

Notes on OLEX2

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Your version of OLEX

Q: How do I install OLEX2?

A: The program is available as a free download from www.olex2.org, just follow the installation instructions from the web. OLEX2 must be installed and launched at least once in an 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/index.html>. SHELXS and SHELXL are necessary for structural solution and refinement, respectively. OLEX2 is smart and if you already have 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: 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.

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.

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.

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.

cell

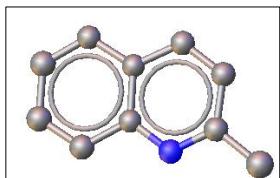
toggles the view of the unit cell boundaries

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

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assembles together the incomplete fragments

compaq -c

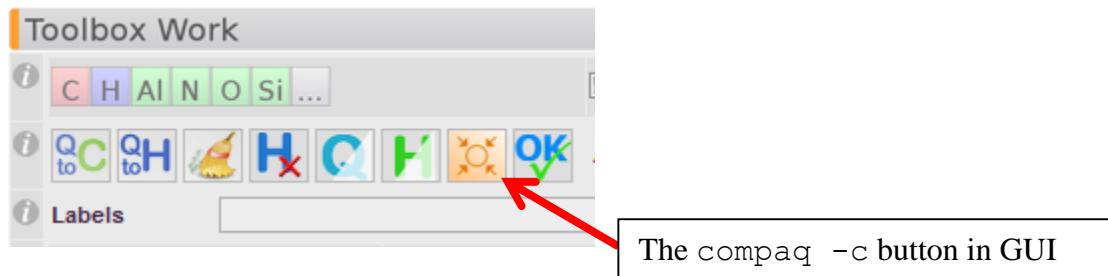
similar to the default behavior, but takes into account the atom-to-atom distances and moves all atoms into the closest possible positions to the largest fragment in the structure

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.



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.

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```
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

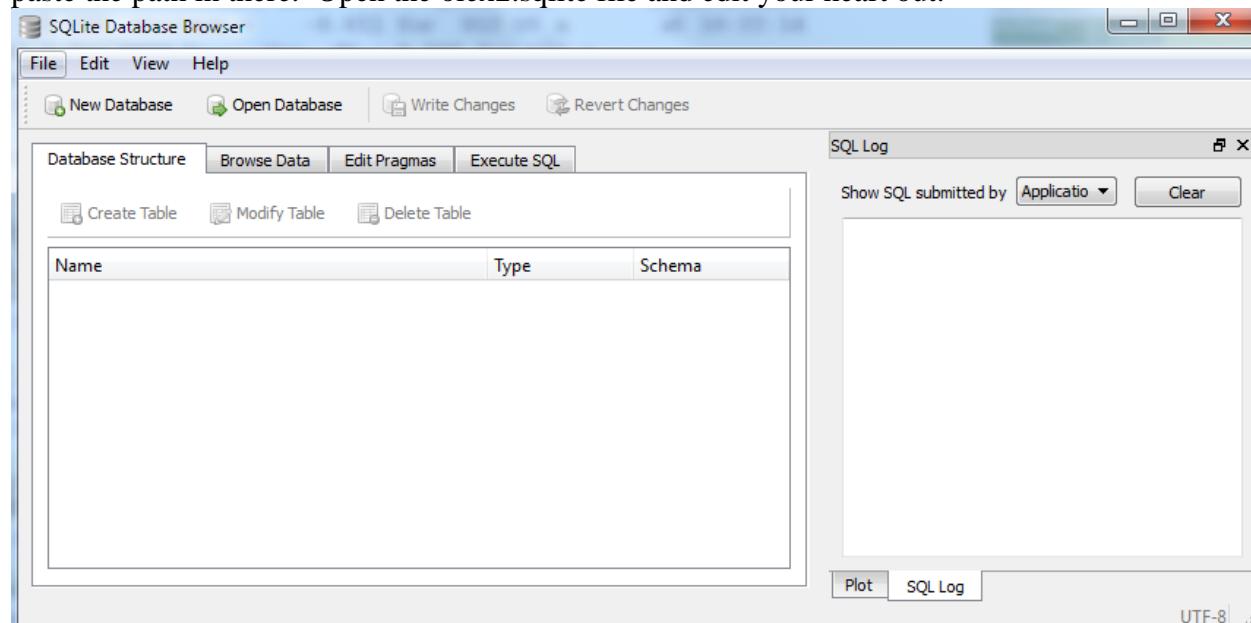
<http://sourceforge.net/projects/sqlitebrowser/files/latest/download>

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.



