**m33.p06**

## Olex$^2$: A Comprehensive Molecular Graphics Tool for Small-Molecule Structures

Horst Puschmann, Oleg Dolomanov

*Department of Chemistry, Durham University, Durham, UK. E-mail: horst.puschmann@durham.ac.uk*

**Keywords: molecular graphics, small molecule, structure model building**

Olex$^2$ is a powerful molecular graphics tool. As can be expected from any molecular viewer, Olex$^2$ provides fully customisable, powerful molecular graphics. Olex$^2$ can interact seamlessly and intelligently with the refinement program ShelXL, setting it apart from most other programs of its kind. The highly sophisticated refinement tools provided by ShelXL can be accessed and addressed intuitively, making building complicated structure models very easy, even for the novice user. The User Interface to Olex$^2$ has a high degree of redundancy: the program can be driven from the command line only (using familiar ShelXP syntax), the context menus (right-click), as well as the highly adaptable (and customisable) Graphics User Interface. This high degree of flexibility allows the program to be accessible to all levels of user experience.

**m34.p01**

## Small molecule crystallography for the future

Luc Bourhis[a], David Watkin[b], Judith Howard[a]
Horst Puschmann[a], Mustapha Sadki[b]

*[a]Department of Chemistry, Durham University, Durham, UK [b]Oxford University, Oxford, UK. E-mail: l_j_bourhis@mac.com*

**Keywords: small molecule, new software, platform**

Almost all crystallographic computing in the area of small molecule crystallography is currently performed using software which is twenty or more years old. Many of the original authors of this software have already left the field, and many more will soon retire. This project is a collaboration between the Universities of Oxford and Durham with the aim to analyze and document existing software and to build from scratch a new, highly modular, maintainable, flexible and extensible computing platform for small molecule crystallography. Modern software tools will be used and a high standard of documentation will be maintained throughout.