note that the Mn1–O4 bond is also highlighted. This is the axis of rotation and this is why it was important to select atom O4 first.
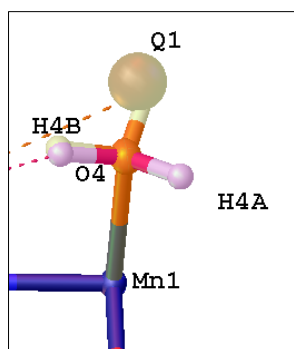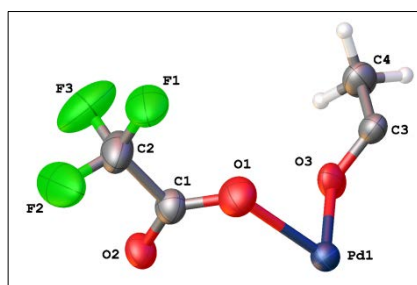

Right-click on the Mn1–O4 bond. Then left-click and drag on the Mn1–O4 bond. The water molecule will rotate about the Mn1–O4 axis. The final position may look like the diagram on the left. It is a little crowded because both the starting and final positions of the H atoms are shown.
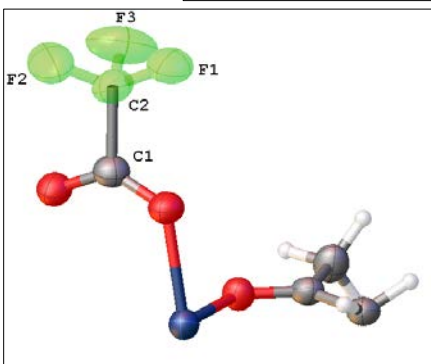

Type `mode off` in the console to exit the `fit` mode and produce the desired outcome:

(3) Splitting a group of atoms into two for the refinement of positional disorder is illustrated with a –CF$_3$ group.
This is seriously cool. The idea is to split atoms F1,F2,F3 into two sets by rotating the CF$_3$ group about the C1-C2 axis.

Select atoms C2 F1 F2 F3 by clicking on them in this order. In general, a selection can be made by drawing a box around the atoms of interest (by holding down the SHIFT key and dragging the mouse with the left button depressed), but in this case the order in which the atoms are selected is important.
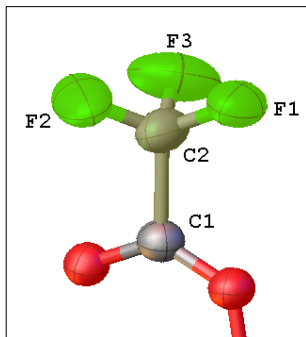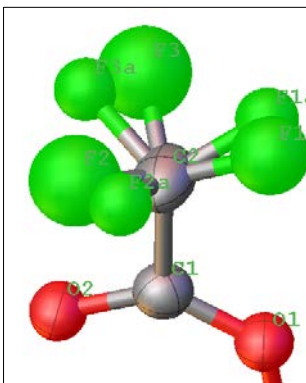
In the GUI type

```
mode fit -s=1
```
to indicate that we will be fitting the whole group to a new location, but one atom (the first atom of the selection) will not be split.

The colors change somewhat, but importantly, the C1–C2 bond is highlighted:

Right click on the C1–C2 bond once.
Press the left mouse button and drag on the C1–C2 bond to rotate the F atoms about the C1–C2 axis.

When you find good positions for the new F atoms, press ESC. The anisotropic F atoms have been split into two sets of isotropic atoms:

```
FVAR 0.20168 0.75
PART 1
F1    5    0.27260  0.87054  0.57380  21.00000  0.07766
F2    5    0.31045  0.91385  0.76109  21.00000  0.10564
F3    5    0.22327  0.78921  0.69629  21.00000  0.11074
PART 2
F2a   5    0.32353  0.93217  0.71783 -21.00000  0.05000
F3a   5    0.24159  0.81252  0.75254 -21.00000  0.05000
F1a   5    0.24608  0.83512  0.57664 -21.00000  0.05000
```

Note that the F atoms are assigned to two parts with occupancies 21 and -21 and that the second free variable with a value of 0.75 has been added to the FVAR line.

mode grow [switch]
Displays clickable bonds to generate symmetry-related molecules.
To display clickable bonds to covalently bonded atoms:
```
mode grow
```

```
mode grow -a
```
Allows to conveniently reposition atoms to symmetry-related sites within the same molecule. It is exceptionally handy when a molecule occupies a special position. [but try
```
compaq -m
compaq
```
first. It may do what you wish to achieve.

To display clickable bonds to generate symmetry related atom that can be used in the refinement with PART -1:
```
mode grow -p
```

The new atoms generated thereby behave as independent atoms and can be used in FRAG commands, but the occupancy of these atoms and their source atoms should be adjusted.

To display clickable bonds to atoms within short contacts:
`mode grow -s`

`mode grow -v`
Example: `mode grow -v=3`
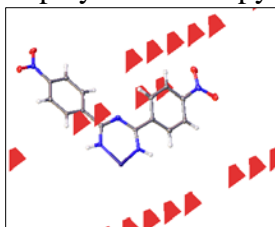The mode will be used with the user-provided delta for connectivity analysis; the default is 2 Å.

mode off
exits the current mode and return the cursor to the default "arrow".

mode pack
displays clickable pyramids that allow generation of additional asymmetric units:

move (for moving atoms see mode fit)
places all entities inside the unit cell, as close to the cell center as possible.

mpln [atoms] [switch]
short for Mean PLaNe. Computes the best LS plane through the selected atoms.
[switch] values are -n or -r.
1. `mpln`
computes the best-fitting LS plane through the atoms selected in the GUI or through all visible atoms if no atoms are selected. The atoms are in the "corners" of the plane
2. `mpln -n`
computes the best least-squares plane and orients the molecule so that the normal to this plane is perpendicular to the screen. Convenient for showing the best molecular orientation.
3. `mpln -r`
similar to mpln -n, but the created plane is rectangular and the atoms are no longer in the "apices" of the plane.
Example:
1. `mpln C1 C2 C3`
computes the LS plane through atoms C1, C2, and C3
2. `mpln C1 C2 C3 -r`
computes a rectangular plane through C1, C2, and C3

name [value]

renames the selected atoms or modifies there labels.
Example:
1. Select a number of atoms and type
`name 1`
to have the atoms labeled sequentially starting with the number 1.
2. Select a number of atoms and type
`name N`
to rename all selected atoms to be nitrogens.
3. Select a number of atoms and type
`name -s=d`
to have the trailer "d" to be added to all the atom labels.
4. Select a number of atoms and type
`name -s=`
to have the trailer removed from all the atom labels.

options

Typing `options` will open your local file `.options` that contains a few commands that you modify to improve the program performance. You may not be aware of these commands because the defaults usually work. All `options` are listed at
http://sourceforge.net/p/olex2/code/HEAD/tree/trunk/options.txt
Any of those commands can be changed Examples: if you are experiencing difficulty with atom selection (too difficult to select an atom by clicking on it) you can insert
`gl_stereo=false`
into your `.options` file. Restart OLEX2 and the problem should go away.
If H atoms cannot be assigned in tricky situations (such as when PART -1 is involved) – insert
`safe_afix=false`
into your `.options` file. Restart OLEX2 and the problem should go away.
Currently my `.options` files looks like this in its entirety:
```
gl_stereo=false
gl_multisample=true
confirm_on_close=false
preserve_restraint_defaults=true
safe_afix=false
```

After you have made your changes restart OLEX2.

panel [value]

The command sets up the width of the menu panel in the GUI. The default is 400 pixels and it works well. A typical problem is that some buttons on the menu panel cannot be seen if the panel width is smaller (sometimes upon the initial installation). This usually results from a suboptimal menu panel width. Type
`panel 400`

OLEX2 Manual

wait several seconds and the default should be restored.

`part number [occupancy]`

assigns the part number and occupancy (optionally) to the selected atoms. The occupancy involve a free variable.

Example.

To assign part number 2 to atoms C1 and C2:

select atoms C1 and C2 and type

`part 2`

Now atoms C1 and C2 belong to part 2.

To assign the selected atoms to part 3 with occupancy of 40% type

`part 3 10.4`

To assign the selected atoms to part 1 with occupancy defined by the third free variable:

`part 1 31`

To remove the symmetry relationship between symmetry-generated atoms, option `-c` is the ticket. This function is handy when one is modeling a molecule disordered over a symmetry element, such as an ethyl acetate over an inversion center.

Example:

Assume you see four peaks of electron density in the asymmetric unit. Type

`grow`

to generate the symmetry-related peaks. Rename them to be carbons. To be able to model this molecule as `part -1` you should select all these atoms and type

`part -1 -c`

`fuse`

At this point the extra atoms can be deleted and the remaining atoms refined in `part -1` with an occupancy of 50%. That is achieved by selecting this molecule and typing either

`part -1 10.5`

or

`fix occu 0.5`

`pictCODE filename` [CODE = STL, VRML, PLY]

will generate a respective file for 3D printing. To prepare an STL file for 3D printing type

`pictSTL filename`

However, before this command would work the 3D print extension module should be installed as follows. Go to HOME→Extension modules, enter your e-mail address in the e-mail field, select "3D plus - Install" in the Modules drop-down menu and click the Install.

An e-mail with an activation link will be sent to you. Once you follow the link and activate it, go back to the Extension modules, select 3D Plus - Install and click on Install to actually install the software. Restart OLEX2 and the pictCODE command will be functional.

To prepare the created STL file for printing download the Autodesk Meshmixer from 123AutoDESK on your computer: http://apps.123dapp.com/3dprint/install.html.
Install the Meshmixer in a typical fashion, start the program, and load in the STL file prepared by OLEX2. To molecule can be moved under the Print tab.

March 30, 2016. Richard Staples shared the following instructions that will fix some errors in the OLEX2-generated STL file. In Meshmixer:

1)   Import your structure
2)   Go to Print menu
3)   Transform, click on fit to build volume (so I can see the compound.)
4)   Click done
5)   Click Repair selected (will take some time)
6)   Export
Now the file can be sent to your 3D printer.

`pim [-l]`
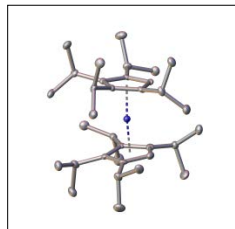generates a metal-π bond. The thickness of the bond is set at 50% of that of a normal bond, as if `BRAD 0.5` has been issued for these metal-centroid bonds.
When the switch `[-l]` is used the metal-centroid bond length is also shown.
Example. In a metallocene complex issuing
`pim`
will remove the ten metal-C(Cp) bonds and create two dashes bonds to the centroids (fig).

To restore the original view type `fuse`.

