MS30 O1

Small Molecule computing - where next?

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Keywords: Computing, automation, structure analysis

With few but important exceptions, computer programming for small molecule crystallography has virtually come to a halt. In recent years the range of software for dealing with small molecule crystallography has reduced as older codes become unsupported and unmaintained. The few remaining programs still in use have excellent track records, and deal with most of the commonly occurring situations. While these programs continue to work, there is little incentive to re-write them in modern programming languages.

New programs are being written in fields which are still developing. JANA [1] is well established for dealing with modulated structures, but is less commonly used for dealing with normal structures. The revolutionary TOPAS [2] program has a small but enthusiastic body of users, and demonstrates a totally new approach to crystallographic software. The charge-flipping algorithm [3] has created a lot of activity in recent years, and has been incorporated into some established programs as well as new, stand-alone, programs. Diffractometer manufacturers continue to develop more powerful packages for reliable automated data collection.

The current situation is that small molecule crystallographers have excellent data collection facilities and many powerful tools for completing a structure analysis. Curiously, since the 1980s there has been very little work aimed at putting these tools together and fully automating crystal structure analysis. Consequently, more time can be spent trying to create a scientifically valid cif than was spent during data collection. A recent small-sample survey in the UK showed that about half a dozen situations were consistently ranked as being most time-consuming in taking a well-crystalline sample through to an Acta Cryst acceptable publication.

None of the time-consuming operations are crystallographically complex – the mathematical tools exist in most programs. The delay is due to the highly branched decision tree that must be searched to find a suitable solution, and the absence of any really effective man-computer interfaces for dealing with anything but essentially trivial problems.

Small molecule crystal structure analysis will remain an art rather than a technology until a wider range of chemical experience can be incorporated into programs.

[1] http://www-xray.fzu.cz/jana/Jana2000/jana.html.
[2] http://members.optusnet.com.au/~alancoelho/
[3] Oszlányi, G. & Süto, A. (2004). *Acta Cryst.* A60, 134-141

MS30 O2

Addressing problems with pseudosymmetry, unknown symmetry and unknown composition by charge flipping

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Keywords: charge flipping, superstructure, structure solution

Since its publication in 2004 the charge-flipping algorithm [1], [2] has gained a considerable attention in the crystallographic community for its simplicity and flexibility. It can be used for a routine solution of inorganic and organic structures with up to several hundred atoms in the unit cell.

One of the crucial features of the algorithm is that it reconstructs the scattering density without any symmetry restrictions, i. e. in the space group $P1$. Thus, the symmetry of the structure need not be known *a priori* and it can be located *a posteriori* in the reconstructed density.

Another appealing property of the algorithm is that it requires only the experimental amplitudes of the structure factors as an input. Neither the normalization of the structure factors, nor the knowledge of the absolute scale of the structure factors is needed. Thus, the chemical composition is not used at all in the structure solution process. This can be a crucial advantage if the chemical composition of the crystal is unknown or only partially known.

Recently the charge-flipping algorithm was generalized to cope also with scattering densities that are not strictly positive [3]. While the main intention of this generalization was to solve the structures measured with neutron diffraction, another exciting application of this method exists: a difference charge flipping. This method allows reconstruction of the difference electron density maps by applying the charge flipping only to a subset of reflections (typically superstructure reflections) and setting the amplitudes of the other reflections to zero. The result of the calculation is a difference density map, showing the deviations of the density from the average that would correspond to the omitted reflections. Such difference density map can reveal shifts of atoms from their average positions and thus allow understanding of the fine superstructure features, a feat that still represents a considerable challenge for the conventional methods.

[1] Oszlányi G.; Sütő A, *Acta Crystallogr. A*, 2004, 60, 134.
[2] Oszlányi G.; Sütő A, *Acta Crystallogr. A*, 2005, 61, 147.
[3] Oszlányi G.; Sütő A, *Acta Crystallogr. A*, in press.

MS30 O3

Olex2: a quick prototyping framework for crystallographers

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Keywords: open source, computer programming in X-ray diffraction, molecular graphics

Olex2 is Graphical User Interface for a set of independent libraries. It provides the user with tools to manipulate the crystallographic model in a comprehensive way. There is also an embedded Python interpreter to perform more complex tasks on the exposed crystallographic model in a non-intrusive way. For example, the latter can be a python script undertaking interactive cctbx refinement procedures. The application is open source and has a very simple design, which eliminates the majority of dependencies up to the GUI level, where wxWidgets is used as a platform for portable GUI.

The crystallographic library provides a pluggable interface for input/output operations and simple objects to operate