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***Ab-initio* structure determination by powders:recent developments in *EXPO2010*.** Anna Moliterni, Angela Altomare, Corrado Cuocci, Carmelo Giacovazzo, Rosanna Rizzi. *Institute of Crystallography, CNR, Bari, Italy*.
E-mail: annagrazia.moliterni@ic.cnr.it

Ab-initio crystal structure determination from powder diffraction data became more and more popular in the last 20 years, thanks to the development of effective novel methods and powerful experimental devices. These enhancements enable to solve, often routinely, organic, inorganic and metallo-organic crystal structures, even if not always they ensure the success because of unavoidable problems like peak overlap, preferred orientation and/or background estimation.
EXPO2010, the evolution of *EXPO2009* [1], is a package able to perform all the steps of the *ab-initio* structure determination process: indexing; space group determination; estimation of the reflection integrated intensities; structure solution (both in reciprocal and direct space) and structure refinement. Special procedures make more straightforward the crystal structure solution process, especially in case of low resolution data and/or organic compounds. They are: 1) a new figure of merit for identifying the correct cell among a set of plausible solutions; 2) new methods, working in direct and reciprocal space, able to correct the truncation effects on the electron density; 3) direct space techniques (simulated annealing and hybrid approach).
Among the new algorithms implemented in *EXPO2010* we quote:

a. new procedures able to improve Direct Methods phasing *via* a suitable selection of the reflections to be phased;
b. a new criterion for ranking the most plausible set of phases provided by Direct Methods.

The main features of *EXPO2010* and its application to experimental data are outlined.

[1] Altomare A., Camalli M., Cuocci C., Giacovazzo C., Moliterni A., Rizzi R., *J. Appl. Cryst*, 2009, 42, 1197.

Keywords: *ab-initio* powder structure determination, computing in cristallography, powder software

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Macromolecular X-ray crystal structure analysis against limited and noisy data. Garib N Murshudov *Chemistry Department, University of York, York, UK, YO10 5EF.*
E-mail: garib@ysbl.york.ac.uk

Despite rapid advances in recent years in Macromolecular crystallography (MX), solution and analysis of structures of large molecules and molecular complexes using low resolution and noisy data from crystals with various peculiarities (e.g. twinning, translocational disorder) is remaining a challenging problem. Extraction chemically and structurally consistent and useful information from such data sets is only possible by a statistically robust combination of prior (structural and chemical) knowledge with experimental data. This talk will cover several recent developments aimed to help analysis of derivation of reliable atomic models using such data sets and their implementations in the macromolecular refinement program – REFMAC. These developments include maximum likelihood analysis (non-)merohedral twinned crystal structures, low-resolution (3-6Å) refinement tools, improved electron density map calculations.
The main focus of the talk will be on several new low resolution crystal structure refinement tools including: 1) using known homologous structures as restraints - information transfer from high resolution to low resolution; 2) internal pattern restraints – retaining structural integrity of macromolecules; 3) jelly body restraints – implicit normal mode refinement; 4) regularized electron density de-blurring – improved structural details in the calculated electron density.
The talk will also include 1) some details of high-resolution protein-ligand complexes; 2) extended dictionary of ligands and building blocks of macromolecules; 3) some statistical properties of crystallographic R-factors.

Keywords: X-ray structure analysis, refinement, ligand dictionary

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One-Stop Small-Molecule Crystallography: Olex2. Horst Puschmann, Luc J. Bourhis, Oleg V. Dolomanov, Richard J. Gildea, Judith A.K. Howard. *Department of Chemistry, Durham University Durham, U.K.*
E-mail: horst.puschmann@gmail.com

Olex2, [1] is an open source molecular graphics program for solution, refinement and manipulation of small-molecule crystal structures.
Powerful and easy-to-learn, Olex2 can be used without any special training, whilst still providing all the tools required by experienced crystallographers.
Task-orientated modules create an elegant interface enabling novices and experts in the field of small-molecule structural analysis to work with crystal structures in an intuitive and modern environment. In addition, the majority of the functionality can be accessed via the command-line or using a custom macro file.
Olex2 also provides a platform to access the full functionality of the Computational Crystallography Toolbox (cctbx). Available from within Olex2 is a new charge flipping algorithm based on the cctbx, as well as a new full matrix least squares minimiser.
It is fair to say that Olex2 has become a fully fledged, one-stop program that allows users of all experience levels to perform all steps that are required for a complete small-molecule structure analysis without the need to employ any third-party software at all. Olex2 now comes with Batteries included.
Olex2 is available free of charge for all common operating systems at www.olex2.org.

[1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.* (2009). 42, 339-341.

Keywords: small-molecule, user interface, refinement