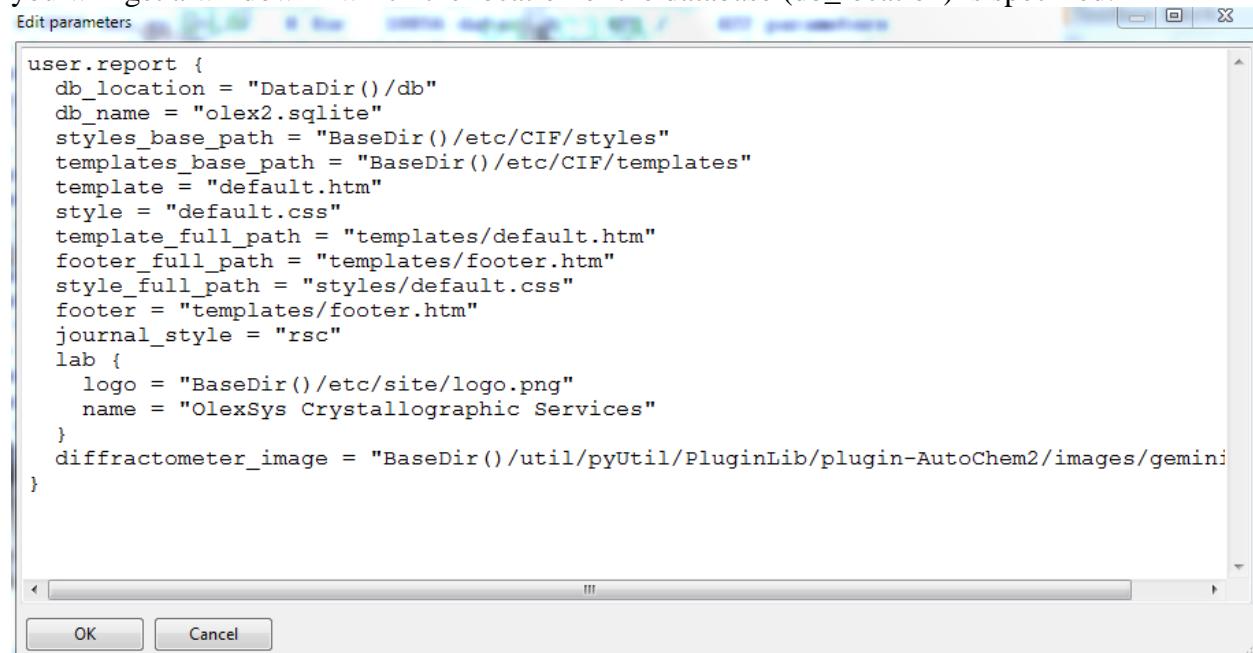
Restart OLEX2 for the changes to take effect.

Also, if you type

```
spy.editparam(user.report)
```

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you will get a window in which the location of the database (db_location) is specified.



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.

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.

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.

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
```

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 tetrานuclear 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

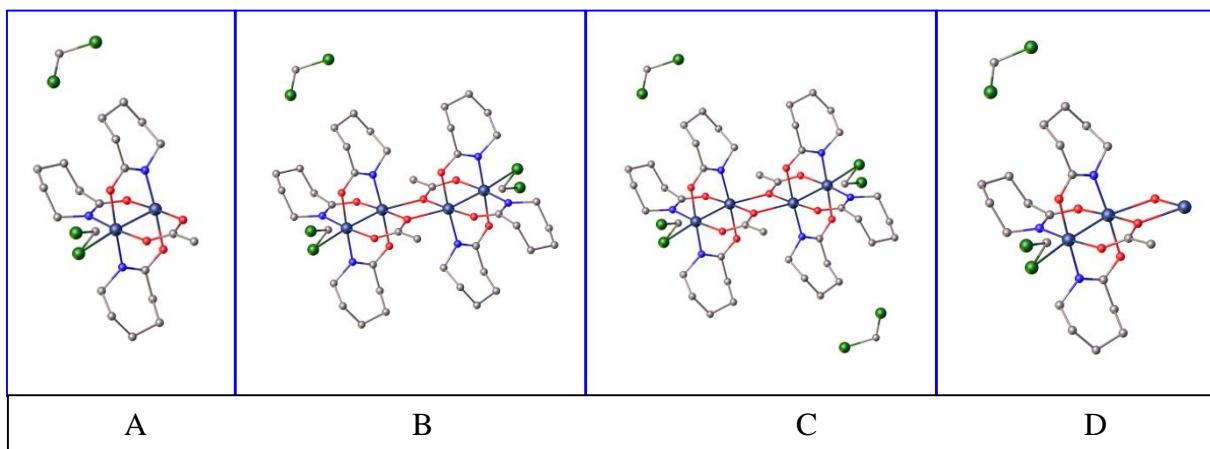
grow -w

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).



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.

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 C2

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 [switch]

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/Å³.

The labels can be hidden by another

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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

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.

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]

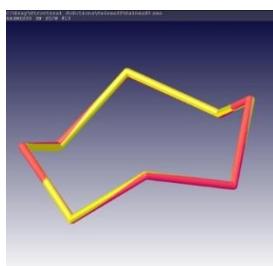
right-click on the molecule→Selection→Group [to group atoms and bonds]

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 S₈ 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 $u_1v_1w_1$ to lattice point $u_2v_2w_2$
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 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
```

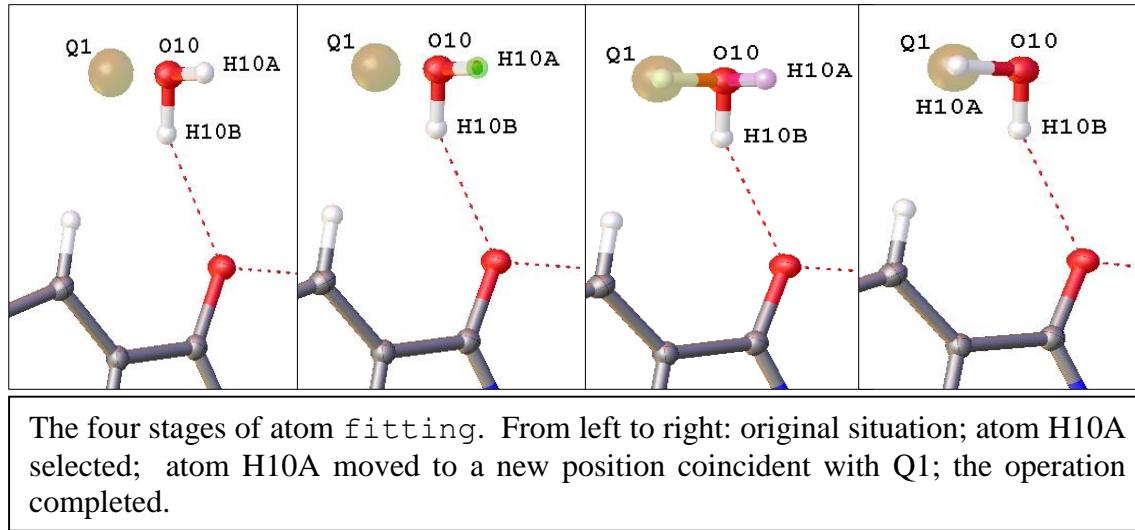
mode fit [switch]

allows one to (1) move an atom or a group of atoms, (2) rotate a group of atoms, (3) split a group of atoms.

