

Notes on OLEX2

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This is work in progress. You are encouraged to e-mail me your comments and suggestions.

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About your version of OLEX2

Q: How do I install OLEX2?

A: The program is available for free download from www.olex2.org, just follow the installation instructions. OLEX2 should be installed and run in an administrator mode. Currently, some options do not work if a non-administrator runs the properly installed OLEX2. You will also likely need programs XS and XL (written by George Sheldrick) available free from <http://shelx.uni-ac.gwdg.de/SHELX/index.html>. XS and XL are necessary for structural solution and refinement, respectively. OLEX2 is smart and if you already have XS and XL (or the entire SHLEXL suite) installed, OLEX2 will find the programs on your computer. See FAQ on the OLEX2 web site.

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 command line type

echo GetCompilationInfo() [provides the compilation date]

Or, hit F7 to highlight the tools tab and expand the Settings tab. The compile date is the top entry.

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.

Q: How do I view where the OLEX2 users reside (not a public option)?

A: **http://www.olex2.org/access_log**

Useful 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 - select everything
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.

Working with molecular graphics

Q: How do I modify the font on the screen?

A: You can modify your font with

setfont console choosefont()

This command is *not* for atom label modification (*vide infra*).

Q: How can I modify atom labels?

A: **setfont Picture_labels choosefont(olex2)** [invokes atom label setting controls]

Q: How do I display atom labels?

A: You can toggle atom labels with **F3**. Additional controls are

labels -l [displays non-hydrogen atom labels]

labels -l -h [display all atom labels including those for the H atoms]

The Q peaks are treated as atoms as far as labeling is concerned except for one unique command

labels -qi [displays the Q peak heights in $e/\text{\AA}^3$]

Note that the word **labels** is plural.

To generate moveable atom labels for diagrams use

label [atom name(s)] [to create movable atom labels].

Examples:

label o1 o2 [will create movable labels for atoms o1 and o2].

label \$o [will create movable labels for all oxygen atoms].

Note that the word **label** is singular.

Q: How do I display the unit cell boundaries?

A: Type

cell

to toggle the unit cell boundaries.

Q: How can I manipulate the molecular image representation?

A: The following commands are handy for manipulating the molecular image:

sfil [to see atomic spheres type]

telp [to switch to the ellipsoid view type]

telph [to switch to the ellipsoid view type with the H atom spheres scaled]

telp 40 [to set the ellipsoid percentage to 40%]

matr 1 [to orient the cell along the a axis type; 2 and 3 work for the *b* and *c* axes]

or

matr 100 [this can also be done with the right click menu]

brad 0.5 [adjusts the bond thickness of ALL bonds. Currently the individual bonds cannot be modified. The default value is 1.0]

grad [to modify the background]

F3 [toggles labels]

F4 [toggles background]

ctrl-t [toggles the molecule and text]

Q: How do I restore the default settings?

A: View→quick drawing styles→default. A shortcut for this is to type

default

Q: How do I save a graphics file with a molecular drawing?

A: After you have created a desired projection with desired labels you can save the drawing with
pict filename.ext resolution[1-10, >100] -pq

Where it is critical to provide the extension “**ext**” to the file. The resolution can be between 1 and 10, but the file size will be VERY large, so don’t go for 10 right off the bat. **-pq** is optional, stands for “picture quality”, and will smooth the bonds and atom boundaries in your diagram. The supported file formats include jpeg, bmp, png, and tiff.

Example:

pict test.jpg 3 -pq

pict test.jpg 640 [will create picture with the width of 640 pixels; option **pq** will be disabled when **resolution** exceeds 100].

In fact if you open the (large) created file with Photoshop and save it anew the file size can be drastically reduced.

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.

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.

To unmatch the molecules type

fuse

or go to Tools→Overlay and click Unmatch.

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].