Platon button

Clicking the button launches PLATON. If this function does not work the first time there is an easy fix. In the PATH for your system environment variable insert the location of the platon.exe, in my case it is C:\pwt. It may help to insert it toward the left end of the PATH line. Restart OLEX2 and it should work. See the installation notes at the beginning of the document.

reap

opens up the Open Dialog in the directory of the current project. Shortcut: CTRL-O.

refine [cycles] [peaks]

Runs a refinement with `cycles` of least-squares cycles and displays `peaks` of electron density peaks. The command resets these numbers in GUI. Example for 12 cycles and five peaks:
`refine  12 5`

run

This command allows one to issue multiple commands on the same line; these commands will be executed consecutively.

Example:
To execute `telp, brad 0.3, sel $H, tubes, brad 0.2` in one command type
`run telp>>brad 0.3>> sel $h>>tubes>>brad 0.2`
This makes sense if you plan to perform these commands several times because the line can be reproduce with the "up arrow" key.

Saving and loading of the current state of the structure
save keyword [name]

records a snapshot of a property of the current model.
`keyword` can be `model`, `scene`, `style`, `view`.
If `name` is not specified a File Save dialog is launched. If `name` is specified a file with this name and proper extension will be saved on the hard drive.

`save model`
saves both crystallographic and graphics information of the current model.
`save scene`
saves the properties of the scene such as background, light parameters, etc. This is equivalent to right-clicking on the GUI background and selecting Draw Style→Scene Properties→Save.
`save style`

saves the properties of atom graphics, such as atom colors. The overall visual appearance depends on the combination of the style and scene properties. Equivalent to right-clicking on an atom and Graphics→Draw Style.
```
save view
```
saves the current projection.

To load the saved item use, in a similar fashion,
```
load keyword [name]
```

Example:
To save the current projection:
```
save view projection1
```
To load projection1:
```
load view projection1
```


sel [arguments] [switch]
```
switches:  a;c;i;l;u;
```
If no arguments provided, prints the information for the current selection. This includes distances (when two atoms are selected) , angles (three atoms), and
torsion angles (four atoms) and other geometrical parameters (such as dihedral angles for planes).

Example:
with three atoms selected
```
sel
```
shows computes the angle defined by the three atoms.

`sel` also selects atoms fulfilling provided conditions, seuch as
`sel $type` - selects any particular atom type where the type is
* - all atoms
m – metals
x – halogens
$ - means all
`sel $*,type` - selects all but `type` atoms

Examples:
`sel C1` – selects atom C1; convenient when one needs to highlight a specific atom in a crowded structure
`sel $c $n` - selects all C and N atoms.
`sel $m` - selects all metals
`sel $*,o` - selects all but the oxygen atoms
To select all atoms
`sel $*`
To select all atoms except hydrogens
`sel $*,h`

To select all atoms but carbons and nitrogens:
`sel $*,c,n`
(it's important that the elements are mentioned after the comma without capital letters.
To deselect a specific, selected atom the selection should be "inverted":
`sel c1 -i`

An extended syntax include keyword 'where' and 'rings' which allow selecting atoms and bonds accordingto their properties, like type and length or rings of particular connectivity like C6 or NC5.
Example:
`sel rings C5` - selects all rings formed by five carbon atoms.

To select all atoms from a PART use
`sel part number`
Example:
`sel part 2` - selects all atoms in PART 2.

If the 'where' keyword is used, logical operators, like and (&&), and or (||) can be used to refine the
selection. For example:
sel atoms where xatom.bai.z > 2 - to select all atoms heavier after H
sel bonds where xbond.length > 2 - to select all bonds longer than 2 A
sel bonds where xbond.b.bai.z == 1 - to select all bonds where the lightest atoms is H
 Switches:
   a - select all
   c - copies printed values to the clipboard
   i - invert selection
   l - consider the list of bonds as independent
   u - unselect all

To select all the bonds:
`sel bonds`
To deselect all the bonds:
`sel bonds -u`
To invert the selection
`sel bonds -i`

To mark bond distances or angles in the CIF as "to be tabulated in print" for Acta Crystallographic purposes the following commands are useful.
To include all bonds to the halogen atoms:
`sel CIF bonds $X`
In general, X designates halogen, M designates metal.
to report all angles involving all nitrogen atoms
`sel cif angles $* $n $*`
or
`sel cif angle $n`

OLEX2 Manual

For a specific atom (e.g. C4):
`sel cif angle c4`
I believe merging CIF from the REPORT section of the GUI is required.

`showp number1 number2 … numberN`
showp = show parts. This command is used to display specified parts.
To display PART 1 type
`showp 1`
to display PARTS 0, 2, and 3 type
`showp 0 2 3`

`skin name`
allows one to customize the uppermost banner of the GUI with a custom image. The `name` is the
name of the new "skin". Create a png of jpg file (115 x 800 pixels), place it in the
C:\Program Files\Olex2-1.2-beta\etc\skins
folder. Let's call it myskin.png.
Then create a new binary file myskin.phil with this content:
gui {
  skin {
    name = uw
    logo_name= etc/skins/myskin.png
 }
}

and in the OLEX2 GUI type
`skin myskin`
OLEX2 will think for a few seconds and then will display the new logo. The rest of the layout
will be default. Whereas extensive customization is possible, this is an example of the simplest
approach.

`standardise`
repositions every atom inside the IUCr-recommended asymmetric unit. Use `compaq` to
reassemble the molecule. Note that you can type the first four-five letters of the command (any
command) and use the TAB key to complete the word.

`text`
displays the DOS prompt text in a separate window
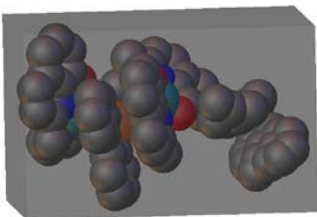

`uniq atomname`
displays the fragment containing the named atom while hiding all other fragments.

wbox

Draws a rectangular Wrapping BOX around the chemical moieties on the screen. The vdW radii employed in the computation are printed.
Example:
typing wbox produces this drawing

and the following text:
```
Using the following element radii:
(Default radii source:
http://www.ccdc.cam.ac.uk/products/csd/radii)
C    1.7
Al   2
N    1.55
O    1.52
Si   2.1
Wrapping box dimension: 13.076 x 15.712 x 20.082 A
Wrapping box volume: 4125.938 A^3
Please note that displayed and used atomic radii might be
DIFFERENT
```

To remove the box right-click on the box→Hide.

GUI equivalent: Tools→Chemical Tools→Bounding Box.

xp

launches the proprietary molecular graphics program XP written by George Sheldrick. Whereas OLEX2 speaks "xp", not all XP commands are implemented in OLEX2. You can manipulate your structure in XP and then save the changes with the file command. The changes will be reflected in OLEX2 GUI, provided the file name was the same.

Space group selection/manipulation

Q: How is the space group selected?
A: In order to see the statistical analysis of the diffracted intensities type the four commands:
wilson_plot [displays Wilson plot and the *E*-statistics.].
sg [to generate the space group info]

text [to show the screen content in an external text editor. Scroll down to see all the stats relevant to the space group selection].
log [to show the full program log for the current session in an external text editor. Scroll down to see all the stats relevant to the space group selection].

Q: How do I display the info on my current space group?
echo sgs() [shows cell choice type selection]
sginfo [space group] [shows the info on the specified space group, not necessarily on your current space group].
Examples:
sginfo fdd2
sginfo P21/c

Q: How do I convert space group P1 with two symmetry-related molecules into P$\bar{1}$ with one molecule?
A: Let us use the following Cr complex $(C_6H_5C_6H_4Br)Cr(CO)_3$ (I) as an example (*Acta Cryst., 2003,* **C59**, m499-m500).
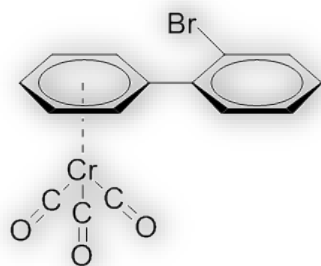

Figure 1. The Cr(0) complex (I) used to illustrate the P1→P$\bar{1}$ switch.

This structure of (I) could not be solved in P1 and had to be solved in P1 with two molecules, Figure 2.
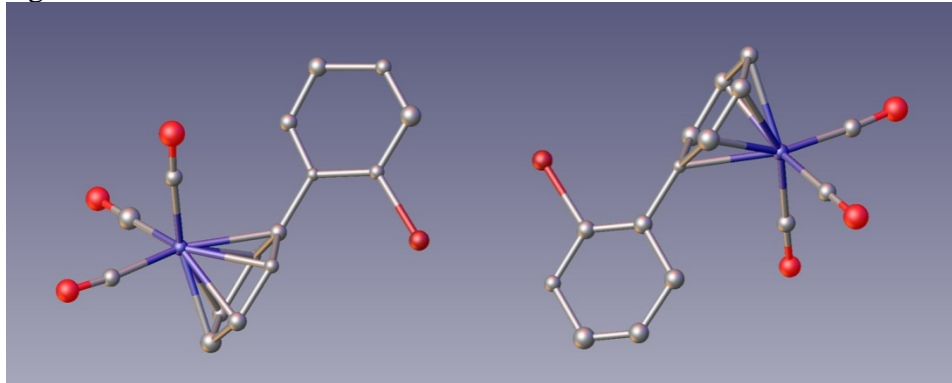

Figure 2. The structure of (I) solved in P1. The two molecules are related by an inversion center.

Now execute the following commands:
1. **Select two symmetry related heavy atoms (e.g. the bromines).**
2. **echo ccrd(sel)** - you will see the three coordinates (x,y,z) of the geometric center between the **sel**ected atoms.
3. **push -x -y -z** [adjust all atomic coordinates so that the observed inversion center be coincident with a crystallographic inversion center at 0,0,0].
4. **Select the same two symmetry related heavy atoms.**
5. **echo ccrd(sel)** [to double check that the geometric center coincides with an inversion center at 0,0,0]
6. **changesg P-1** [merges the molecules].
The space group symbol in the upper right corner of the GUI should be updated.

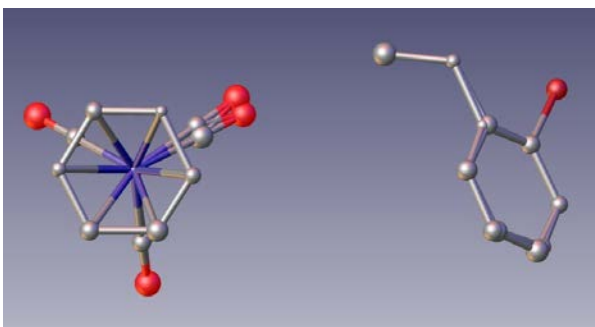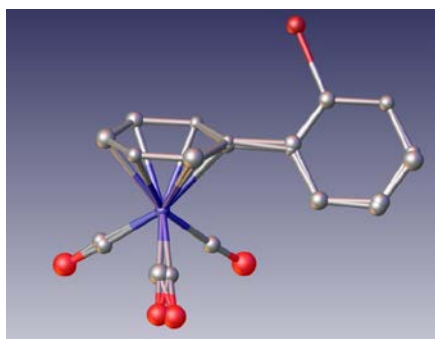Now the structure may look correct *or* like in Figure 3.