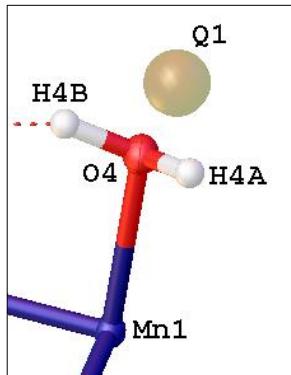
switch can be `-s` followed by the number of atoms to not be displaced as in
`mode fit -s=1` (see part (3) of this section).

- 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.



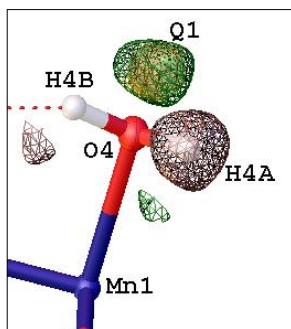
(2) A group of atoms can be rotated about a bond. This is handy, for example, for $-\text{CF}_3$ groups and H atoms.



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:

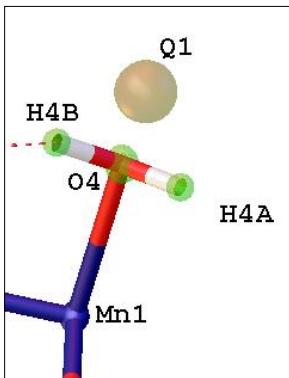


The green color shows areas with excess of electron density (it overlaps with Q1) whereas the brown-purple meshwork indicates holes. Atom H4a is in an incorrect position.

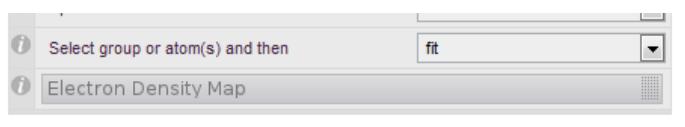
We will rotate the water molecule about the Mn1–O4 vector so that H4a will move to the position of H4b, and H4b will take the position of Q1.

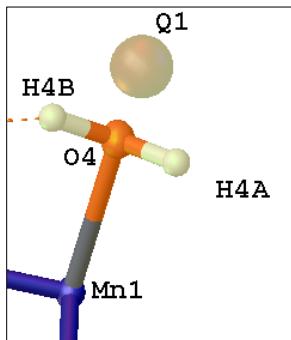
Hide the map by clicking on Work→Toolbox Work→Electron density map.

Select atoms O4, H4a, H4b in that order. The first selected atom will be on the axis of rotation.

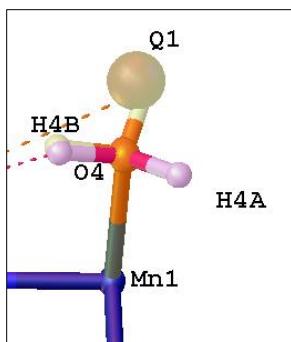


In the console type mode `fit`.
 Alternatively, select “fit” from the dropdown menu under Work→Toolbox Work→Select group of atom(s) and then

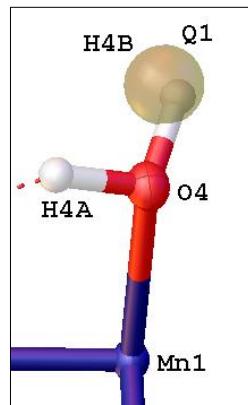




The selection will change the colors. Note that the Mn1–O4 bond is also highlighted. This is the axis of rotation and this is why it was important to select atom O4 first.

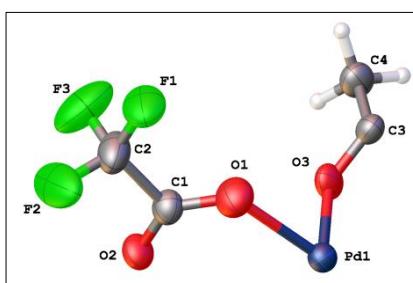


Right-click on the Mn1–O4 bond. Then left-click and drag on the Mn1–O4 bond. The water molecule will rotate about the Mn1–O4 axis. The final position may look like the diagram on the left. It is a little crowded because both the starting and final positions of the H atoms are shown.

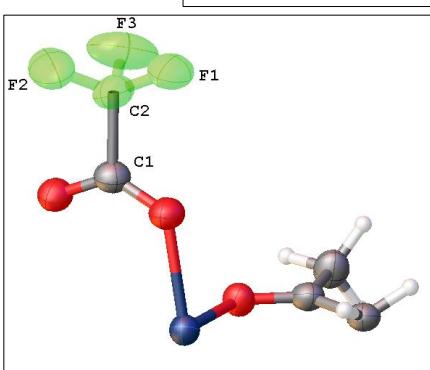


Type `mode off` in the console to exit the `fit` desired outcome:

mode and produce the



(3) Splitting a group of atoms into two for the refinement of positional disorder is illustrated with a $-\text{CF}_3$ 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.



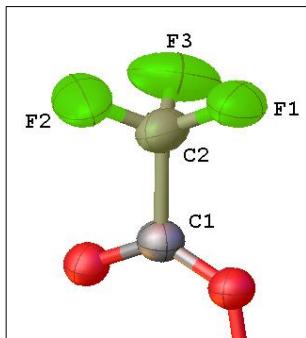
Select atoms C2 F1 F2 F3 by clicking on them in this order. In general, a selection can be made by drawing a box around the atoms of interest (by holding down the SHIFT key and dragging the mouse with the left button depressed), but in this case the order in which the atoms are selected is important.