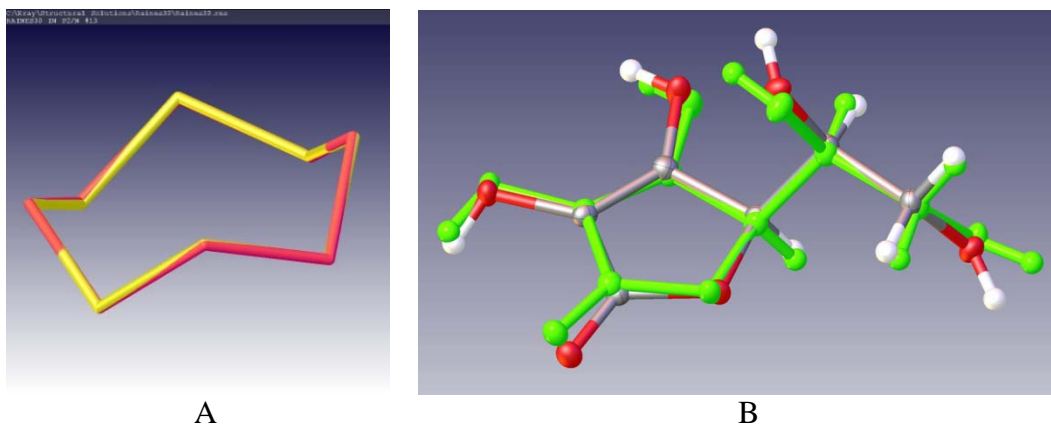


Figure 1. a) Two superimposed symmetry-independent molecules of S_8 shown with the "tubes" drawing style; b) two superimposed symmetry-independent molecules of vitamin C shown with the "ellipses and sticks" drawing style. One molecule is colored whereas the other shows atomic identities.

To color one of the superimposed molecules

right-click on the molecule→Fragment→Show this only [to display the molecules by itself]

ctrl-a [to select the molecule, both atoms and bonds]

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

right-click on the molecule→Draw style [to display the Material Parameters palette]

In the Material Parameters palette double-click on the color rectangle corresponding to Ambient Front and select the color of your choice followed by OK.

Then type

fmol [to bring back all the molecules on the screen]

Repeat as necessary for other molecules.

Q: How do I generate a packing diagram?

A: Use menu Structure→Generate, and in Generation Options select the box size.

Alternatively, you can use

mode pack [displays the positions of other molecule positions as maroon pyramids]

and then click on the pyramids that you want to turn into molecules. Hitting the ESC key will end the **pack** mode.

Another way it to control the diagram creation manually:

pack [generates a packing diagram. The default for **pack** is “**pack -1.0 1.5 -1.0 1.5 -1.0 1.5**” Olex 2 generates all the fragments with the centers of gravity within the defined parallelepiped]

or

pack 0 1 0 1 0 1 [fills the unit cell with molecules; the numbers are pairwise limits for the *a*, *b*, and *c* axial vectors and can be adjusted as necessary].

Q: Can I display the basis vectors?

A: The basis vectors can be toggled by typing

basis

and moved with the left mouse button when the SHIFT key is depressed. Right-click on the basis to resize it.

Q: Is there an easy way to label several symmetry-independent molecules (with the same composition) similarly?

A: Yes. The following procedures work well on structures with two molecules, but I have not tested it on structures with $Z' > 2$. It is important to eliminate all the Q peaks prior to the **match** operations. It is necessary to execute **kill \$q** rather than **ctrl-Q**, because the latter will only hide them.

Example: two molecules with similar geometries in the asymmetric unit.

Section A.

1. Label one molecule (let's call it molecules **A**) to your liking. Maybe you have O1,O2,C1,C2... atoms with suffixless labels.

2. Select any atom in molecule **A** (by left-clicking on it).

3. Select any atom in molecule **B** (by left-clicking on it).

4. In order to label molecule **B** similarly with suffix "a" type

match sel -n=a [n stands for "name of the suffix"]

Now you have two identically named molecules with names such as C1 in molecule **A** and C1a in molecule **B**.

Section B.

The GUI alternative to the procedure in Section A is now available:

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

Section C.

But perhaps you want your two molecules to have suffixes "a" and "b". [Since the atom names cannot be longer than four characters in XL the procedure above may not work. This is because if you have a molecule with names such as C1a and want to mimic the other molecule with suffix "b" you will end up with names such as C1ab.] Here is the correct procedure.

1. Label one molecule (let's call it molecules **A**) to your liking. Maybe you have O1,O2,C1,C2... atoms with labels but no suffixes.
2. Select any atom in molecule **A** (by left-clicking on it).
3. Select any atom in molecule **B** (by left-clicking on it).
4. Now to label molecule **B** similarly with suffix "a" type **match sel -n=b** [**n** stands for "name of the suffix"]
5. Select any atom in molecule **A** (by left-clicking on it).
6. Isolate this molecule by typing **uniq sel**
7. Select the molecule with **ctrl-a**.
8. Add the suffix to the atom labels with **name sel -s=a** [**s** stand for "suffix"].
9. Bring back the other molecule with **fmol**

Section D.

