MS45-1-2 Olex2: what's in the black box?
#MS45-1-2

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Abstract
Olex2 [1] is now firmly established as a major software package in the field of small-molecule crystallography and it is safe to claim that the majority of structures are now processed with Olex2.
For many, Olex2 is a convenient interface to the ShelX software, and rightly so: users can concentrate on what matters in their structures and there is no need to be overly familiar with the computer language that interfaces the structure with the refinement program.
But there is so much more to Olex2, and recent developments have seen the coming-of-age of our native refinement program olex2.refine [2]. Recent developments have seen an enormous increase in speed and it is now also fully compatible with ShelXL refinements (you can switch easily between the two). But in addition, with olex2.refine we can now also
-- refine using non-spherical form factors (NoSpherA2) [3,4]
-- access constantly evolving new Quantum Crystallographial functionality [5]
-- refine atoms anharmonically
-- refine the anomalous dispersion parameters f' and f'' [6]
-- use various unique constraints and restraints
Olex2 is extensible on many levels: be it through simple macros, small python scripts, fully functional complex extension modules (which anyone can create) and, at a deeper level, powerful new developments on the level of the underlying cctbx.
In this contribution, I will dissect what is in Olex2, and explain how it is all organised. You will be interested in this if you
-- would like to get an overview of what's new in Olex2
-- are interested in gaining a deeper understanding of how it all works
-- would like to learn how to teach Olex2 new tricks
-- would like to contribute new science to Olex2
Olex2 is open-source, multi-platform and free of charge for all users

References
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