In the GUI type

mode fit -s=1

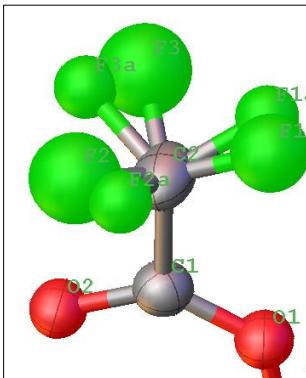
to indicate that we will be fitting the whole group to a new location, but one atom (the first atom of the selection) will not be split.

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

To display clickable bonds to atoms within short contacts:

mode grow -s

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.

mode grow -a

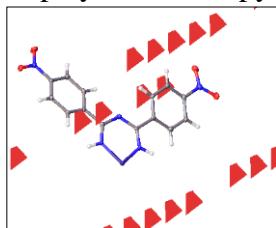
Allows to conveniently reposition atoms to symmetry-related sites within the same molecule. It is exceptionally handy when a molecule occupies a special position. [but try
compaq -m
compaq
first. It may do what you wish to achieve.

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.

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

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
```

pim [-1]

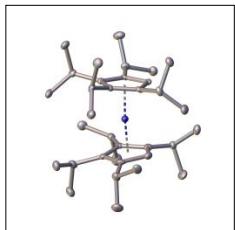
generates a metal- π bond. The thickness of the bond is set at 50% of that of a normal bond, as if BRAD 0.5 has been issued for these metal-centroid bonds.

When the switch [-1] 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.

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 reproduced 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.

```
item 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, such 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 includes keyword 'where' and 'rings' which allow selecting atoms and bonds according to 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 than H

`sel bonds where xbond.length > 2` - to select all bonds longer than 2 Å

`sel bonds where xbond.b.bai.z == 1` - to select all bonds where the lightest atom is H

Switches:

`a` - select all

`c` - copies printed values to the clipboard

`i` - invert selection

`l` - consider the list of bonds as independent

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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

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 or 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/uw1.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

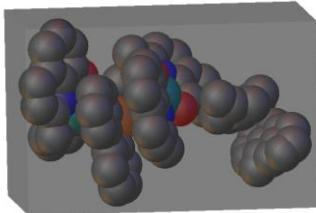
displays the DOS prompt text in a separate window

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 Å

Wrapping box volume: 4125.938 Å³

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 $\bar{P}1$ 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).

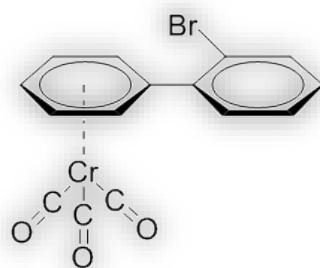


Figure 1. The Cr(0) complex (I) used to illustrate the $P1 \rightarrow \bar{P}1$ switch.

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

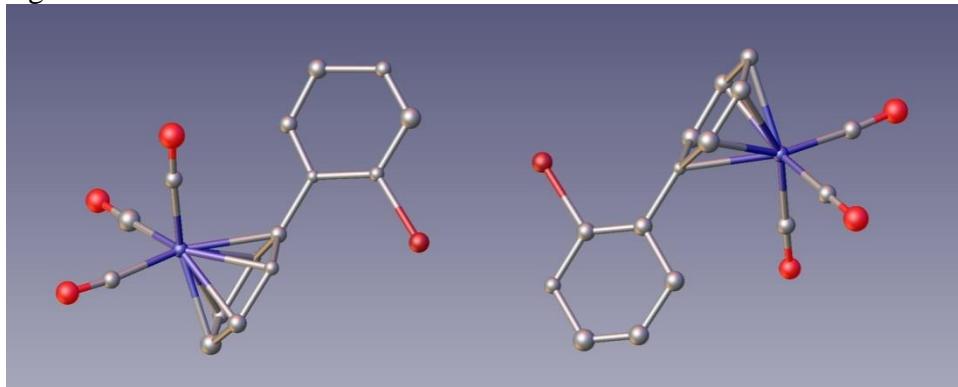


Figure 2. The structure of (I) solved in P1. The two molecules are related by an inversion center.

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 selected 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.

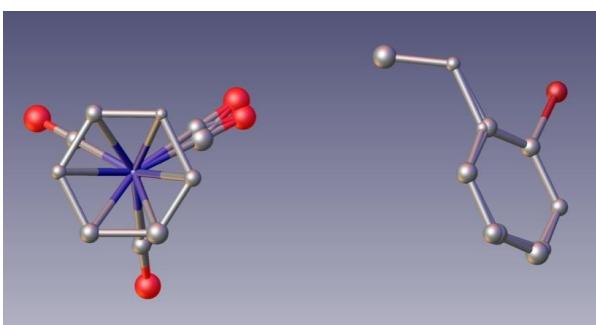
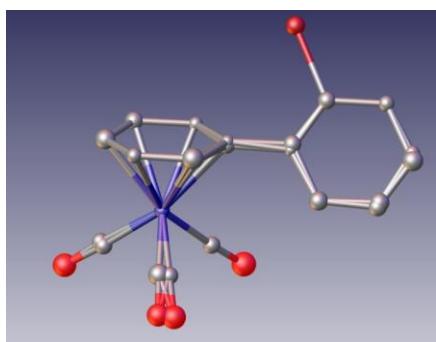


Figure 3. The structure of (I) immediately after converting the space group to the correct $P\bar{1}$.



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.

