MS20 ADVANCES IN COMPUTATIONAL METHODS FOR SMALL MOLECULE CRYSTALLOGRAPHY
Chairpersons: Simon Parsons, Giovanni Luca Cascarano

MS20.25.1
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Phasing via full Pattern Powder Decomposition by Monte Carlo and Patterson Methods

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In a recent paper [1] a new full pattern decomposition technique has been suggested using linear ternary codes resulting from modifications of the Hamming codes. The resultant decomposition procedure consists of only 27 decomposition trials: to each of them 20 direct methods trials are applied, for a total of 540 tangent processes among which the correct solution may be found.

The above method has been combined with a technique [2] which modifies the Patterson map to obtain, by inversion, better estimates of the structure factor moduli.

The resultant procedure has been introduced in EXPO2005, and proved quite useful to solve crystal structures from powder diffraction data.

[1] Altomare A., Caliandro R., Cuocci C., da Silva I., Giacovazzo C., Moliterni A.G.G., Rizzi R., *J.Appl. Cryst.*, 2004, **37**, 204-209. [2] Altomare A., Foadi J., Giacovazzo C., Moliterni A.G.G., Burla M.C., Polidori G., *J.Appl. Cryst.*, 1998, **31**, 74-77.
Keywords: direct phasing, powder diffraction, ab-initio structure determination

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Ab-initio Structure Solution without the Use of Atomicity

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Charge flipping [1] is an amazingly simple ab-initio structure solution method that is based on the existence of extended zero regions in the electron density, but not directly on atomicity. The algorithm is iterative: the real-space modification simply changes the sign of electron density below a threshold, while in reciprocal space observed moduli are prescribed without any weighting. It was tested using synthetic data for a wide range of structures [1], and was shown to work on real data of both normal [2] and modulated [3] crystals. Recently, we have found an efficient modification of the charge flipping algorithm [4] that complements the phase exploration in reciprocal space. In the modified algorithm weak reflections are treated separately, their calculated moduli are let to change freely and their calculated phases are shifted by $\pi/2$. Paradoxically, it is better not to use observed moduli of weak reflections, in the search for a solution they create only unwanted constraints. The improvement is drastic, in some cases the success rate is increased by a factor of ten, in other cases a previously unsolvable structure becomes solvable by the modified algorithm.

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[1] Oszlányi G., Sütő A., *Acta Cryst. A*, 2004, **60**, 134. [2] Wu J.S., Spence J.C.H., *et al.*, *Acta Cryst. A*, 2004, **60**, 326. [3] Palatinus L., *Acta Cryst. A*, 2004, **60**, 604. [4] Oszlányi G., Sütő A., *Acta Cryst. A*, 2005, **61**, 147.
Keywords: ab-initio structure determination, algorithms, single-crystal diffraction

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A DS5 (Direct-Searcher Automatic System Version 5) Program for small Molecules Running on Windows PCs

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New developed **DS5** (Direct-Searcher automatic system ver. 5) for the crystal structure analysis of organic compounds running on PCs is one program that is integrated into one from more than 20 main programs and subroutine/graphic libraries of the *DS*SYSTEM* series [1,2]. Three features of the **DS5** are: input instruction data have compatibilities with *Shelx* series [3], calculation sequences are controlled by subprogram names that are prepared by user, and graphical outputs are displayed on PC with Postscript/HP-GL files. All functions of the **DS5** are inherited from the *DS*SYSTEM4*.

1) Data reduction (6): *ABSORP, AFCR, CONVERT, LQPARM, RDEDIT, SPACEG*
2) Calculation (8): *COMPARE, DISTAGL, LSBF, PARST, ROTEN, SFFR, Shake (ShakePSD), THMA*
3) Display and Plot (4): *DISTAGL, ORTEP3, PLUTO, ROTENP*
4) Publication (3): *DISTAGL, PARSTC, TABLES*
5) Document (2): *Manual, Help File*

[1] Okada S., Okada K., *Z. Kristallogr.*, 2000, **215**, 131. [2] Okada K., Okada S., *J. Chem. Inf. Comput. Sci.*, 1997, **37(3)**, 522. [3] Sheldrick G. M., SHELXL97: Program for the Refinement of Crystal Structures. University of Göttingen, 1997.
Keywords: computer programs, organic compounds, structural analysis software

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Maximising the Information Obtainable from Diffraction Experiments

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In this presentation I will describe some of the methods we have been developing in recent years for the analysis of both single crystal and powder diffraction data. In particular I will address how using modern and flexible software, such as the Topas-Academic package written by Alan Coelho, one can perform innovative analysis without needing access to source code. Complex analytical approaches can then be rapidly developed to address specific problems by those without high levels of computational expertise.

To illustrate the importance of software flexibility I will describe how simulated annealing techniques widely use for structure solution from powder diffraction data can be used to solve complex oxide superstructures from single crystal data. I will also describe methods we've developed for "surface fitting" diffraction data. By treating a set of variable temperature/time/pressure powder or single crystal data as an ensemble rather than as unconnected individual measurements, one can dramatically increase the useful information extractable from experimental data. Whilst specific examples will be used to highlight possibilities, the methods to be described have wide ranging applicability.

Keywords: methodology of diffraction analysis, powder diffraction, single-crystal X-ray methods

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Small Molecule Crystallographic Computing – What is the future?

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A well known proverb amongst programmers is 'If it's not broken, don't mend it'. This is good advice, but what should be done if it is clear that very soon something is going to stop working?

In recent years small molecule crystallographic programs have disappeared one by one. This usually happens when there is no one left who really understands the program, and who can support it in a changing environment. For a short while after the programs become unavailable, old crystallographers bore young crystallographers by repeating 'I remember when it was easy to do …. with program X'. Then people forget that it was ever possible, and then some one re-discovers the process. The wheel is re-invented.