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Density modification for macromolecular and small molecule phasing. George M. Sheldrick[a]. [a]*Lehrstuhl für Strukturchemie, Georg-August-Universität, Göttingen, Germany.*
E-mail: gsheldr@shelx.uni-ac.gwdg.de

Experimental phasing of macromolecules almost always requires a step known as ***density modification*** [1-4], in which the electron density is modified iteratively so that it looks more like that expected for a macromolecule, before an interpretable map can be obtained. The quality of the resulting map depends on the quality of the initial phases, the resolution of the native data and the solvent content. Modern direct methods of solving small molecule structures also often involve a density modification step, but with the important differences that the initial phases may be random and that the data are expanded to the space group P1 and the true space group is determined after solving the ***phase problem*** [5-8]. A particularly effective form of density modification is simply to set negative density to zero [9] but the radius of convergence can be increased by using additional criteria for modifying the density [2-4,10,11] and by perturbing the density in some way, e.g. by ***charge flipping*** [12-14]. However care is needed when this approach is applied to the solution of small molecule structures because both the extension to space group P1 and the perturbation of the density can degrade the quality of the electron density maps, especially when the experimental data do not extend to high resolution. This talk will discuss a new implementation of ***random omit maps*** [8], a robust alternative to charge flipping for solving small molecule structures, and the incorporation of chemical information with the help of the ***sphere of influence algorithm*** [10] and ***iterative chain tracing*** [15] in the experimental phasing of macromolecular structures. It is to be expected that some of the density modification algorithms that have proved useful for phasing macromolecules will also assist the solution of small molecule structures and *vice versa*.

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Keywords: density modification, direct methods, SAD phasing

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XPRESSO: Automation in Routine Crystallography. Holger Ott[a], Joerg Kaercher[b]. [a]*Bruker AXS GmbH, Karlsruhe, Germany.* [b]*Bruker AXS Inc, Madison, WI, USA.*
E-mail: info@bruker-axs.de

Single crystal X-ray diffraction (SC-XRD) has become a routine tool for structure validation in analytical chemistry. Due to tremendous improvements in available hardware, smaller and more weakly diffracting crystals can now be measured. In consequence, the workload of staff crystallographers has increased significantly. At the same time software tools became available for processing data files more easily, e.g. for structure solution, structure refinement and absorption correction. In particular on routine data sets these tools allow for quick processing of the entire data set based on reasonable defaults and some clever decisions of an experienced user. In many cases only little crystallographic knowledge is required for successful processing. However, the routine work delays investigation of crystallographically more challenging samples and problems in a number of cases.

To alleviate experienced crystallographers from day-to-day routine work an automated software interface (XPRESSO) is available as part of the APEX2 software. This software builds a layer on top of established programs, such as SAINT, SADABS and the SHELXTL suite, which makes a number of crystallographic decisions to attempt for a successful structure solution, refinement and validation.

XPRESSO (Figure 1) also provides an entirely automated process from an initial quality check to the fully refined structure for processing previously collected data. A general description of the program flow and a number of examples will be presented.

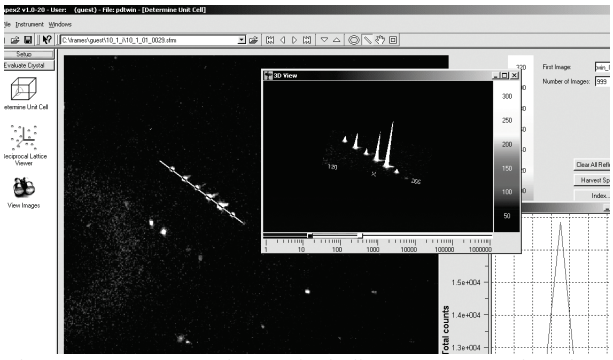

Figure 1: APEX2 software including XPRESSO interface, facilitating routine crystallography

Keywords: automation in chemistry, crystallographic software development, service crystallography

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Technologies for structural determination and validation using the CSD. Tracy Allgood, Ian Bruno *Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK*
E-mail: allgood@ccdc.cam.ac.uk