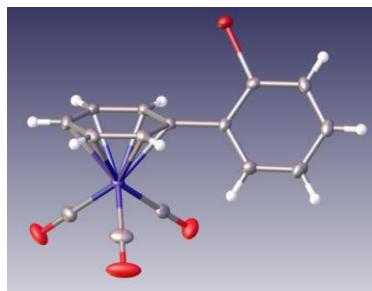


Figure 5. The finished structure of (I) in the correct space group $P\bar{1}$.

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]

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 -1` to see the length of the bond)

in order to obtain a cleaner view as in Fig. 1.

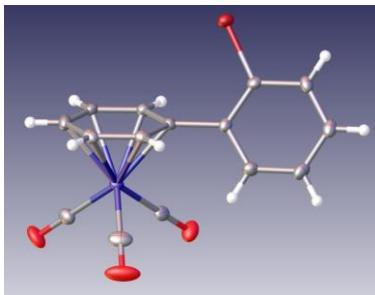


Fig. 1. The Cr complex.

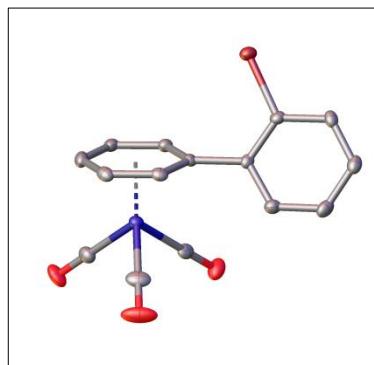


Fig 2. Complex (I) with a different coordination depiction.

To go back to the previous display delete the dashed line and then type
`conn 9 Cr1`

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`.

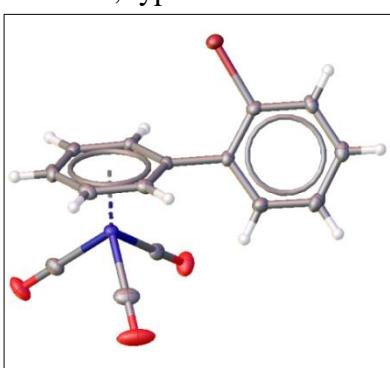


Fig 3. Display of the delocalized electron density in rings.

To compute the dihedral 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

mp1n

to generate a plane confined to a ring with a selector (black dot) in the middle.

Fig. 4 shows the two created planes.

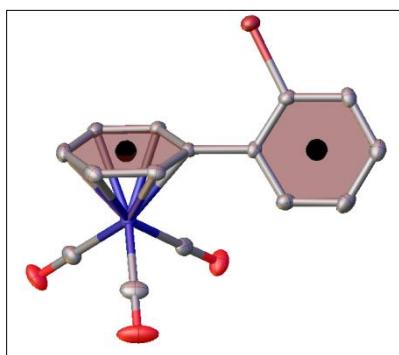


Fig. 4. Two rings are ready for computation.

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 $58.86(1)^\circ$.

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

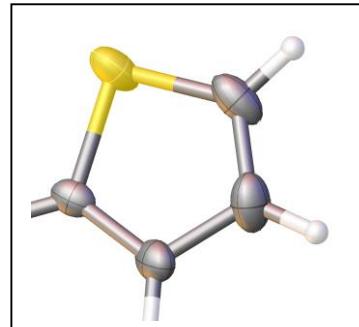
```
esd
Using shelxl matrix for the calculation
Plane C7 C8 C9 C10 C11 C12 to plane angle: 58.86(10)
Plane centroid to plane centroid distance: 4.343(2) A
Plane [C7 C8 C9 C10 C11 C12 ] to plane centroid distance: 0.092(5) A
Plane [C7 C8 C9 C10 C11 C12 ] to plane shift: 4.342(2) A
Plane [C1 C2 C3 C4 C5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

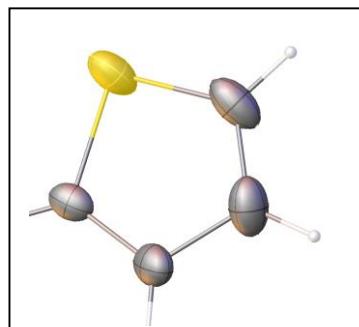
By Nattamai Bhuvanesh

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">
>
>
>

```

- Where bhtelp is going to be the new custom Macro's name
- "Change **telp** Settings for Bhuv" is what OLEX2 will show if we type "help bhtelp"
- If necessary, you may add args – arguments.
- 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**".
- 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 "`>`".
- After you are done, save the **custom.xld** file.
- Go back to OLEX2 and type

reload macro

and we are done.

Now you can use **bhtelp** to get the new styled **telp**.

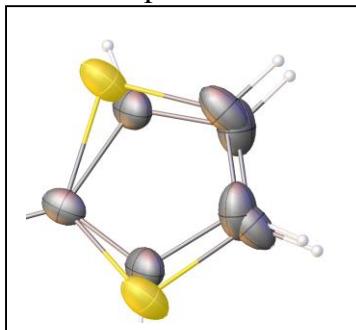
Q: Is it possible to show only one or more (selected) "part" of the disordered atoms?

A: Absolutely, only selected "part" numbers can be shown by using

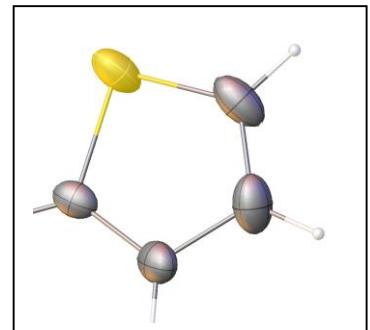
showp 0 1

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

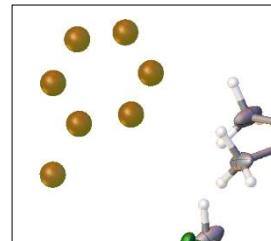
Constraining the molecular geometry

EXAMPLE 1.

