Poster

Olex2 and olex2.refine

Oleg Dolomanov

OlexSys Ltd
oleg@olexsys.org

Over the years, Olex2 has established itself as user-friendly software, enabling novice users to quickly solve and refine X-ray structures. But what also comes in the box - and is often overlooked - is olex2.refine. This presentation will highlight olex2.refine's development directions and the new features it introduces in addition to the well-established refinement performed by ShelXL.

In the last several years, olex2.refine has been adopted to perform refinements based on tabulated atomic form factors computed by NoSperA2, thus providing easy access to Quantum Crystallography (QC). Olex2.refine can now also refine against intensities that take the dynamic nature of the Electron Diffraction (ED) into account. Refinement of anharmonic thermal parameters up to the 4th order and refinement of the anomalous dispersion terms has also been implemented and is readily available.

Olex2.refine brings in new restraints, like ADP “volume” similarity and constraints - rotated ADP and shared ADP, same group constraint and others. The well-known linear equation SUMP restraint from ShelXL can also be used as a constraint in olex2.refine.

We also extended olex2.refine to be executed remotely—either on the same computer or externally. This recognises that ED and QC refinements and computation can be time-consuming processes. We are always looking for further directions that olex2.refine might take. What do you want to see in olex2.refine?

Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009).J. Appl. Cryst., 42, 339-341.

Bourhis L.J., Dolomanov O.V., Gildea R.J., Howard J.A.K, Puschmann H., The anatomy of a comprehensive constrained, restrained refinement program for the modern computing environment - Olex2 dissected (2015), Acta Cryst. A71, 59–75.