Figure 3. The structure of (I) immediately after converting the space group to the correct $P\bar{1}$.

In order to reassemble the two separate parts execute
7. **compaq**
and now the structure looks like in Figure 4.

Figure 4. The structure of (I) is in the correct space group $P\bar{1}$, but needs polishing.

Sometimes the resultant merged molecule contains extra atoms near the expected positions (Figure 4). This is because some symmetry-equivalent atoms were not perfectly related by an inversion center. These redundant atoms should be eliminated. In the case of (I) there are four extra sp^2-carbons and two extra carbonyl carbon and one oxygen atoms.

The extra atoms can be deleted manually (it does not matter which one of the two you delete at each site) or by issuing

8. **`fuse 0.4`**

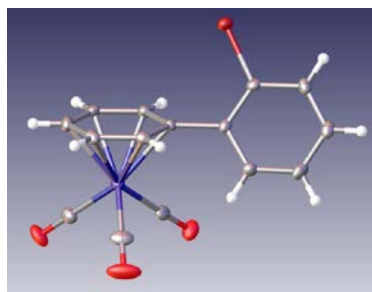This command will "fuse together" all atoms that are closer to each other than 0.4 Å.

Figure 5. The finished structure of (I) in the correct space group P$\bar{1}$.

Space group changes

Q: How can I change the space group choice?
A: Currently this is implemented for monoclinic space groups only.
`echo sgs()` [shows the current setting]
Then to change the cell setting issue
`sgs [unique axis][cell choice] [name.hkl]` [converts the unit cell type].
Example:
`sgs b1 mydata.hkl`
transforms the unit cell to cell choice 1 with the *b* axis unique, creates a new hkl file for the structure, transforms the atomic coordinates to correspond to the new choice. But the unit cell parameter esd's will be overestimated in the new INS file. Note that the space group symbol in the upper right corner of GUI does not get updated. Run a refinement and then reload the res file into OLEX2 to rectify.

Example of a space group change from P2_1/n to P2_1/c.
This corresponds to a change from cell choice 2 into cell choice 1.
`sgs b1 mydata.hkl`
will do the desired transformation.

Q: How can I change the space group?
A: This action is performed prior to structure solution. Click "Suggest SG" under the work→solve→Space group, and select a space group from the drop-down menu.
Alternatively, use the CMD line, for example:
`reset -s=P21` [resets the current space group space group to be P21]

OLEX2 Manual

Additional structure manipulations.

The display of the coordinated ring of binding to the metal in (I), Fig. 6 is easily adjusted to one dashed line:
1.   select the coordinated ring and the metal center
2. `pim`   (or `pim -l` to see the length of the bond)
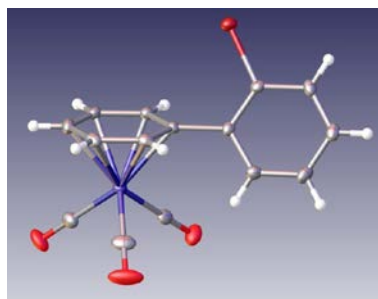**in order to obtain a cleaner view as in Fig. 1.**
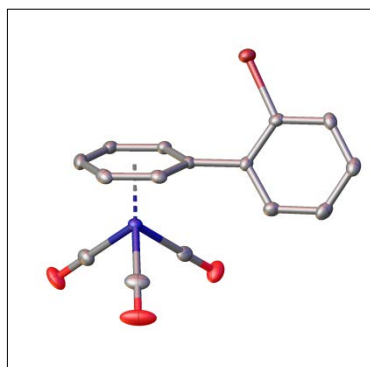

Fig. 1. The Cr complex.

Fig 2. Complex (I) with a different coordination depiction.

To go back to the previous display delete the dashed line and then type
`conn 9 Crl`
to force the metal center to make nine bonds.

To show delocalization of the electron density in the rings type
`chemdraw`
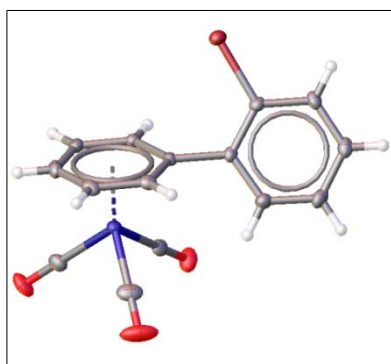to produce a drawing similar to that in Fig. 3.
To undo, type `fuse.`

Fig 3. Display of the delocalized electron density in rings.

To compute the dihederal angle between the ring planes one needs to rerun refinement with card
MORE -1
in the INS file. This card can be added to the INS file manually, or from OLEX2 GUI by typing
/ more -1
The forward slash tells OLEX2 to add a command into the INS file.
Note that more -1 is incompatible with the wpdb card.

This writes out a variance-covariance matrix into a file that is used by OLEX2 for further computations.

Select a ring and type
mpln
to generate a plane confined to a ring with a selector (black dot) in the middle.
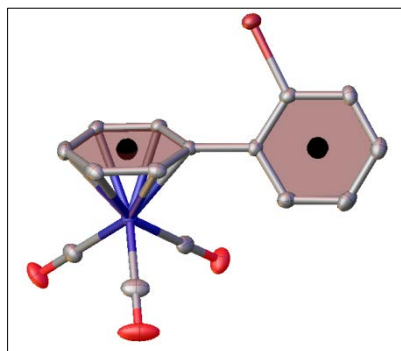Fig. 4 shows the two created planes.

Fig. 4. Two rings are ready for computation.

Select the rings by clicking on the selectors (selected rings turn green) and type
esd

to show some statistics with standard deviations on the screen. The dihedral angle of interest is
58.86(1)°.

This is a sample output on the OLEX2 GUI (the rings are labeled C1-C6 and C7-C12):

```
esd
Using shelxl matrix for the calculation
Plane C7 C8 C9 C10 C11 C12 to plane angle: 58.86(10)
Plane centroid to plane centroid distance: 4.343(2) A
Plane [C7 C8 C9 C10 C11 C12 ] to plane centroid distance: 0.092(5) A
Plane [C7 C8 C9 C10 C11 C12 ] to plane shift: 4.342(2) A
Plane [C1 C2 C3 C4 C5 C6 ] to plane centroid distance: -0.027(5) A
Plane [C1 C2 C3 C4 C5 C6 ] to plane shift distance: 4.343(2) A
```
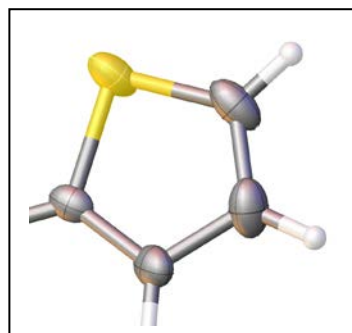

# How to combine / concatenate two or more commands into a macro command:

By Nattamai Bhuvanesh

It is possible to modify the macro file ***custom.xld*** in OLEX2 to your great advantage.

For example, a **telp** command will give you, by default, a display shown across:

But if you are like me, I am more inclined to do **telp**, followed by a **brad 0.3** (to make the radius thinner, and also selecting the hydrogens and making them smaller as well; and, finally unselecting the hydrogen atoms. This would result in a display which looks better for publications:
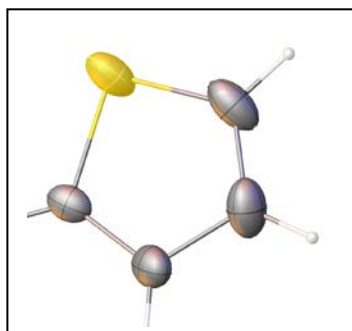
The commands **telp**, **brad 0.3**, followed by selecting the Hydrogens, making them smaller can all be combined into one macro:

1. Open Olex2
2. Type
"**emf**"
This will open the custom.xld file; where the custom macros reside.
3. You can start adding the commands, if you know the style, or copy one of the already existing macros and paste it at the end. Modify the commands in the macro.
    e.g.,

<bhtelp help="Change TELP Settings for Bhuv"
  <body
      <args>
      <cmd
          <cmd1 "telp">

        <cmd2 "brad 0.3">
        <cmd3 "sel $H">
        <cmd4 "arad 0.08">
        <cmd5 "sel -u">

    >

  >

>

a. Where bhtelp is going to be the new custom Macro's name
b. "Change **telp** Settings for Bhuv" is what OLEX2 will show if we type "help bhtelp"
c. If necessary, you may add args – arguments.
d. List all the commands to be combined within the <cmd …… > as above. In our examples, we are concatenating "**telp**", "**brad 0.3**", "**sel $H**", "**arad 0.08**", and "**sel –u**",
e. You may run these commands one by one and verify the end result before making them a macro. It is imperative that all the "<" should be matched to its corresponding ">".
f. After you are done, save the **custom.xld** file.
g. Go back to OLEX2 and type
reload macro
    and we are done.
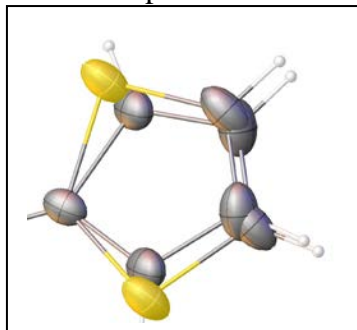Now you can use **bhtelp** to get the new styled **telp**.

Q: Is it possible to show only one or more (selected) "part" of the disordered atoms?
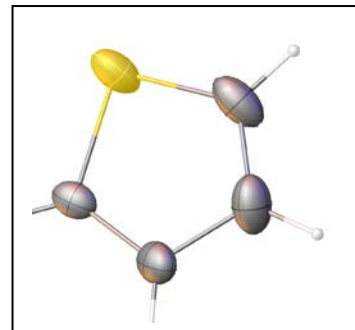A: Absolutely, only selected "part" numbers can be shown by using
showp 0 1
the parts under part 0 (zero and not "oh"), and 1 are shown.
For example:

This changes, on executing **showp 0 1,** to :

The command can be reversed by:
showp

If more parts need to be shown, they have to be added, *e.g.*,
**showp 0 1 3**

Constraining the molecular geometry

EXAMPLE 1.

There are several way to model molecular disorder. One of them to constrain the geometry of an entire molecule or fragment with an idealized geometry. This is based on the FRAG/FEND cards of SHELXL, but a lot will happen behind the scenes in OLEX. Concrete examples should help.

Example 1. Imposing an idealized geometry using peaks of electron density.