There are several ways 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.



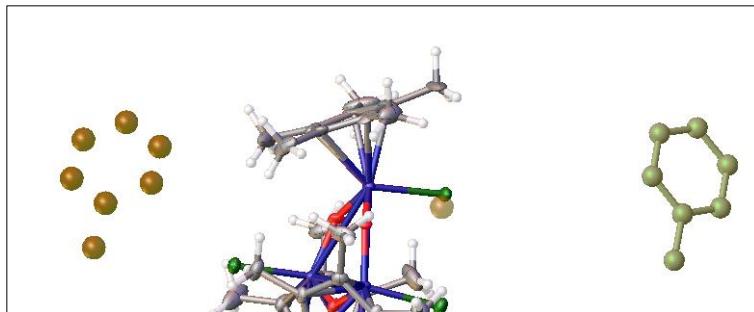
1. Prepare an idealized geometry of the molecule of choice (toluene in this case). It should look like a typical FRAG/FEND command:

```
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
```

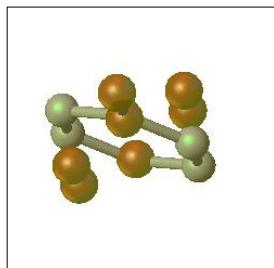
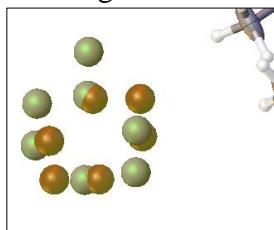
Many DFT-optimized molecular geometries are available free at <http://xray.chem.wisc.edu/Projects/IdealizedMolecularGeometry.html>. Of course one can use a reasonable geometry from the Cambridge Structural Database or any other reliable source.

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).

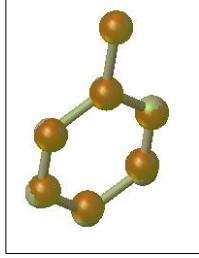


3. Match at least three atoms. We start with the Me carbons by clicking on the Me carbon of the green molecule and then on the Q peak corresponding to the toluene Me carbon:

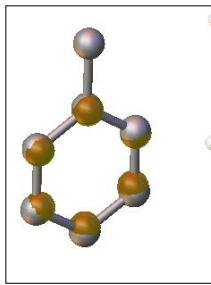


Next we click on the pair corresponding to the para atoms:

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
```

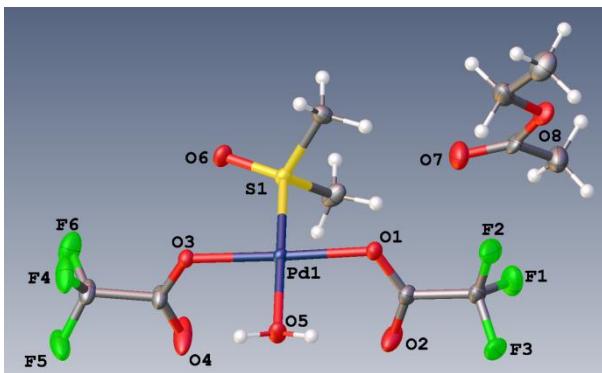
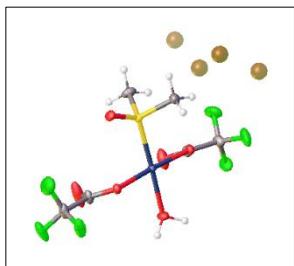
The original molecule has been deleted, the idealized one is left in the proper orientation and we can proceed with step 4 and 5.

EXAMPLE 3.

A Pd complex that co-crystallizes with $\frac{1}{2}$ equivalent of ethyl acetate, figure on the right. The solvent molecule is disordered over an inversion center and should be refined with part -1.

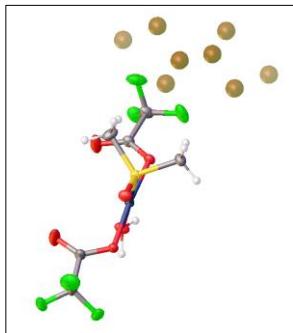
Use file disorder 3.res and disorder 3.hkl to follow the steps.

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:



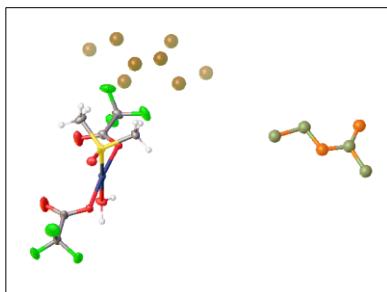
4. Prepare an idealized geometry of the molecule of choice (ethyl acetate in this case). It should look like a typical FRAG/FEND command:

```
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).



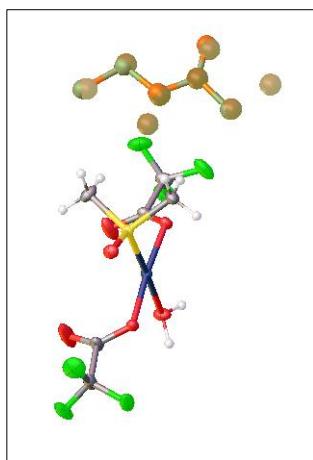
The inserted molecule can be overlaid on the Q peaks in the MATCH mode. Prior to that is may be beneficial to move the inserted molecule manually as follows:

Left click on the molecule and keep the left button depressed to rotate the molecule.

