Olex2 1.2.6. Change log

Mac 64 bit distribution, fixing stability issues on some Mac platforms.

Added user database management (Home->Settings->User Database) and the report publication section is reviewed.

Changes to the atom naming – now no duplication allowed at any point. Previously the program could undo the users labelling if there were duplications left.

Extended atom labelling in the reports (combinations of brackets super and subscript is possible disregarding the actual naming in the CIF).

Extension to the ‘sadi’ command to generate a set of restraints for rotor like groups (e.g. CF3 ) when the user selects two atoms

Olex2 now transforms EQIV commands when the user modifies the asymmetric unit so that existing like information table definitions (HTAB/RTAB) and restraints still make sense after the symmetry transformations

Small atoms now can be temporarily represented by tetrahedrons using the ‘special’ drawing mode which is activated by pressing Ctrl+Spacebar. Besides this the mode also renders the EXYZ atoms in spatially separated position.

Shelxl-2014/7 compatibility regarding modified HKL and version comments in the INS header

Extending mpln –r parameter which now can take the number of the polygon edges, e.g. ‘mpln -r=6’ constructs a regular plane with hexagon representation

Atom sorting now applies to SAME groups other restraint atom lists

ShowR for working with residues

Reworked context menus for connectivity and occupancy; the Atom Type menu now also contains elements in current formula; ‘Brad’ command is now accessible from the bond context menu

Extending ‘info’ command to print the formula and number of electrons for the input

Extensions to the ‘wbox’ added so that it can adopt spherical shape. The shape can be controlled using ‘wbox.Type’ command with sphere/box argument. This object can be used for packing and various map display trimming.

HAdd now can put restraints rather when constraints (rigid groups) when placing H atoms onto water molecules (use ‘–r’ option to control it)

Improvements to handling the complete CIF – now the metadata will also be exported and the CIF resulting from the refinement should be nearly identical to the original one. The exported values list is controlled by the ‘export\_metacif’ section of the customisation.xld file.

More work on the solid angles (Guzei, I.A., Wendt, M.Dalton Trans., 2006, 3991-3999), representation and analysis (ProjSph)

Fixing rims rendering in PS (if the atom has no rims – they are not rendered, thus adding one more rendering option for atoms)