In the structure on the right we want to constrain the toluene geometry with an idealized geometry. The electron density peaks (golden spheres) are fairly consistent with the geometry. All you need for this procedure are three non-linear peaks regardless of the total number of atoms in the molecule.
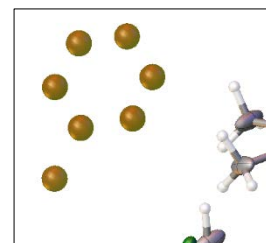
1. Prepare an idealized geometry of the molecule of choice (toluene in this case). It should look like a typical FRAG/FEND command:

```
FRAG 17
C1  1  1.198402 -0.033739  3.629224
C2  1  1.201835 -0.000101  2.122450
C3  1  0.001012 -0.000301  1.398484
C4  1  0.000813 -0.000261  0.002140
C5  1  1.208427  0.001721 -0.699221
C6  1  2.412741  0.006115  0.007778
C7  1  2.406015  0.006056  1.404106
FEND
```

Many DFT-optimized molecular geometries are available free at http://xray.chem.wisc.edu/Projects/IdealizedMolecularGeometry.html. Of course one can use a reasonable geometry from the Cambridge Structural Database or any other reliable source.

2. Copy the entire `frag/fend` list (including the `frag` and `fend` command) and paste them with CTRL-V into the GUI.
The idealized molecule will be inserted in green (on the right in the diagram below) and OLEX2 goes into the MATCH mode (the cursor is no longer an arrow).
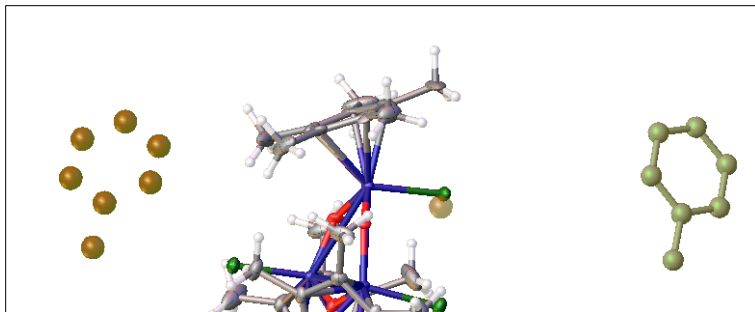
3. Match at least three atoms. We start with the Me carbons by clicking on the Me carbon of the green molecule and then on the Q peak corresponding to the toluene Me carbon:
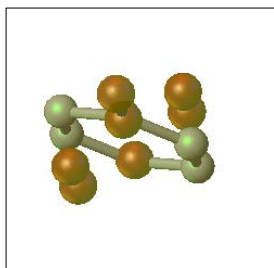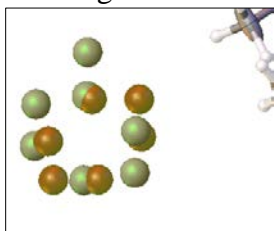
     Next we click on the pair corresponding to the para atoms:
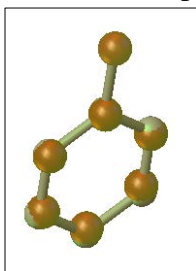
and then on a pair of meta atoms:
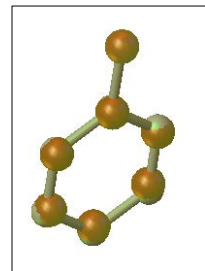
Now that a good match is obtained keep pressing the ESC key until you are out of the MATCH mode (the cursor becomes an arrow and the toluene molecule turns grey) or type mode off:

To manipulate the FRAG molecule:
Left click on the molecule and keep the left button depressed to rotate the molecule.
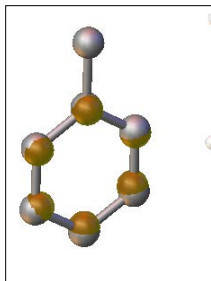Hold down the SHIFT key to drag the molecule with a depressed left click.
You can rotate the entire structure as usual if you click elsewhere on the GUI.

Once the inserted molecule is close to the proper place its position can be fine-tuned in the MATCH mode, by pairwise matching of the atoms and Q peaks:

4.   We are ready for a refinement. Note that this idealized toluene molecule has been incorporated into the ins file as a fixed geometry moiety:

```
AFIX 6
C1      C      0.21400   0.32710   0.26920   1.00000   0.05000
C2      C      0.23497   0.37425   0.18633   1.00000   0.05000
C3      C      0.15957   0.32139   0.14236   1.00000   0.05000
C4      C      0.18136   0.36307   0.06565   1.00000   0.05000
C5      C      0.27935   0.45902   0.03133   1.00000   0.05000
C6      C      0.35491   0.51286   0.07436   1.00000   0.05000
C7      C      0.33263   0.47074   0.15105   1.00000   0.05000
AFIX 0
```

The actual atom labels will depend on the content of your structure.

5.   If the refinement goes well re-label the toluene atoms, add the H atoms and make sure the occupancy of the atoms are correct.

EXAMPLE 2. Imposing an idealized geometry using atoms from a poorly behaved molecule.

The procedure is essentially the same, and the "old" atoms of the fragment being modeled will be deleted if they are within 0.5 Å from an atom from the FRAG unit.

When the pretty good default of 0.5 Å does not work the trick is to delete the atoms of the molecule being modeled after the idealized molecule has been matched, and leave the idealized molecule. If the "old", poorly behaved molecule remains present then there will be two molecules in the same space – which is obviously a problem.

Here is the procedure from the start (before any matching done).
Start by selecting the molecule you want to model and type
```
sel part 100
```

to assign part 100 to this molecule.

Now follow the matching procedure, steps 1 – 3 above.

Prior to the refinement and with no atoms selected type:
```
sel part 100
kill part 100
```

The original molecule has been deleted, the idealized one is left in the proper orientation and we can proceed with step 4 and 5.

EXAMPLE 3.

A Pd complex that co-crystallizes with ½ equivalent of ethyl acetate, figure on the right. The solvent molecule is disordered over an inversion center and should be refined with `part -1`.

Use file disorder 3.res and disorder 3. hkl to follow the steps.

1. Begin by deleting the solvent molecule and refining the structure.
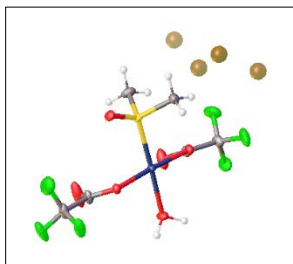
2. The refinement reveals, among other things, four residual peaks higher than the rest:

3. Optional: the four residual peaks can be reassembled with `compaq -c`.
   In the GUI make sure only the Pd complex and the four highest Q peaks are shown. Type `grow` to generate the symmetry related Q peaks:

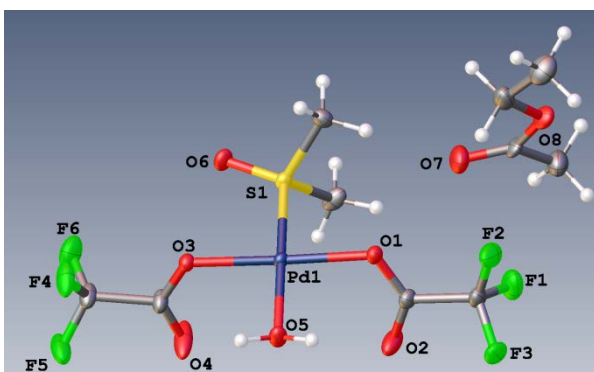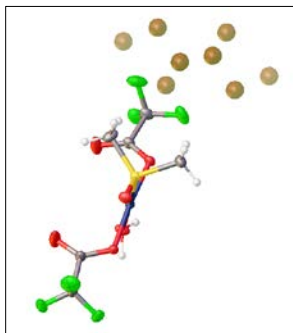4. Prepare an idealized geometry of the molecule of choice (ethyl acetate in this case). It should look like a typical FRAG/FEND command:

```
FRAG 17
O1   3 -0.787135   1.361478 -1.826069
O2   3 -1.250238   2.162490  0.179184
C1   1 -0.072846   0.126000  0.077980
C2   1 -0.733637   1.268944 -0.645662
C3   1 -1.903975   3.293234 -0.386436
C4   1 -2.401190   4.153250  0.753379
FEND
```

Many DFT-optimized molecular geometries are available free at http://xray.chem.wisc.edu/Projects/IdealizedMolecularGeometry.html. Of course one can use a reasonable geometry from the Cambridge Structural Database or any other reliable source.

5. Copy the entire `frag/fend` list (including the `frag` and `fend` command) and paste them with CTRL-V into the GUI.

The idealized molecule will be inserted in green(ish) (on the right in the diagram below) and OLEX2 goes into the MATCH mode (the cursor is no longer an arrow).
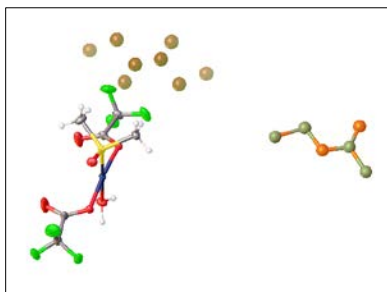
The inserted molecule can be overlaid on the Q peaks in the MATCH mode. Prior to that is may be beneficial to move the inserted molecule manually as follows:

      Left click on the molecule and keep the left button depressed to rotate the molecule.
      Hold down the SHIFT key to drag the molecule with a depressed left click.
      You can rotate the entire structure as usual if you click elsewhere on the GUI.

Once the inserted molecule is close to the proper place its position can be fine-tuned in the MATCH mode, by pairwise matching of the atoms and Q peaks:
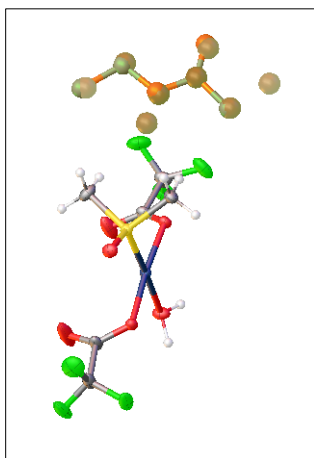
To exit from the MATCH mode either keep pressing the ESC button or type `mode off`:
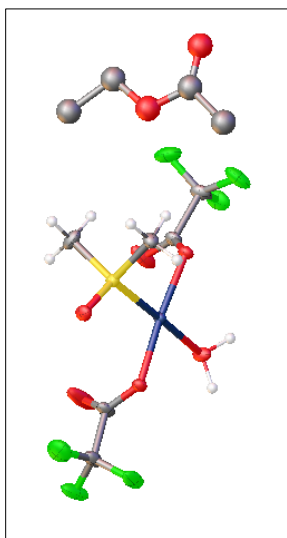
Because the solvent molecule is disordered over an inversion center it should be refined with PART -1 and occupancy of 50%.

First, we will assign part -1 to the solvent molecule.
Double click on the solvent molecule to select it. Then type
`part -1`

OLEX2 Manual

```
labels -p
```
The latter command serves to prove that the atoms belong to PART -1. The part numbers are displayed next to the atoms that are in a PART:
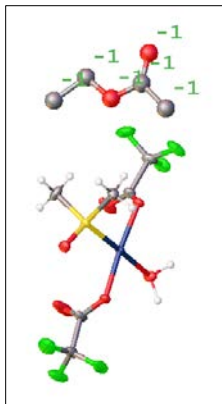
Next, the solvent molecule should be given the proper occupancy.