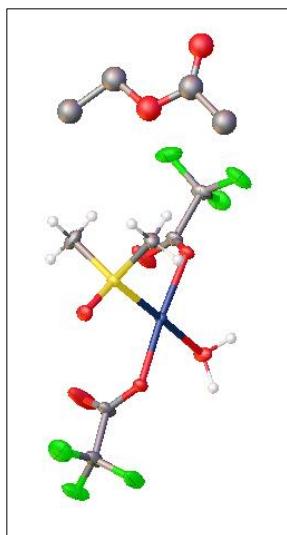
Hold down the SHIFT key to drag the molecule with a depressed left click.

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%.

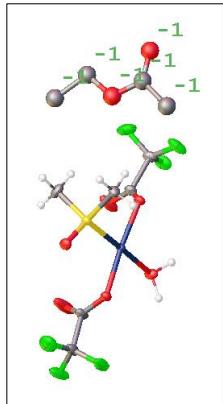
First, we will assign part -1 to the solvent molecule.

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:

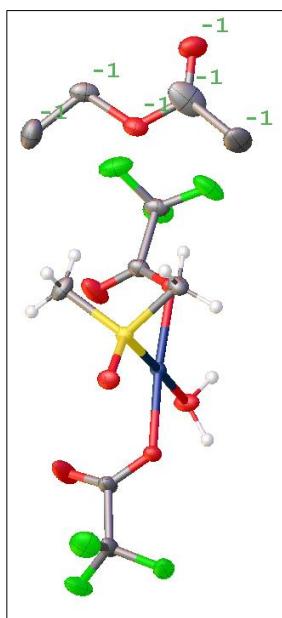
```
FVAR 0.38625
PART -1 10.5      ! modified line
AFIX 6
O7      O      0.98336  0.46279  0.43296  11.00000  0.05000
```

OLEX2 Manual

```
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.

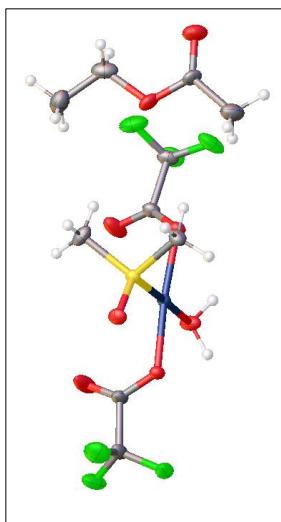


The refinement indicators have improved, but the ellipsoid of the carbonyl atom looks somewhat enlarged. In this case it is a good idea to remove the idealized geometry constraint:

-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.]

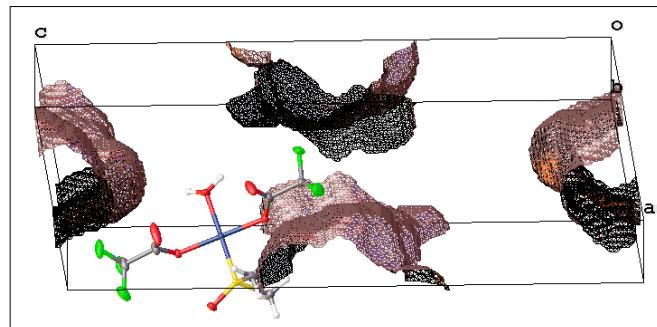
An alternative procedure, implemented in OLEX2, is based on the paper “Bulk-solvent correction in large macromolecular structures” by B. Rees, L. Jenner, and M Yusupov in *Acta Cryst. D*, 2005, 61(9), 1299-1301.

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 \AA^3 with 51.7 electrons in each. Ethyl acetate contains 48 electrons and the estimated volume of the molecule is 124 \AA^3 . For comparison, PLATON (with the default settings) estimated the volume of each of the two voids at 145 \AA^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.

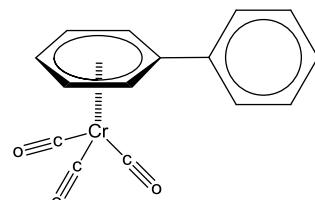
To proceed with the refinement return to the Work menu (F5), expand the Refine menu, mark the “Use solvent mask” checkbox and run a refinement. You can also elect to “Recompute mask” by checking its box.

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.

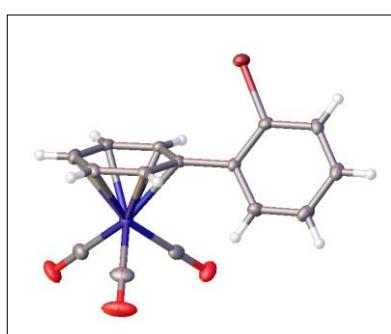
It goes without saying that this type of refinement should be documented in the experimental.

Working with molecular graphics

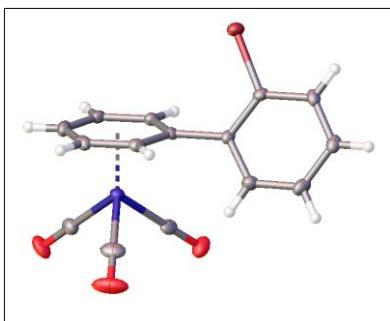
OLEX2 is great for generating publication quality diagrams. As an example consider the Cr(0) complex on the right. We will generate a very similar looking diagram with atom labels.



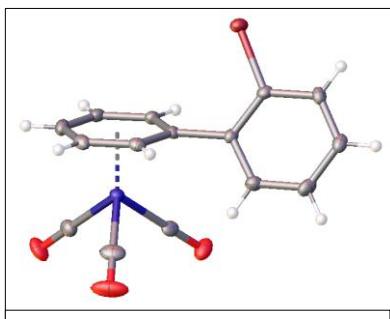
What you see on the screen is what you get in the graphics file.



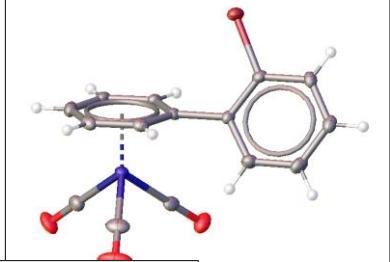
This is the default diagram.



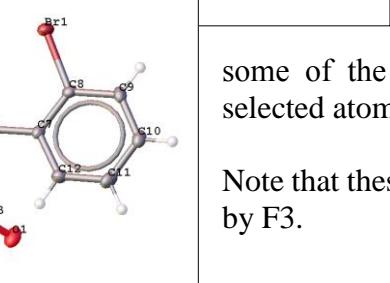
To remove the six Cr–C bonds and generate a dashed line to the center of the coordinated Ph ring type
pim



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



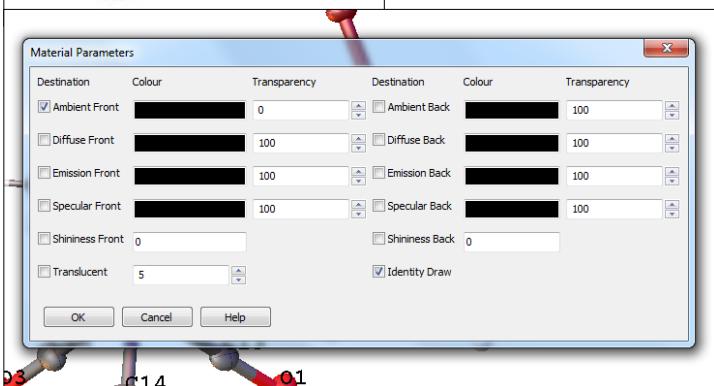
To add atom labels go to Tools→Images. If you want to label only some of the atoms first select them and then click under Images→1)Label selected atoms. To label all non-H atoms click on Images→non-H atoms.

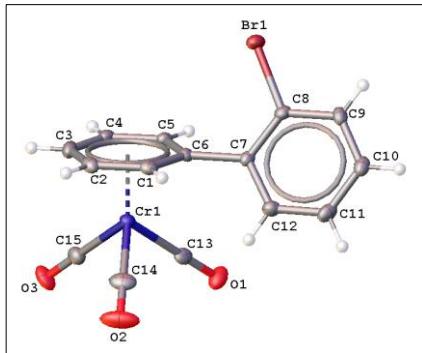
Note that these labels differ from the green working labels that can be toggled off by F3.

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.





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 -1 [displays non-hydrogen atom labels]
```

```
labels -1 -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/Å³]
```

