Commands and Modes in Olex2

There is no special console window in Olex2 - the commands described here can be typed at any time and the text you type as well as the program response will appear in the bottom right hand corner of the main window. The text will then scroll up behind the displayed molecule. The number of lines of text that are visible can be set with the command **lines** *n*.

Many commands in Olex2 are modelled on the SHELX syntax: four letter commands, where the letters often provide a hint about the function of the command. Many commands that are available in ShelXP, for example, can be used in Olex2. Also, all all commands of the ShelXL and ShelXS syntax are interpreted by Olex2 and used to construct the internal Olex2 structure model. This model is then used directly to carry out a smtbx-refine refinement, whereas a shelx.ins file is generated on the fly if ShelXL/XH is chosen for the refinement.

All commands in Olex2 will auto-complete when pressing the TAB key. If the completion is not possible, because there are more than one commands starting with the letter that have been typed, a list of these commands will be printed. It is good practice to use the auto-complete feature!

Understanding the Syntax

Selection: If one or more atoms are selected on the screen, then any command that acts on a selection will apply to the selected atoms only. If there is no selection, it will apply to **all** atoms. Instead of making a selection on the screen, a list of atom names can also be supplied. *If a command has been successful, the selection will disappear.*

Mode: If Olex2 is in a **Mode**, the chosen action will be applied to all subsequently clicked atoms.

Syntax used below:
{a, b, c}: choice of a, b or c. For example: fix {occu, xyz, Uiso} [atoms] means 'fix occu [atoms]', 'fix xyz [atoms]', 'fix Uiso [atoms]'.

[val=2]: optional parameter. This parameter is not required for the command to work, and if it is not supplied, the default value will be used.

-**k:** This is an option switch.

i: Italic characters are used for variables.

[atoms] means an optional list of atoms. Any atoms that are selected will automatically be present in this list. If there are no selected atoms, **all** atoms will be in this list. Alternatively, the atom names of the atoms that should appear in this list can be typed by hand.

atoms means a compulsory list of atoms. Any atoms that are selected will automatically be present in this list. Alternatively, the atom names of the atoms that should appear in this list can be typed by hand.

Capital Letters are used for commands that will directly affect the structure model in the refinement. These commands will become part of the structure model and will appear in the ShelX input file. Please note that these commands can be typed either in upper or lower case.

Fixed/Refined Parameters		
fix	{occu, xyz, Uiso} [atoms]	Fixes the specified refinement parameter, ie these parameters will not be refined in subsequent refinement cycles. **occu**: will fix the occupancy **xyz**: will fix the xyz coordinates **Uiso**: will fix the whole ADP
free	{occu, xyz, Uiso} [atoms]	The opposite of fix - makes the specified parameters for the given atoms refineable. Feeing the occupancy is also available from the context menu.
mode	fixu	Fixes Uiso or ADP for subsequently clicked atoms.
mode	fixxyz	Fixes coordinates for subsequently clicked atoms.
mode	occu occupancy_to_set	Sets atoms occupancy to the povided value for subsequently clicked atoms.
labels -f show currently fixed atomic parameters, **labels -f -r** show labels for fixed atoms and also the number at which the occupancy of riding atoms is fixed		

Atom Connectivity Table Manipulation		
conn	*n* [*r*] atoms	Sets the maximum number of bonds for the specified atoms to *n* and changes the default bond radius for the given atom type to *r.* **Examples:** **conn 5 $C** sets the maximum number of bonds all C atoms can have to 5, **conn 1.3 $C** changes the bonding radius for C atoms to 1.3 (the floating point is used to distinguish between *n* and *r* in this case!), **conn 5 1.3 $C** combines the two commands above
compaq	[**-a**] [**-c**]	Moves all atoms or fragments of the asymmetric unit as close to each other as possible. If no options are provided, all fragments are assembled around the largest one. **-a:** assembles broken fragments

		• **-c**: similar as with no options, but considers atom-to-atom distances and will move all atoms to the closest possible position to the largest fragment in the structure.
addbond	**A1 A2** *or* atoms	Adds a bond to the connectivity list for the specified atoms. This operation will also be successful if symmetry equivalent atoms are specified.
delbond	**A1 A2** *or* Selected bond(s)	Removes selected bonds from the connectivity list.
Olex2 will display the altered connectivity table in the case if structure is grown or packed		

