

**MS30 O1**

**Small Molecule computing - where next?** David Watkin, Chemical Crystallography Laboratory, University of Oxford, England. E-mail: [david.watkin@chem.ox.ac.uk](mailto:david.watkin@chem.ox.ac.uk)

**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. & Sütö, A. (2004). *Acta Cryst.* A60, 134-141

**MS30 O2**

**Addressing problems with pseudosymmetry, unknown symmetry and unknown composition by charge flipping** Lukas Palatinus, Gervais Chapuis *Laboratory for Crystallography, EPF Lausanne, Switzerland.*

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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.; Sütö A, *Acta Crystallogr. A*, 2004, 60, 134.

[2] Oszlányi G.; Sütö A, *Acta Crystallogr. A*, 2005, 61, 147.

[3] Oszlányi G.; Sütö A, *Acta Crystallogr. A*, in press.

**MS30 O3**

**Olex2: a quick prototyping framework for crystallographers** Oleg Dolomanov and Horst Puschmann, *Department of Chemistry, Durham University, Durham, UK*

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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

with the crystallographic model. The graphics library is independent of the crystallographic library and provides an interface sufficient for the implementation of complex graphical objects.

#### MS30 O4

**News from DirAx and Indexing** Jürgen Kopf  
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**Keywords:** Auto-indexing; Dirax-algorithm; Programming

Auto-indexing routines [1] have been used extensively for single crystal diffractometers with point-detector devices in the seventies and eighties of the last century. Without indexing routines data collection is impossible on such instruments. They depend on the accurate measurements of the diffractometer angles of a few selected (between 10 to 15) reflections.

In cases of non-merohedral twinning these techniques fail generally to find suitable cell parameters. By exclusion or replacement of unfavorable reflections, changing tolerances or other, mostly undocumented activities, indexing problems can be solved sometimes.

In 1992 Duisenberg [2] described a new algorithm for single-point-detector data. The method presented by Duisenberg takes the whole reflection list and constructs so-called "direct axes" vectors from all data. Then, the projections of the reciprocal lattice points onto these vectors are calculated and each line projection is searched for the one-dimensional lattice with the shortest period that represents the maximum number of projected reflections. The final primitive cell is determined from a reduced set of properly averaged "direct axes" vectors that give the best fit.

Nowadays only single crystal diffractometers with area detectors are in use, but an intrinsic problem of area-detector data is that the measured positions are less accurate than measured with point-detector devices. Therefore, other approaches are necessary for fast and reliable indexing in these cases.

A new method for auto-indexing of area-detector data was introduced by Steller et al. [3] in 1997. Steller also constructs "direct axes" vectors, but unlike the method of Duisenberg his routine tests all possible directions over a hemisphere and analyzes the frequency distribution of these vectors in each case. Also unlike the procedure of Duisenberg the periodicity is determined using fast fourier transform.

The concept of the reciprocal lattice is very important in xray-crystallography. In connection with the development of a new graphically oriented program for the visualization and the 3D presentation of the reciprocal lattice both algorithms were re-implemented. This program, called **QTRECLAT**, uses the Qt 4 and the OpenGL libraries and can handle an almost unlimited number of reflections. It reads a file that contains all relevant information about the positions and the intensities of the reflections, as can be produced with the Bruker-AXS *SMART* software. With the help of two projections on the x- and y-axis the extraction of periodic information of the reciprocal lattice is trivial

for the human eye. However, extracting the periodic length for a computer program is much more difficult to realize. The program is written in C++ using the Qt 4 class library [4]. Qt is the leading framework for native cross-platform application development that run on Windows, Unix/Linux and Mac OS X.

An important part of the program **QTRECLAT** is the refinement of the orientation matrix. This allows the definitive discrimination between reflections of the basic lattice and possible twin or other satellite reflections. Another feature of the program is that it can consider the intensity distribution of the reflections. Thus, the program may also serve as a good starting point for the following integration procedures.

[1] Sparks R.A., *Crystallographic Computing Techniques*, 1976, 452.

[2] Duisenberg A.J.M., *J. Appl. Cryst.*, 1992, 25, 92.

[3] Steller I., Bolotovskiy R., Rossmann M.G., *J. Appl. Cryst.*, 1997, 30, 1036.

[4] <http://www.trolltech.com/>

#### MS30 O5

**Comparing Entire Crystal Structures: Structural Genetic Fingerprinting** Andrew Parkin<sup>a</sup>, Gordon Barr<sup>a</sup>, Wei Dong<sup>a</sup>, Christopher J. Gilmore<sup>a</sup>, Dylan Jayatilaka<sup>b</sup>, Joshua J. McKinnon<sup>b</sup>, Mark A. Spackman<sup>b</sup> and Chick C. Wilson<sup>a</sup>  
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**Keywords:** Structural Comparison, Structural Similarity, Cambridge Structural Database

A method is described that is both robust and generally applicable, which allows the calculation of a similarity index between whole molecular crystal structures [1]. It is based on the use of fingerprint plots derived from Hirshfeld surfaces coupled with cluster analysis and associated multivariate statistics. Using this formalism, it is possible to show quantitatively that naphthalene is more similar to anthracene than to benzene, and moreover that benzodicyclopentadiene is more similar to anthracene than naphthalene is to anthracene. Whereas the correlation coefficients themselves obtained say nothing about the ways in which the patterns of intermolecular interactions are similar or different for two different structures, the fingerprint plots do contain such information. For the first time structural analysts have a robust method for quantifying structural similarities of whole molecular crystal structures; this has been termed 'Structural Genetic Fingerprinting'. A number of examples will be presented. There is no reason why this method cannot be applied to datasets consisting of many hundreds or even thousands of structures.

[1] Parkin A., Barr G., Dong W., Gilmore C.J., Jayatilaka D., McKinnon J.J., Spackman M.A., Wilson C.C., *CrystEngComm.*, 2007, Accepted for publication.