One way to do so is to select the molecule by double-clicking on it and then type
```
fix occu 0.5
```

Another way is to select the molecule by double clicking on it and then click on the "atom edit"

 button to modify the instructions in the context menu:

Prior to modification:
```
FVAR 0.38625
PART -1    ! the line to be modified
AFIX 6
O7     O      0.98336  0.46279  0.43296  11.00000  0.05000
O8     O      0.98510  0.56586  0.51732  11.00000  0.05000
C7     C      1.10254  0.28937  0.50910  11.00000  0.05000
C8     C      1.01760  0.44680  0.48150  11.00000  0.05000
C9     C      0.90473  0.72118  0.49622  11.00000  0.05000
C10    C      0.88189  0.83477  0.54498  11.00000  0.05000
AFIX 0
```

Only the occupancy must be modified, and that is achieved by addition 10.5 to the PART line:
Upon modification:
```
FVAR 0.38625
PART -1 10.5   ! modified line
AFIX 6
O7     O      0.98336  0.46279  0.43296  11.00000  0.05000
```

```
O8      O        0.98510   0.56586   0.51732   11.00000   0.05000
C7      C        1.10254   0.28937   0.50910   11.00000   0.05000
C8      C        1.01760   0.44680   0.48150   11.00000   0.05000
C9      C        0.90473   0.72118   0.49622   11.00000   0.05000
C10     C        0.88189   0.83477   0.54498   11.00000   0.05000
AFIX 0
```

Click OK and run a refinement. If the resultant structure looks "strange" and some solvent atoms are missing - type `fuse`. A proper view should be restored.

Refine the structure anisotropically.
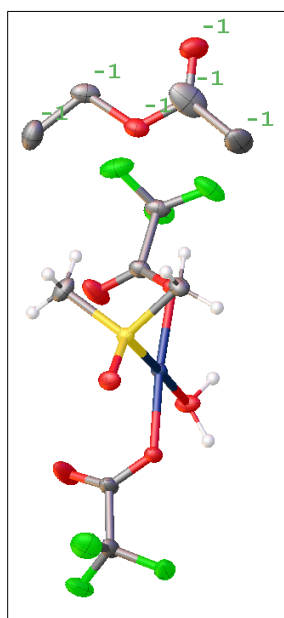
The refinement indicators have improved, but the ellipsoid of the carbonyl atom looks somewhat enlarged. In this case it is a good idea to remove the idealized geometry constraint:
-double click on the solvent molecule to select it.
-type `afix 0`.

Run a refinement. Then position H atoms on this molecule and run another refinement:

The solvent molecule looks much better and the overall refinement is stable. The R factor is 2.04%.

To remove the "-1" labels from the GUI type `labels`.

When a solvent cannot be modeled

Sometimes a solvent molecule can be neither identified nor modeled. In such cases option SQUEEZE of Ton Spek's PLATON can be used. The SQUEEZE procedure accounts for diffuse electron density. For people interested in the void algorithm of PLATON ("CALC SOLV"), you can check the following presentation:
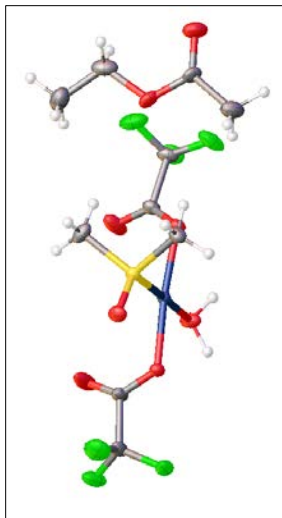http://www.cryst.chem.uu.nl/spek/ppp/PLATON-SQUEEZE.pdf
(pages 6-12) . An application in microporous crystals can be found in:
H. Küppers, F. Liebau and A. L. Spek (2006). J. Appl. Cryst. 39, 338-346.

[Solvent accessible voids can be displayed with Mercury. For an introduction to crystal porosity I recommend "Crystal porosity and the burden of proof" by Len Barbour, Chem. Commun., 2006, 1163-1168. But I digress.]

An alternative procedure, implemented in OLEX2, is based on the paper "Bulk-solvent correction in large macromolecular structures" by B. Rees, L. Jenner, and M Yusupov in Acta Cryst. D, 2005, 61(9), 1299-1301.

Let us proceed with the previous example Disorder3 with ethyl acetate. In this case it is known what the solvent is and thus the structure is a good test.
1. Delete the ethyl acetate solvent molecule and run a refinement.
2. Go to Tools→Maps→Mask and click on the Mask button to run a computation with the default parameters.

The program draws the solvent accessible voids in the GUI (unit cell drawing below) and generates a numerical output (also available in file name-mask.log) the bottom portion of which is copied here:

```
Void  Vol/Ang^3  #Electrons
   1     152.2        51.7
   2     152.2        51.7
```
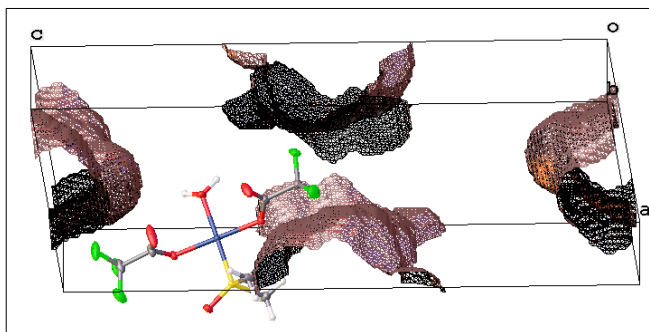
OLEX2 has identified two voids of 152.2 $Å^3$ with 51.7 electrons in each. Ethyl acetate contains 48 electrons and the estimated volume of the molecule is 124 $Å^3$. For comparison, PLATON (with the default settings) estimated the volume of each of the two voids at 145 $Å^3$ with 48 electrons in each. Similarly to this case, in my experience PLATON's algorithm frequently works better than OLEX's. With electron counts, anyway.

   To proceed with the refinement return to the Work menu (F5), expand the Refine menu, mark the "Use solvent mask" checkbox and run a refinement. You can also elect to "Recompute mask" by checking its box.

   You can proceed to completion in this fashion, or you can select file name-mask.hkl from the Work→Refine→Reflection file and uncheck the "Use solvent mask" and "Recompute mask" boxes.

   It goes without saying that this type of refinement should be documented in the experimental.

Working with molecular graphics

OLEX2 is great for generating publication quality diagrams. As an example consider the Cr(0) complex on the right. We will generate a very similar looking diagram with atom labels.

What you see on the screen is what you get in the graphics file.
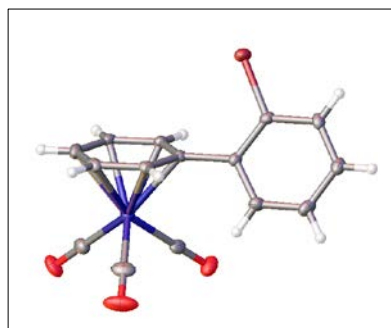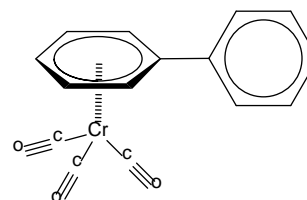
This is the default diagram.

OLEX2 Manual
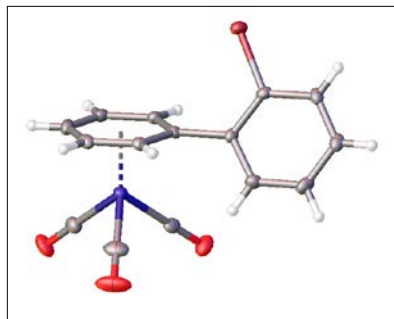
To remove the six Cr–C bonds and generate a dashed line to the center of the coordinated Ph ring type
`pim`
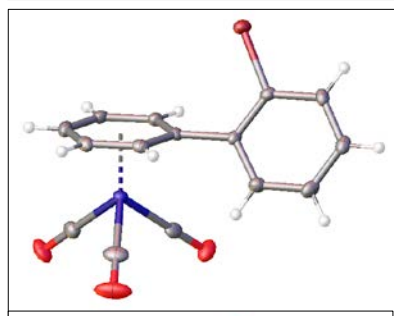
To change the thickness of the C–H bonds select one of the C–H bonds by clicking on it and type
`brad 0.5`
to make the C–H bonds 50% thinner. [For more on `pim`, `brad`, and other commands see the "Alphabetical list of commands"]
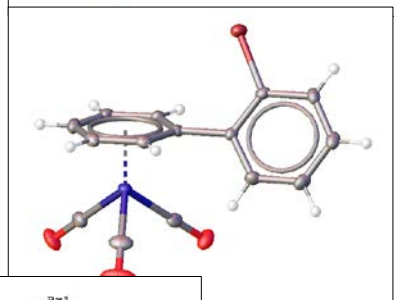
To illustrate delocalization of electron density in the Ph rings type
`chemdraw`
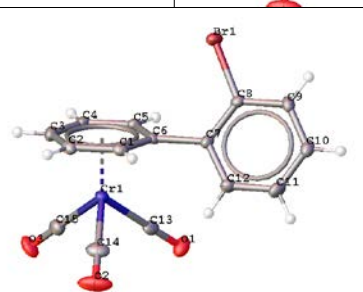
To add atom labels go to Tools→Images. If you want to label only some of the atoms first select them and then click under Images→1)Label selected atoms. To label all non-H atoms click on Images→non-H atoms.

Note that these labels differ from the green working labels that can be toggled off by F3.
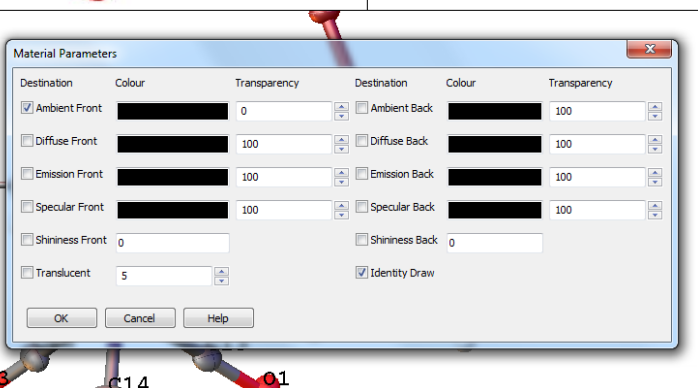
If the label color is not black (usually that happens when you run it for the first time) click on Images→3)Choose label color and in the menu Material Parameters double click on the color in the Ambient Front box and choose the color of your liking. I prefer black, my settings are shown in the figure to the left.

If you need to delete the labels type
`kill labels`
or follow the tip under Images→Tip.