Symmetry Operations		
lstsymm		Prints symmetry operations and their codes for current structure.
envi	*r* [2.7 Å] **A1** *or* one selected atom [**-h**] [**-q**] **Note:** if more than one atom is selected the first one is used	Prints a list of those atoms within a sphere of radius *r* around the specified atom. • **-h**: adds hydrogen atoms to the list • **-q**: option adds Q-peaks to the list
mode	**grow** [**-s**] [**-v**] [**-b**]	Displays the directions in which the molecule can be grown • *-s***:** also shows the short interaction directions • *-v:* [2.0 Å] shows directions to the molecules within *v* value of the Van der Waals radii of the selected atoms which can be generated by clicking on the direction representations, only unique symmetry operations (producing shortest contacts are displayed) • *-r***:** shows directions to all symmetry equivalent atoms atoms of the selected one(s) within 15 Å • shortcut **Ctrl+G** is used to enter the '**mode grow**'
mode	**pack**	Displays the position of symmetry equivalent asymmetric units as tetrahedra. These asymmetric units can be generated by clicking on the corresponding tetrahedron.
sgen	atoms The Symmetry operation is represented as 1_555 or -1+X,Y,Z and atoms as a selection or a names list	Generates symmetry equivalents of the provided (or all atoms, if there is no selection) using the provided symmetry operation. **Note:** For symmetry operations starting with '-' and letter, a leading zero must be added, for example, **0-x,-y,-z**, otherwise Olex2 confuses this with an option.
pack	**-a a -b b -c c** [atoms]	Packs all or specified atoms within given dimensions • **-c:** prevents clearing existing model **Example:** **pack $O** will pack all O atoms with the default of -1.5 to 1.5 cells range.
pack	**cell**	Shows content of the unit cell.
pack	*r*	Packs fragments within radius *r* of the selected atom(s) or the centre of gravity of the asymmetric unit.

grow	[atoms] [-w]	Grows all possible/given atoms; for the polymeric structures or structures requiring several grows Olex2 will continue grow until the comes to already used symmetry element • **-w:** allows to apply already used symmetry operations to other fragments of the asymmetric unit **Example:** If the main molecule is grown, but only one solvent molecule is shown, using '**grow -w**' will produce other solvent molecules using symmetry operators used to grow the main molecule
	If some atoms are deleted after growing operations, Olex2 will use existing unique atoms as the asymmetric unit atoms; this can be helpful to avoid a sequence of sgen/kill commands	

Disorder Modelling: Constraints and Restraints		
EXYZ	atom types (to add for the selected atom) [-**EADP**] [-**lo**]	Makes the selected site shared by atoms of several atom types. • **-EADP:** adds the equivalent ADPs command for all atoms sharing one site. • **-lo:** links the occupancy of the atoms sharing the site through a free variable.
EADP	atoms	Makes the ADP of the specified atoms equivalent.
SADI	atoms or bonds [esd=0.02]	For selected bonds or atom pairs **SADI** makes the distances specified by selecting bonds or atom pairs similar within the esd. If only **one** atom is selected it is considered to belong to a regular molecule (like PF_6) and adds similarity restraints for P-F and F-F distances. For **three** selected atoms (**A1,A2,A3**) it creates similarity restraint for **A1-A2** and **A2-A3** distances.
DFIX	*d* atom pairs or pairwise selection in order *[esd=0.02]*	For selected bonds or atom pairs **DFIX** will generate length fixing restraint with the given esd. If only **one** atom is selected, all outgoing bonds of that atom will be fixed to the given length with provided esd. For **three** selected atoms (**A1,A2,A3**) the A1-A2 and A2-A3 restraints will be generated.
DANG	*d* atom pairs or pairwise selection in order [esd=0.04]	For selected bonds or atom pairs, distance restraints similar to dfix will be generated.
tria	*d1 d2 angle* [esd=0.02]	For given set of bond pairs sharing an atom or atom triplets generates two dfix commands and one dang command. **Example: tria 1 1 180 C1 C2 C3** will generate 'DFIX 1 0.02 C1 C2 C2 C3' and 'DANG 2 0.04 C1 C3' it will calculate the distance for dang from d1 d2 and the angle.
FLAT	[atoms][esd=0.1]	Restrains given fragment to be flat (can be used on the grown structure) within given esd.

CHIV	[atoms][*val*=0] [esd=0.1]	Restrains the chiral volume of the provided group to be *val* within given esd
SIMU	[*d*=1.7] [esd12=0.04] [esd13=0.08]	Restrains the ADPs of all 1,2 and 1,3 pairs within the given atoms to be similar with the given esd.
DELU	[esd12=0.01] [esd13=0.01]	'rigid bond' restraint
ISOR	[esd=0.1] [esd_terminal=0.2]	Restrains the ADP of the given atom(s) to be approximately isotropic
SAME	N	Splits the selected atoms into the N groups and applies the SAME restraint to them. Olex2 will manage the order of atoms within the in file, however mixing rigid group constraints and the 'same' instructions might lead to an erroneous instruction file.
showp	[any]; space separated part number(s)	Shows only the parts requested: **showp 0 1** will show parts 0 and 1, **showp 0** just part 0. **showp** by itself will display all parts.
split	[-**r**={eadp, isor, simu}]	Splits selected atom(s) along the longest ADP axis into two groups and links their occupancy through a free variable. -**r** adds specific restraints/constraints for the generated atoms • **eadp**, **isor** or **simu**
AFIX	shelx afix number{mn} [-n]	-n option considers N-atoms as parts of rings. If no are atoms provided and afix corresponds to a fitted group where n is 6 or 9 (such as 106 or 79), all the rings which satisfy the given afix will be automatically made rigid (this is useful in the case of many PPh3 fragments); alternatively a single ring atom can be selected to make that ring rigid. In other cases, depending on afix either 5,6 or 10 atoms will be expected. Special cases of afix 0, 1 and 2 can be used to remove afix, fix all parameters or leave just the coordinates refinable, all other afix instructions will consider the first atom as a pivot atom and the rest - dependent atom.
part	[part=new_part] [atoms] [-p=1]	Changes part number for given/selected atom; -lo options links occupancies of the atoms through a +/-var or linear equation (SUMP) depending on the -p[=1] option which specifies how many parts to create. if -p=1, -lo is ignored and the given or new part is assigned to the given atoms.
fvar	[*value*] [atoms]	This command links two or more atoms through a free variable. • If **no *atoms*** are given the current free variables are printed. • If **no *value*** is given but two atom names are give, the occupancies of those atoms are linked through a new free variable. • If a **value of 0** is given, the occupancy of the specified atoms will be refined freely