Suppose that you have an organometallic complex with two identical ligands that you would like to label similarly, such as two molecules in Section A. The procedure described in Sections A-C are valid, but the trick is to isolate each ligand first by disconnecting the central atom from them.

conn 0 Ti

[connects the specified atom (Ti) to exactly 0 atoms; in this case, Ti will be disconnected from all other atoms].

or, click on the metal atom to select it and type

conn 0

Now you can follow any routine from Sections A-C to label the atoms to your liking. Re-refine the structure to restore connectivity.

Working with hydrogen atoms

Q: What control over H atoms do I have?

A: These two commands are frequently useful:

ctrl-H [to toggle hydrogen atoms and hydrogen bonds on the screen]

telph [to switch to the ellipsoid view type with the H atom spheres scaled]

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

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

Q: How do I show the hydrogen bonding interactions of my choice?

A: To show hydrogen bonds adjust the slider in the WORK panel, click on the bonds you want to expand, then ESC to remove the hanging bonds.

Q: How do I tabulate the hydrogen bonding interactions?

A: This is achieved with

htab [dist][angle][keywords]

If you issue

htab

with no arguments OLEX2 will insert HTAB card(s) (and the necessary EQIV cards) for the hydrogen bonds in the INS file. The defaults for the H-bond determination are Donor-Acceptor distance of 2.85 Å and Donor-H...Acceptor angle of 150°.

To survey more interactions one may use

htab 3 120 -t=C,N

where **3** is the D...A distance in Angstroms, **120** is the D-H...A angle in degrees, and **-t=C,N** will add additional atom types that can serve as donors and acceptors, the default atom types are N, O, F, S, and Cl.

It may be convenient to display the H-bonds as connected sets with

compaq -a [to reposition molecules to form H-bonds]

Q: How do I remove all the H atom constraints? My data are that good!

A: In the command line type

sel \$h

afix 0

and run a refinement.

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]

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:

wp [to generate info about the *E*-statistics. This command will result in the Wilson plot which can be closed].

sg [to generate the space group info]

text [to show the screen content in an external text editor. Scroll down to see all the stats relevant to the space group selection].

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

Q: How do I display the info on my current space group?

echo sgs() [shows cell choice type selection]

sginfo [space group] [shows the info on the specified space group, not necessarily on your current space group].

Examples:

sginfo fdd2

sginfo P21/c

Q: How do I convert space group P1 with two symmetry-related molecules into $P\bar{1}$ with one molecule?

A: Let us use the following Cr complex (C₆H₅C₆H₄Br)Cr(CO)₃ (I) as an example (*Acta Cryst.*, 2003, **C59**, m499-m500).

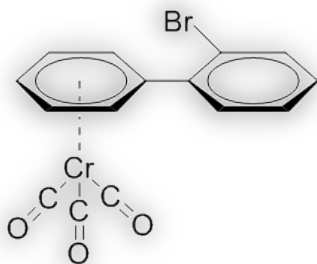


Figure 2. The Cr(0) complex (I) used to illustrate the $P4 \rightarrow P\bar{1}$ switch.

This structure of (I) could not be solved in $P1$ and had to be solved in $P1$ with two molecules, Figure 3.

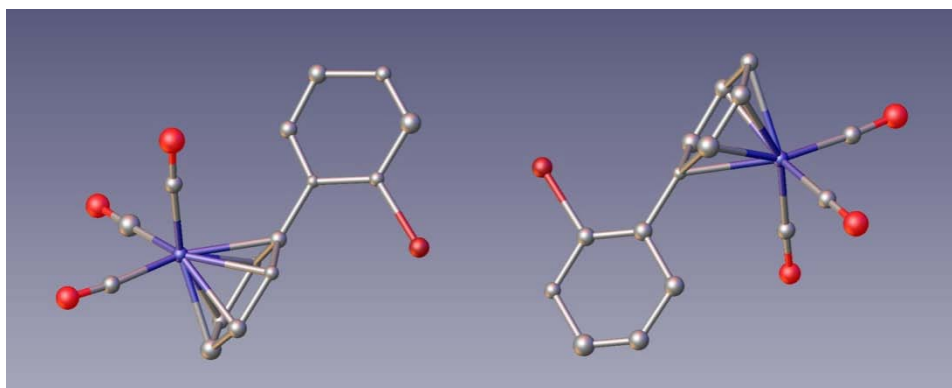


Figure 3. The structure of (I) solved in $P1$. The two molecules are related by an inversion center.

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 4.