60
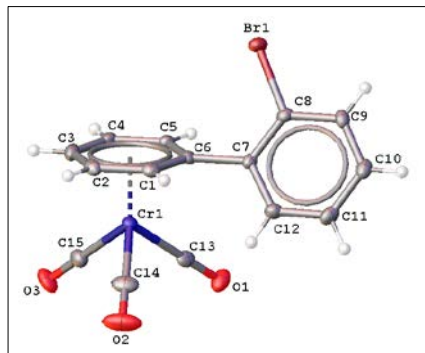
To position the labels so that they don't overlap with the atoms depress the SHIFT key and move the atom with the left mouse button.

To save the properties of the image for the future type
```
save view nameofyourchoice
```
To load it back at some point in the future type
```
load view nameofyourchoice
```

To save a high quality image go to Tools→Images→Bitmap Images, enter the name of your file, select the file type (png works well), the size (think of it as quality; the default 2 is adequate), and click on the Go button. A file with the specified name and extension will be generated in your structure folder.

Other types of images are created in a similar fashion.

Q: How do I display atom labels?
A: You can toggle atom labels with **F3**. Additional controls are
labels –l [displays non-hydrogen atom labels]
labels –l –h [display all atom labels including those for the H atoms]
The Q peaks are treated as atoms as far as labeling is concerned except for one unique command
labels –qi [displays the Q peak heights in e/Å^3]
Note that the word **labels** is plural.

To generate moveable atom labels for diagrams use
label [atom name(s)] [to create movable atom labels].
Examples:
label o1 o2 [will create movable labels for atoms o1 and o2].
label $o [will create movable labels for all oxygen atoms].
Note that the word **label** is singular.

Q: How do I display the unit cell boundaries?
A: Type
cell
to toggle the unit cell boundaries.

Q: How can I manipulate the molecular image representation?
A: The following commands are handy for manipulating the molecular image:
sfil [to see atomic spheres type]
telp [to switch to the ellipsoid view type]
telph [to switch to the ellipsoid view type with the H atom spheres scaled]
telp 40 [to set the ellipsoid percentage to 40%]
matr 1 [to orient the cell along the a axis type; 2 and 3 work for the *b* and *c* axes]
or
matr 100 [this can also be done with the right click menu]
brad 0.5 [adjusts the bond thickness of ALL bonds. Currently the individual bonds cannot be modified. The default value is 1.0]
grad [to modify the background]
F3 [toggles labels]
F4 [toggles background]
ctrl-t [toggles the molecule and text]

Q: How do I restore the default settings?
A: View→quick drawing styles→default. A shortcut for this is to type
default

Structure matching

For the **match** operation to work properly it is important to eliminate all the Q peaks prior to running it. Thus, it is necessary to execute
kill $q
fuse
Note that **ctrl-Q** would not work because it hides the Q peaks rather than eliminates them.

See command info for help with troubleshooting match.

Q: How can I overlay two symmetry-independent molecules within one structure?
A: This procedure is called MATCH and can be applied to two or more molecules. By default, the program matches all atoms, hence if you don't want to include the H atoms they should be killed explicitly:
kill $h $q [to kill all the h and q peaks]
fuse [ensures the correct connectivity after atom elimination – very important command!]
match [number of molecules]
Typing **match** will overlay the selected molecules (or all molecules if none is selected). If only some atoms should be matched, do the following:
select atoms to match in one molecule
select atoms to match in other molecules

type **match N**, where N is the number of molecules with selected atoms.

To unmatch the molecules type
fuse
or go to Tools→Overlay and click Unmatch.
To unmatch the molecules but keep the grown fragments/groups use
match -u

It is possible to superimpose molecules based on five or more atoms. The atoms should be selected in the respective MATCHing order, for example by clicking on C1,C2,C3,C4,C5 in one molecule, and C1a,C2a,C3a,C4a,C5a in another. Then type
match sel [to match the **sel**ected atoms].

A	B
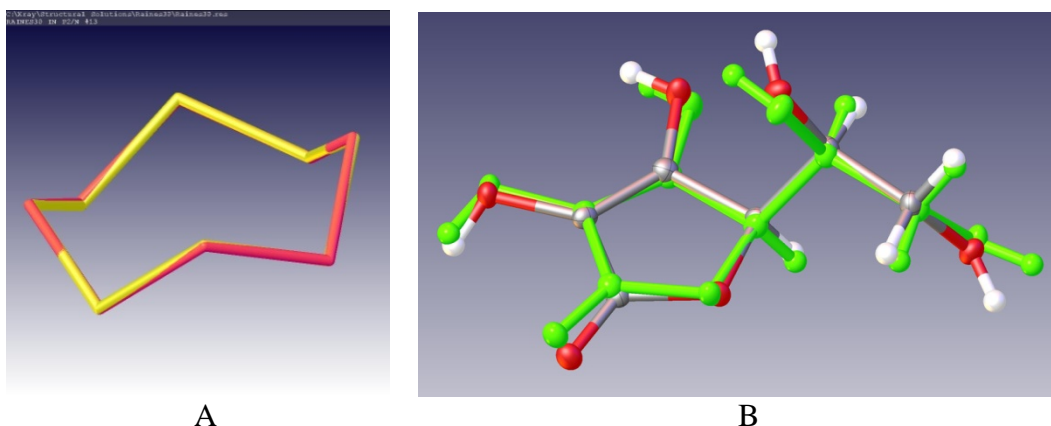
Figure 1. a) Two superimposed symmetry-independent molecules of S_8 shown with the "tubes" drawing style; b) two superimposed symmetry-independent molecules of vitamin C shown with the "ellipses and sticks" drawing style. One molecule is colored whereas the other shows atomic identities.

To color one of the superimposed molecules
right-click on the molecule→Fragment→Show this only [to display the molecules by itself]
ctrl-a [to select the molecule, both atoms and bonds]
right-click on the molecule→Selection→Group [to group atoms and bonds]
right-click on the molecule→Draw style [to display the Material Parameters palette]
In the Material Parameters palette double-click on the color rectangle corresponding to Ambient Front and select the color of your choice followed by OK.
Then type
fmol [to bring back all the molecules on the screen]
Repeat as necessary for other molecules.

Q: How do I generate a packing diagram?
A: Use menu Structure→Generate, and in Generation Options select the box size.

Alternatively, you can use
mode pack [displays the positions of other molecule positions as maroon pyramids]
and then click on the pyramids that you want to turn into molecules. Hitting the ESC key will end the **pack** mode.

Another way it to control the diagram creation manually:
pack [generates a packing diagram. The default for **pack** is "**pack -1.0 1.5 -1.0 1.5 -1.0 1.5**" Olex 2 generates all the fragments with the centers of gravity within the defined parallelepiped]
or
pack 0 1 0 1 0 1 [fills the unit cell with molecules; the numbers are pairwise limits for the *a*, *b*, and *c* axial vectors and can be adjusted as necessary].

Q: Can I display the basis vectors?
A: The basis vectors can be toggled by typing
basis
and moved with the left mouse button when the SHIFT key is depressed. Right-click on the basis to resize it.

Q: Is there an easy way to label several symmetry-independent molecules (with the same composition) similarly?
A: Yes. The following procedures work well on structures with two molecules, but I have not tested it on structures with Z'>2. It is important to eliminate all the Q peaks prior to the **match** operations. It is necessary to execute **kill $q** rather than **ctrl-Q**, because the latter will only hide them.

Example: two molecules with similar geometries in the asymmetric unit.
Section A.
1. Label one molecule (let's call it molecules **A**) to your liking. Maybe you have O1,O2,C1,C2... atoms with suffixless labels.
2. Select any atom in molecule **A** (by left-clicking on it).
3. Select any atom in molecule **B** (by left-clicking on it).
4. In order to label molecule **B** similarly with suffix "a" type
match sel -n=a   [**n** stands for "name of the suffix"]
Now you have two identically named molecules with names such as C1 in molecule **A** and C1a in molecule **B**.
Tricks of the trade:
match sel -n=a   [adds the suffix **a** to the atom names]
match sel -n=-b   [replaces the last character of the atom name with **b**]
match sel -n=$2   [changes the first character after the element symbol with the provided value (**2** in this case). If your base molecule has atom names C11a, C12a, and C13a, the second molecule will have labels C21a, C22a, C23a. However, if you start with C1a, C2a, C3a... you will end up with C2a C2a C2a.

Section B.
The GUI alternative to the procedure in Section A is now available:
1. Label one molecule (let's call it molecules **A**) to your liking. Maybe you have O1,O2,C1,C2... atoms with suffixless labels.
2. Select any atom in molecule **A** (by left-clicking on it).
3. Select any atom in molecule **B** (by left-clicking on it).
4. Go to work→Naming, type letter "a" in the Suffix box next to Equivalent Fragments (Z'>1) option.
5. Click on the Equivalent Fragments (Z'>1).

Section C.
        But perhaps you want your two molecules to have suffixes "a" and "b". [Since the atom names cannot be longer than four characters in XL the procedure above may not work. This is because if you have a molecule with names such as C1a and want to mimic the other molecule with suffix "b" you will end up with names such as C1ab.] Here is the correct procedure.
1. Label one molecule (let's call it molecules **A**) to your liking. Maybe you have O1,O2,C1,C2... atoms with labels but no suffixes.
2. Select any atom in molecule **A** (by left-clicking on it).
3. Select any atom in molecule **B** (by left-clicking on it).
4. Now to label molecule **B** similarly with suffix "a" type
match sel -n=b   [**n** stands for "name of the suffix"]
5. Select any atom in molecule **A** (by left-clicking on it).
6. Isolate this molecule by typing
uniq sel
7. Select the molecule with **ctrl-a**.
8. Add the suffix to the atom labels with
name sel -s=a [**s** stand for "suffix"].
9. Bring back the other molecule with
fmol

Section D.
Suppose that you have an organometallic complex with two identical ligands that you would like to label similarly, such as two molecules in Section A. The procedure described in Sections A-C are valid, but the trick is to isolate each ligand first by disconnecting the central atom from them.
conn 0 Ti
  [connects the specified atom (Ti) to exactly 0 atoms; in this case, Ti will be disconnected from all other atoms].
or, click on the metal atom to select it and type
conn 0
Now you can follow any routine from Sections A-C to label the atoms to your liking. Re-refine the structure to restore connectivity.

Working with hydrogen atoms

Q: What control over H atoms do I have?
A: These two commands are frequently useful:
ctrl-H [to toggle hydrogen atoms and hydrogen bonds on the screen]
telph [to switch to the ellipsoid view type with the H atom spheres scaled]

The GUI alternative to **ctrl-H**: view(or F6)→Show, and clicking on Hydrogen Atoms will toggle them while H-Labels will display their labels.

The GUI alternative to **telph**: view(or F6)→Quick Drawing Styles→click on the H symbol in the "Ellipsoid | H" button to show scaled H atoms. Click on Ellipsoids in the "Ellipsoid | H" button to return to the regular ellipsoid view.

Q: How do I show the hydrogen bonding interactions of my choice?
A: To show hydrogen bonds adjust the slider in the WORK panel, click on the bonds you want to expand, then ESC to remove the hanging bonds.