		• if the **value is not 0**, the occupancy value of the specified atoms is set to the given value.
sump	[**val**=1] [esd=0.01]	Creates a new linear equation. If any of the selected atoms has refinable or fixed occupancy, a new variable is added with value 1/(number of given atoms), otherwise already used variable is used with weight of 1.0. **Example:** If 3 atoms (A1, A2, A3) are selected this command will generate three free variables and insert the **r2 1.0 var 3** instruction (equivalent to 1.0 = 1.0*occu(A1) + 1.0*occu(A2) + 1.0*occu(A3).
mode	split [-**r**={eadp, isor, simu}]	Splits subsequently clicked atoms into parts, or in combination with the Shift key can be used to drag an atom to change its position. -r option can be used to generate extra restraints/constraints for original and generated atoms; values are eadp, isor or simu. While in the mode the newly generated atoms can be selected and moved as a group with Shift down or rotated when dragging the selection. The original and generated atoms will be placed into different parts.

HKL file Operations		
hklstat		Prints detailed information about reflections used in the refinement.
omit	h k l	Inserts 'OMIT h k l' instruction in the ins file
omit	val	Inserts 'OMIT h k l' for all reflections with $|Fo^2 - Fc^2| > val$.
omit	s 2theta	Inserts 'OMIT s 2theta' instruction in the ins file
edithkl	[h k l]	Brings up a dialogue, where 'bad' reflections from the Shelx lst file and all its constituent symmetry equivalents can be inspected and flagged to be excluded from the refinement. In constrast to the OMIT h k l instruction, which excludes the reflection and *all it equivalents*, this dialogue allows to exclude those equivalents that are actually outliers. If a particular reflection is specified, this particular reflection and all its constituent equivalents can be viewed.
excludehkl	-h=h1;h2;.. -k=k1;k2.. -l=l1;l2.. [-c]	This function provides a mechanism to reversibly exclude some reflections from refinement (these reflections will be moved to the end of the hkl file so they appear after the 0 0 0 reflection). • **-c:** option controls how the given indices are treated, if not -c option is provided, then any reflection having any of the given h, k or l indices will be excluded, otherwise only reflections with indices within provided h, k and l will be excluded.

appendhkl	-h=h1;h2;.. -k=k1;k2.. -l=l1;l2..	Acts in the opposite way to excludehkl

Customising the Olex2 GUI

setfont	{console, Picture_labels} choosefont()	Will bring up the dialogue to choose the font
grad	[C1 C2 C3 C4]	Choose the colour of the four corners of the graduated background.
brad	brad *r*	Adjust the bond radius in the display.

Output: Tables, Reports and Images

pictPS	filename.ps [color_fill] [color_line]	Generates a post-script file of what is visible in the molecule display. • **-color_fill:** Fills the ellipses with colour. • **-color_bond:** Bonds will be in colour. • **-color_line:** Lines representing the ellipses will be in colour. • **div_pie:** number [4] of stripes in the octant • **lw_ellipse:** line width [0.5] of the ellipse • **lw_font:** line width [1] for the vector font • **lw_octant:** line width [0.5] of the octant arcs • **lw_pie:** line width [0.5] of the octant stripes • **p:** perspective • **scale_hb:** scale for H-bonds [0.5]Label Labels The bond width is taken from the display. This can be changed with **brad**
pict	filename.*ext* [-pq] [*n*]	Generates a bitmap image of what is visible on the molecule display. • ext {png, jpg, bmp}. png is best. • **-pq:** print quality • *n:* refers to the size of the output image. If *n* is smaller than 10, it refers to a multiple of the current display size, if it is larger than 100, it refers to the width of the image in pixels.
picta	filename.*ext* [-pq] [*n*]	A portable version of **pict** with limited resolution, which is OS and graphics card dependent. This may not be stable on some graphics cards • **-pq:** print quality
label	label [atoms]	Adds labels to the selected atoms. These labels can be moved by pressing the SHIFT key while holding down the left mouse button • **type:** {subscript, brackets, default}