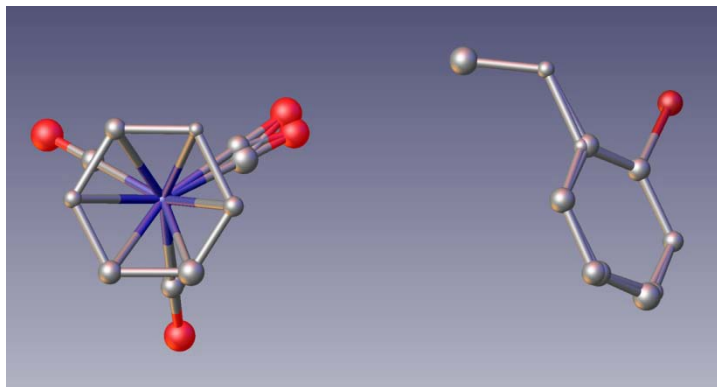


Figure 4. The structure of (I) immediately after converting the space group to the correct $P\bar{1}$.

In order to reassemble the two separate parts execute
7. `compaq`
and now the structure looks like in Figure 5.

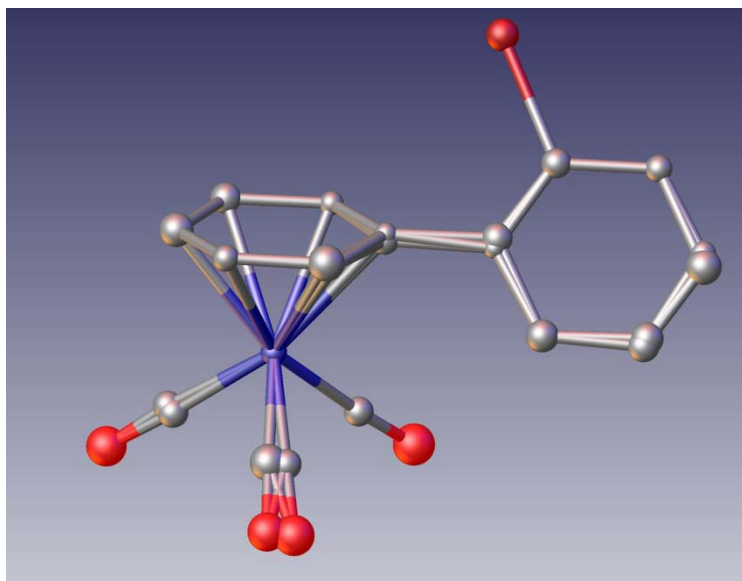


Figure 5. The structure of (I) is in the correct space group $P\bar{1}$, but needs polishing.

Sometimes the resultant merged molecule contains extra atoms near the expected positions (Figure 5). 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.

8. Delete the redundant atoms and proceed with the refinement.

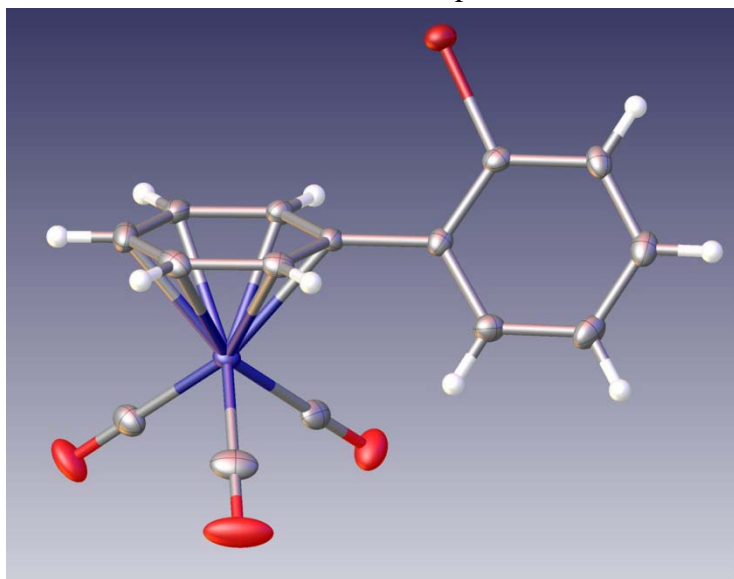


Figure 6. The structure of (I) in the correct space group $P\bar{1}$.

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 type issue

sgs [axis][cell choice] [converts the unit cell type].

Example:

sgs b1 [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 *a*'s will be overestimated in the new INS file].

Q: How can I change the space group?

A: Either by using a menu under the work→solve→Space group, click "Suggest SG" 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]

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 & Label". The H atoms will follow the atoms they are attached to in the instruction file. If you click on "Moieties" the moieties will also be sorted by size; this is achieved by splitting the atoms according to their moieties. The order in which the sorting routines are executed matters. Thus, it's a good idea to sort by "Mass & 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.

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, then 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()

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.