Q: How do I tabulate the hydrogen bonding interactions?
A: This is achieved with
htab [dist][angle][keywords]
If you issue
htab
with no arguments OLEX2 will insert HTAB card(s) (and the necessary EQIV cards) for the hydrogen bonds in the INS file. The defaults for the H-bond determination are Donor-Acceptor distance of 2.85 Å and Donor-H…Acceptor angle of 150°.
To survey more interactions one may use
htab 3 120 –t=C,N
where **3** is the D…A distance in Angstroms, **120** is the D-H…A angle in degrees, and –t=C,N will add additional atom types that can serve as donors and acceptors, the default atom types are N, O, F, S, and Cl.

It may be convenient to display the H-bonds as connected sets with
compaq –a [to reposition molecules to form H-bonds]

Q: How do I remove all the H atom constraints? My data are that good!
A: In the console type
afix 0 $h
free uiso $h

and run a refinement. The first command removes the constraints, the second frees the thermal displacement parameter.

Q: I can't seem to be able to assign the H atoms!
A: To modify how atoms are bonded (if H atoms cannot be assigned):
delta 0.2 [modifies the default delta for atomic connectivity]
fuse
hadd
delta 0.5
fuse

Q: How can I adjust the element-H distances?
A: Select the H atoms to be moved and type
himp [+/-][value]
Examples:
Select an H atom by clicking on it, then
himp 1.1 [positions the selected H atom at 1.1 Å from the atom closest to this H atom]
or
himp +0.1 [lengthens the distance from the specified H atom to the closest atom by 0.1 Å]

Q: How do I select all N–H distances? I refined the H atoms freely, but want to constrain the distance?
A: Right click on an N–H bond, Graphics→Select Group. Then navigate to Tools→Shelx Compatible Restraints.

Making the structure look professional

Q: How do I sort the atoms?
A: Very good sorting options are available under work→sorting. I recommend sorting by Mass, then Label. The H atoms will follow the atoms they are attached to in the instruction file. Moieties can be sorted by size. The order in which the sorting routines are executed matters. Thus, it's a good idea to sort by Mass and Label first and by Moieties second.

An older alternative is to sort the atoms by atomic mass with
file -s [saves the INS file with sorted atoms]
type
help sort
to learn more about sorting options.

If you have two identical molecules with labels such as (C1, C2… and C1a, C2a) it is good idea to sort them first by Suffix. Then the first molecule will have consistent labels.

One has a lot of control over sorting if the command line is used. For example
sort +szl
Will sort atoms by suffix, then mass, then label.

Q: How can adjust the unit cell content in the UNIT card of the SHELXL INS file?
A: The command of choice is
fixunit [Z'] [Z' must be supplied if different from 1]
example:
fixunit 3 [for the case with three symmetry independent molecules].
fixunit 0.5 [for the case with a molecule on a special position].
Note that the number of formula units on the ZERR card in the INS file will be updated accordingly.

Q: How do I reposition the molecules to be inside the unit cell and to show H-bonding interactions?
A: The following two commands are handy:
compaq –a [to reposition molecules to form H-bonds]
move [to move the molecule(s) inside the asymmetric unit]

Q: I have a warning indicating that the structure should be inverted. How do I go about that?
A: The entire structure can be inverted by typing
inv [inverts the structure].
Other inverting commands include
inv –f [forces the inversion of the non-centrosymmetric structures]
inv sel [inverts the specified molecule; **inv -f** can also be used for a selected molecule]

Deriving metric data using GUI

sel and **esd** are the universal commands for various mathematical computations. They deal with the **sel**ected items such as atoms or least=squares planes.

Q: How can I measure interatomic distances, angles, and dihedral angles?
A: To compute an interatomic distance, angle, or torsion angle select two, three, or four atoms, respectively, by clicking on them and type
sel [displays the metric parameter value. The parameter will correspond to the number of atoms selected].

Q: How can I measure a dihedral angle between planes of my choice?
A: To define a plane select three or more atoms and type

mpln sel [computes a LS planes through the **sel**ected atoms].
Follow by defining your second plane. Then click on each plane to select it (the plane color will change to green) and type
sel [when two planes are defined **sel** will show the dihedral angle and the distance between the planes' centers].

GUI alternative: To define a plane select three or more atoms, the go to view→geometry→Mean Plane (of active selection) and the plane will be generated.
sel [when two planes are defined **sel** will show the dihedral angle and the distance between the planes' centers].

Q: How do I compute the distance from an atom to a plane?
A: Define your plane, select the defined plane and the atom of interest, and type **sel**

Q: How do I compute the angle between a plane and a vector?
A: Define your plane, select the defined plane and two atoms of your vector, and type **sel**
Currently this option is not working.

Q: How do I obtain a standard uncertainty for my metric parameter?
A: Great question, and this is where OLEX2 has the upper hand relative to other programs. George Sheldrick's XL, of course, is very instrumental here. In XL there is an undocumented feature, namely card "MORE -1". A structural refinement with MORE -1 in the INS file will generate a file with the covariance matrix that allows the computation of the s.u.'s. Thus, the first step is to re-refine the structure as follows:
/ more -1 [note the forward slash and spaces before and after the word **more**. This command inserts "more -1" into the INS file]
ctrl-r [to run a refinement; note that currently you can't simultaneously have cards "WPDB -2" and "MORE -1" in your INS file].
Define the planes or select atoms as you would for **sel**, but now type
esd [computes metric parameters similarly to **sel**, only with s.u.'s].

Thus, **sel** and **esd** are congeners and work in the same fashion, only **esd** will also produce standard uncertainties if the structure has been refined with the MORE -1 card.

General useful commands

Q: How do I obtain help with a specific command?
A: **help** [command] [displays info on the specified command]

Q: How do I keep track of OLEX2's operation?
A: Use command
log [to show the full program log file for the current session in an external text editor].

Q: How do I generate the symmetry-related parts when my molecule occupies a special position?
A: Let's say you have a structure residing on a special position. In order to generate the symmetry related parts you can type
grow
However, if your asymmetric unit contains moieties both on special and in general positions, **grow** will only complete the fragments on special positions. To correctly multiply the content of the asymmetric unit (for example, when you have a complex on an inversion center and a solvent molecule in a general position) two commands are necessary:
grow
grow -w
This sequence is equivalent to a properly executed command SGEN in program XP.

Q: How do I execute Fourier atom type analysis?
A: By running
fata()
or
fata
fata stands for "free atom type analysis". A positive number indicates that the atom is too light, a negative - the atom contains too much electron density. This command yields the list of atoms. Analyses volumes of at least 1.5 Å^3. Threshold is 3σ. analyses spherical blobs of electron density around atoms with value of at least 3σ of the electron density map. Currently, this option is experimental.

Q: What should I do if a solution fails?
A: You can type, for example, 'TREF 5' after ShelXS has finished. The top 5 solutions will show on your screen and you can browse through them using CTRL+UP/DOWN. When you recognize a real solution, hit ENTER and you can take it from there.

Q: How can keep the Refine panel from closing after each refinement?
A: By default the panel closes. If you want to change this setting type
spy.EditParams(user)
and set the auto_close_settings_panel to False as in
auto_close_settings_panel = False

Q: How do I generate a lattice with atoms in the corners?
A: In the RES file remove the symm cards. Introduce a new atom at the origin, for example a phosphorous and pack the new atoms:

xf.au.newatom(P,0,0,0)
xf.endupdate()
pack P
It is likely the P atoms would have to be manually connected with `addbond`.

How to include instrument specifications in the CIF file

One of OLEX2's strengths is the ability to incorporate metadata from various sources into the final Crystallographic Information File (CIF). Here I am showing how to include your instrument and typical data collection parameters into the CIF file.

1. Prepare a metadata CIF file with the instrument and typical data collection parameters metadata. Two examples (A and B) of my complete CIF files are below.

A. A complete CIF file for a Bruker APEX2 sealed tube Cu instrument with an APEX2 detector called Bucky. You are welcome to copy it into a brand new ASCII file in its entirety and modify according to your specifications.

```
#=======================================================================
#Single-crystal diffractometer Bucky,
#Molecular Structure Laboratory,
#Chemistry Department, UW-Madison
#Updated January 12, 2015

_diffrn_radiation_type            'Cu K\a'
_diffrn_radiation_probe           x-ray
_diffrn_radiation_xray_symbol     K-L~3~
_diffrn_source                    'sealed X-ray tube'
_diffrn_source_type               'Siemens, K FFCU 2K 90'
_diffrn_measurement_device        'three-circle diffractometer'
_diffrn_measurement_device_type   'Bruker SMART APEX II'
_diffrn_measurement_method        '0.60\% \w and 0.6\% \f scans'

_diffrn_detector_area_resol_mean  7.9
_diffrn_detector           'charge-coupled device (CCD) area detector'
_diffrn_detector_type             'Bruker APEX II'
_diffrn_radiation_detector        'Bruker APEX II'
_diffrn_radiation_collimation     '0.5 mm double-pinhole'
_diffrn_radiation_monochromator   'equatorially mounted graphite'


_diffrn_standards_number          .
_diffrn_standards_interval_count  .
_diffrn_standards_interval_time   .
_diffrn_standards_decay_%         .

_computing_data_collection        'APEX3 Ver. 2016.5-0 (Bruker-AXS, 2016)'
```

```
_computing_cell_refinement          'SAINT+ Ver. 2016.5-0 (Bruker-AXS, 2016)'
_computing_data_reduction           'SAINT+ Ver. 2016.5-0 (Bruker-AXS, 2016)'
_computing_structure_solution       'XT (Sheldrick, 2015a)'
_computing_structure_refinement     'XL (Sheldrick, 2015b)'
_computing_molecular_graphics       'OLEX2 (Dolomanov et al., 2009)'
_computing_publication_material     'OLEX2 (Dolomanov et al., 2009)'
_exptl_crystal_density_meas         ?
_exptl_crystal_density_method       'not measured'

_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_process_details
;
SADABS-2016/2 (Krause et al., 2015) was used for absorption correction.
;


_publ_section_references
;
Bruker-AXS (2016). APEX3. Version 2016.5-0. Madison, Wisconsin, USA.

Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.
"OLEX2: a complete structure solution, refinement and analysis program".
(2009), J. Appl. Cryst. 42, 339-341.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015).
J. Appl. Crystallogr. 48, 3-10.

Sheldrick, G.M. (2015a). "SHELXT - Integrated space-group and crystal-
structure
determination". Acta Cryst. A71, 3-8.

Sheldrick, G.M. (2015b). "Crystal structure refinement with SHELXL".
Acta Cryst. C71, 3-8.
;
#=======================================================================
```