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 [will superimpose the molecules with all atoms used for matching].

To see how well the molecules fit, on the right-hand panel select Tools→Overlay to see the root-mean-square deviation table. The RMS deviations are also listed in the main window. The table will refer to individual molecules as A, B, C..., which of course has nothing to do with the way your molecules are labeled. This feature may be obsolete as of July 9, 2012.

To unmatched the molecules type

fuse

or go to Tools→Overlay and click Unmatch.

To unmatched 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 selected atoms].

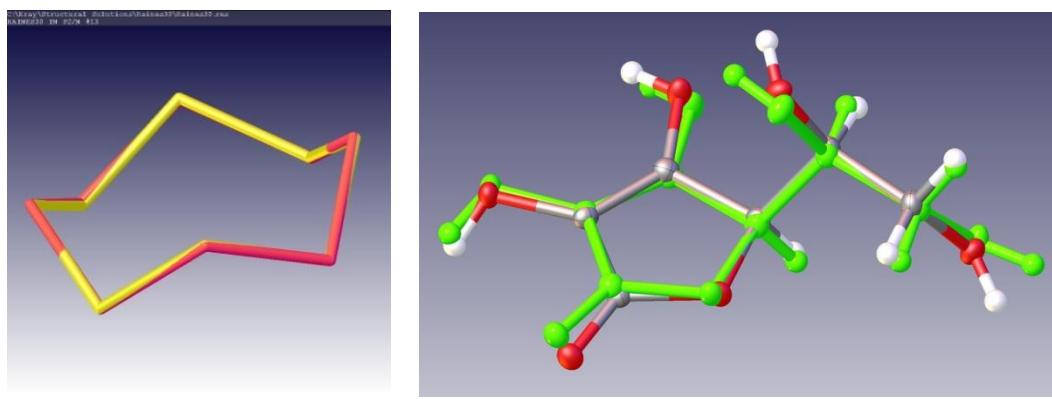


Figure 1. a) Two superimposed symmetry-independent molecules of S₈ shown with the "tubes" drawing style; b) two superimposed symmetry-independent molecules of vitamin C shown with the "ellipses and sticks" drawing style. One molecule is colored whereas the other shows atomic identities

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 molecule **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 molecule **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 molecule **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]

Deriving metric data using GUI

sel and **esd** are the universal commands for various mathematical computations. They deal with the **selected** 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 selected 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 \AA^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`

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

proj sph

or

proj sph -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.

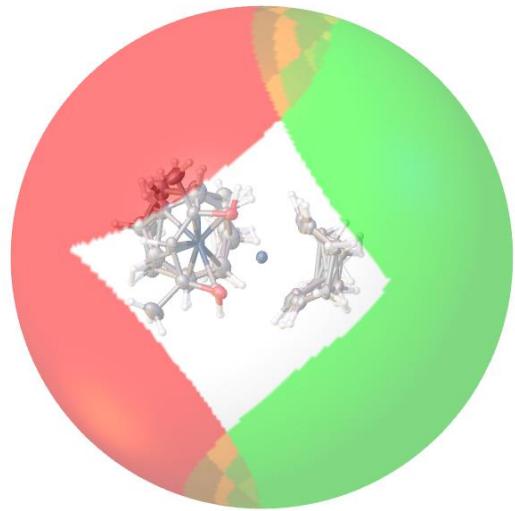
Type

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 your 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.