OLEX^2 Quick Reference

Files	
reap	brings up the Open File dialog (also accessible using CTRL-O)
close	closes current structure
save model	saves the current model and display settings to a ".oxm" file
load model	retrieves a saved model file (defaults to current_filename.oxm)
edit [filetype]	edits current INS, LST, CIF (or any other extension (defaults to INS)

Model Building	
fuse	displays only the asymmetric unit
compaq	moves all atoms of the asymmetric unit as close together as possible
compaq [–q,–a,–c,–m]	as above, but considers Q-peaks, fragments, atoms, or non-metals
move	moves all fragments as close to the unit cell center as possible
uniq **atoms**	displays the fragment connected to selected or named atom(s)
fmol	displays all fragments
grow	grows incomplete molecules or fragments using symmetry
grow –w	grows structure using symmetry generators already applied
mode grow	shows clickable "bonds" to grow fragments using symmetry
mode grow –s	shows clickable "bonds" to grow to atoms with short interactions
pack	generates packing diagram with default (large) number of unit cells
pack 0 1	packs atoms/fragments between zero and one (other #'s possible)
pack cell	packs all atoms that fall within unit cell (combine with grow –w)
mode pack	Displays asymmetric units as a set of tetrahedral (click to add units)
kill $q	kills (deletes) all Q-peaks
conn *n* **atoms**	sets maximum number of bonds for selected or specified atoms to *n*
addbond **atoms**	adds a bond to connectivity list for selected or specified atoms pairs
delbond **bond** (or **atoms**)	removes selected bond (or bond between specified atoms) from list
hadd [**atoms**]	adds hydrogen atoms to all (default), selected, or named atoms

Refinement	
refine [*n m*]	runs *n* cycles of refinement and displays *m* Q-peaks
CTRL-R (⌘-R on Mac)	runs the refinement with the current number of cycles/peaks
weight	updates the weighting scheme to the (SHELX) suggested scheme
anis [**atoms**]	makes selected or named atom(s) anisotropic (defaults to all atoms)
isot [**atoms**]	makes selected or named atom(s) isotropic (defaults to all atoms)
addins *instruct*	adds the SHELX *instruct*ion to the current INS file (*e.g.* addins EXTI)
fixunit [Z']	sets SFAC and UNIT to content of asymmetric unit (default Z'=1)

Selections	
sel $*x*	selects all atoms (or peaks) of type *x* (*e.g.* sel $h or sel $q)
sel C1 > C10	selects all the carbon atoms in the range C1 through C10
sel part *n*	select all atoms in PART *n*
selback	re-selects the last set of selected atoms and/or bonds
SHIFT + lclick	drag to select atoms within a given rectangle
CTRL-A	select all atoms, bonds, and objects
CTRL-I	inverts the current selection
ESC (escape)	unselects the current selection (also exits current MODE)
DEL **atoms**	deletes selected atom(s) or object(s) (CTRL-DEL on Mac)
sort +ml moiety +s	sorts atoms by mass and label and forms moieties by size

Model Style	
telp [*n*]	displays atoms as thermal ellipsoids (percentage *n*)
pers	displays the model in typical ball and stick style
proj	displays the model in a simple wireframe style
tubes	displays the model in the "tubes" drawing style
sfil	displays atoms as spacefilling spheres

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Naming	
F3	toggles display of atom names labels
name $q C	changes of the element type of all Q-peaks to C (Q-peaks become carbon)
name 1 **atoms**	names the selection (*e.g.* C1, C2, …) starting with the number given
name **atoms** P	changes the atom type of the selected atom(s) to phosphorus

Display	
matr *n*	orients the model along the *a* (*n*=1), *b* (*n*=2), or *c* (*n*=3) axis
cell	toggles display of the unit cell boundaries
F2, F4	toggles the background color white and solid (F2), or gradient (F4)
lines *n*	sets the number of text lines to display to *n*, use –1 for all lines
CTRL-T	toggles display: 1) structure and text, 2) text only, 3) structure only
CTRL-Q	toggles Q-peaks: 1) Q-peaks, 2) Q-peaks w/bonds, 3) no Q-peaks
CTRL-H	toggles H's: 1) show hydrogens, 2) w/H-bonds, 3) hide hydrogens
qual {–l,–m,–h}	sets drawing quality to low, medium or high

Information	
envi **atom**	prints distances and angles to all atoms within 2.7Å of selected atom
fvar	if nothing selected, prints current values of all free variables (FVAR)
hklstat	prints detailed information about reflections used in the refinement
info [**atoms**]	prints information about the selected, named, or all atoms
sel **atoms/obj**	prints geometric information about the selected atoms or objects
esd **atoms/obj**	prints geometric information *with esd* information (requires MORE –1)

Analysis	
mpln **atoms**	creates a best plane from the selected or named atoms (at least 3)
cent **atoms**	creates a centroid for all selected or named atoms (at least 2)
pipi	analyzes the structure for π-π stacking interactions
htab	analyzes structure for hydrogen bonds and adds HTAB to INS file

Disorder	
part *n* **atoms**	assigns selected or named atoms to PART *n*
fvar *n* **atom** (1)	links occupancy of atom to the n^{th} free variable (use –*n* for 1-FVAR)
fvar **atom** (2*n*)	creates new free variable and links occupancies of 2 halves of selection
split **atoms**	splits the selected atom(s) into two groups and links occupancies
mode fit **atoms**	move atoms, SHIFT-drag (on atom) to move, lclick-drag to rotate set rclick on atom to set rotation center, rlick on bond to set rotation axis
showp 0 1	shows only PARTs 0 and 1, (can show any number of PARTs)
showp	shows all PARTS
labels {–p,–o,–v}	labels atoms with PART number, occupancy, or FVAR number
eadp **atoms**	constrains the ADPs of the selected or named atoms to be equal (EADP)
sadi **bonds**	all selected bonds will be restrained to be equal (within esd=0.02)
sadi **atoms** (2*n*)	bonds between *n* selected pairs will be restrained to be equal (esd=0.02)
sadi **atom** (1)	all outgoing bonds of that atom will be restrained to be equal (esd=0.02)
dfix *d* **bonds**	all selected bonds will be restrained to the distance *d* (esd=0.02)
dfix *d* **atoms** (2*n*)	bonds between *n* selected pairs will be restrained to the distance *d*
dfix *d* **atom** (1)	all outgoing bonds of that atom will be restrained to the distance *d*
simu [d] **atoms**	restrains ADPs of 1,2 and 1,3 pairs within *d* Å to be similar (1.7Å)
delu **atoms**	applies a 'rigid bond' restraint to selected or named atoms
isor **atoms**	restrains the ADPs of the atoms to be approximately isotropic
flat **atoms**	restraints selected or named group of (at least 4) atoms to be FLAT

Syntax for left column:

- keys are in ALL CAPS, variables are in *italics*
- optional parameters are in [square brackets]
- required parameters are in {curly brackets}
- **atoms/bonds** refers either to one or more selected atoms, selected bonds, or one or more named atoms
- **atoms** (*n*) refers to a selection of *n* atom(s), when the number of selected atoms is significant

Right column: SHELX keywords are in ALL CAPS