B. The following is a file for a Bruker microsource Mo Kα radiation source diffractometer with an APEX2 detector called Gromit. Copy it into a brand new ASCII file and modify according to your specifications.

```
#=======================================================================
#Single-crystal diffractometer Gromit,
#Molecular Structure Laboratory,
#Chemistry Department, UW-Madison
#Updated August 9, 2016

_diffrn_radiation_type              'Mo K\a'
_diffrn_radiation_probe          x-ray
_diffrn_radiation_xray_symbol    K-L~3~
_diffrn_source                      'microfocus sealed X-ray tube'
_diffrn_source_type                 'Incoatec I\ms'
_diffrn_measurement_device          'three-circle diffractometer'
_diffrn_measurement_device_type     'Bruker APEX II Quazar'
_diffrn_measurement_method          '0.5\% \w and 0.5\% \f scans'

_diffrn_detector            'charge-coupled device (CCD) area detector'
_diffrn_detector_type               'Bruker APEX II'
```

```
_diffrn_radiation_detector              'Bruker APEX II'
_diffrn_detector_area_resol_mean         7.9
_diffrn_radiation_collimation            'focusing mirrors'
_diffrn_radiation_monochromator          'mirror optics'

_diffrn_standards_number                .
_diffrn_standards_interval_count        .
_diffrn_standards_interval_time         .
_diffrn_standards_decay_%               .

_computing_data_collection          'APEX3 Ver. 2016.5-0 (Bruker-AXS, 2016)'
_computing_cell_refinement          'SAINT+ Ver. 2016.5-0 (Bruker-AXS, 2016)'
_computing_data_reduction           'SAINT+ Ver. 2016.5-0 (Bruker-AXS, 2016)'
_computing_structure_solution       'XT (Sheldrick, 2015a)'
_computing_structure_refinement     'XL (Sheldrick, 2015b)'
_computing_molecular_graphics       'OLEX2 (Dolomanov et al., 2009)'
_computing_publication_material     'OLEX2 (Dolomanov et al., 2009)'
_exptl_crystal_density_meas         ?
_exptl_crystal_density_method       'not measured'

_exptl_absorpt_correction_type     multi-scan
_exptl_absorpt_process_details
;
SADABS-2016/2 (Krause et al., 2015) was used for absorption correction.
;

_publ_section_references
;
Bruker-AXS (2016). APEX3. Version 2016.5-0. Madison, Wisconsin, USA.

Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.
"OLEX2: a complete structure solution, refinement and analysis program".
(2009), J. Appl. Cryst. 42, 339-341.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015).
J. Appl. Crystallogr. 48, 3-10.

Sheldrick, G.M. (2015a). "SHELXT - Integrated space-group and crystal-
structure
determination". Acta Cryst. A71, 3-8.

Sheldrick, G.M. (2015b). "Crystal structure refinement with SHELXL".
Acta Cryst. C71, 3-8.
;
#=========================================================================
```
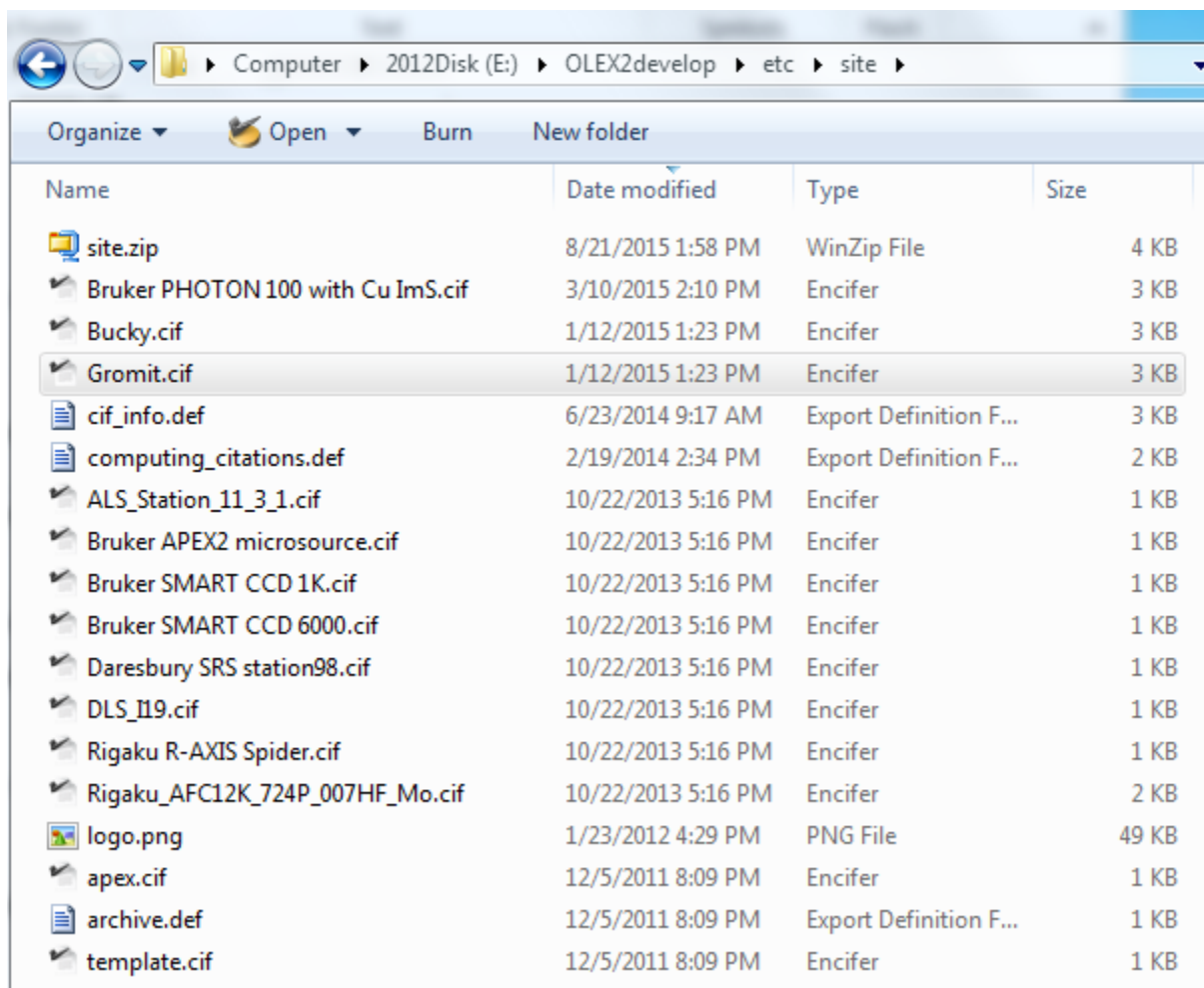
2. Place the files into the ETC\SITE folder of the OLEX2 install folder as follows:

3. Now you are ready to use it for the final report. From the WORK→REPORT module in OLEX expand the DIFFRACTION menu and from the drop-down menu select the instrument on which the data were collected. In the example below the data were collected on the instrument called Gromit and the location of the definition file is shown. If you are doing this for the first time you may have to locate the instrument CIF file from the "Definition file" menu.
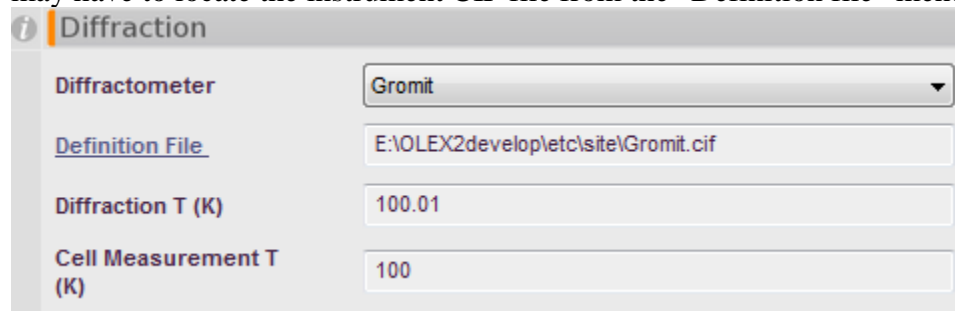
3. After you prepare a merged CIF file using the [Merge Cif] button the data from the selected CIF (Gromit.CIF in the example above) will be incorporated in the final structure CIF.

Comments on the Report feature

When a structural report is created OLEX2 examines the contest of the directory where you have you RES/HKL files and extracts a lot of information from the files present therein. Thus it is a good idea to correct for absorption, solve and refine the structure in the same directory. The following are some of the file extensions for the files OLEX2 uses to resolve many CIF entries (http://svn.olex2.org/olex2-gui/trunk/util/pyUtil/PyToolLib/FileReaders/):

.ABS
.INI
.LST
.P4P
.PCF
.DAT
._LS
.CIF

Working with Solid Angles

To display ligand shadow projections on a sphere of an arbitrary radius (effectively using solid angles) the following commands are used.
Select the metal and type
`conn 0`
to "disconnect the ligands from the central metal.
Select the central metal and type
`projsph`
or
`projsph -g=7`
to generate ligand projections onto a sphere. g stands for generation quality, the numerical value is the exponent, increase it judiciously.
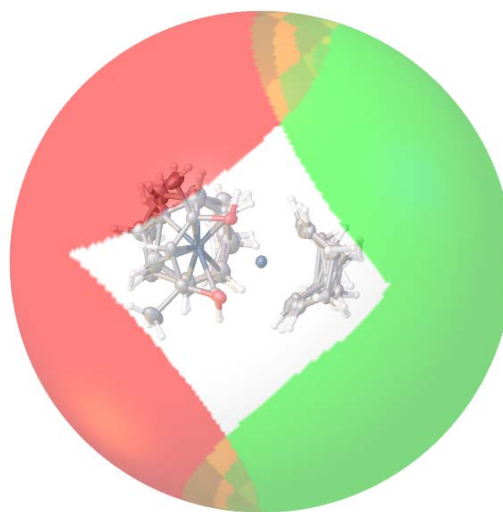To change atom types to van der Waals spheres one uses
`arad vdW`
To change it to ellipsoids use
`telp`
Command
`molinfo -g=7`
works as well.

The sphere can be deleted by right-clicking on it and selecting Hide from the menu. If the option is unavailable you need modify your options as follows.

Type
```
options
```
and file .options will be open in Notepad. Add a new line:
```
gl_selection = true
```
Save the file, restart OLEX2, and this problem should be resolved.

Some known issues

Q: I have difficulty selecting atoms – when I click on them a bond is selected instead.
A: Update you graphics card driver, and if it does not help (did not help me) type 'options' in Olex2 and place this line in the file:
gl_selection=False
It should fix the issue temporarily, but it seems to have fixed it permanently for me.

Q: When I submit my file to CheckCIF at http://checkcif.iucr.org/ for complete validation the site asks me to upload the FCF file separately, despite the fact that it's in the CIF. Why?
A: There may be two reasons.
1. You may have manually changed CIF and invalidated the _shelx_res_checksum.
2. You have OLEX inserting HKL/RES files in the CIF, but you want this option to be turned off. Go to Work→Report and select "Ignore HKL/RES" in the drop down menu: