[MS45-P09] Olex2 – A Complete Package for Molecular Crystallography H. Puschmann, L.J. Bourhis, O.V. Dolomanov, R.J. Gildea, J.A.K. Howard,

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Olex2 [1] has become established in the community of small-molecule crystallographers as an easy-to-use unified package that provides tools needed for day-to-day analyses of small molecule structures. There many thousand installations of the software world-wide and our user base is growing rapidly. Olex2 is under active development and our users are fully supported. **Structure Solution** is achieved by our own charge-flipping implementation, *Olex2-Solve*, based on E^2, but SIR, ShelXS, ShelXD and SUPERFLIP link seamlessly with Olex2 **Structure Refinement** can be carried out with *Olex2-Refine*. The refinement engine is based on the cctbx and provides all the functionality required for a meaningful structure refinement. A general system allows the implementation of any constraints, which has been used to provide all ShelXL constraints. Alternatively, all versions of ShelXL are also fully supported. **Structure Analysis** tools covering most requirements are an integral part – growing, packing, geometric measurements, void, molecular and solvent accessible volume calculation, π-π analysis and many more. **Structure Publication** is made easy. Complete and correct CIFs result automatically, the generation of reports is easy and images – bitmaps or ORTEP-style drawings – can be generated with minimum effort. **Olex2 is Open Source** free of charge for academic users. Compiled versions for Windows, Linux and MaxOSX are available from our site.

[1] www.Olex2.org

[2] 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.

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