

## ADVANCES IN CRYSTAL STRUCTURE SOLUTION BY EXPO2008

A. Altomare<sup>1</sup>, C. Cuocci<sup>1</sup>, C. Giacovazzo<sup>2</sup>, A. Moliterni<sup>1</sup> & R. Rizzi<sup>1</sup>

<sup>1</sup> Istituto di Cristallografia, CNR, via Amendola 122/o, 70126 Bari Italy

<sup>2</sup> Dip. Geomineralogico, Università di Bari, via Orabona 4, 70125 Bari Italy

In the last twenty years the role of powder diffraction has considerably increased. Powder technique is widely adopted for the characterization of new materials: organic, inorganic, metallorganic, biological, as well as pharmaceutical. Several sophisticated new computing programs have been developed in order to solve crystal structures from powder data. EXPO2008 is the updated version of EXPO2004 [1]. EXPO is a package able to carry out automatically the full pathway of the *ab-initio* structure solution process, both for organic and inorganic compounds, from the unit cell determination up to the Rietveld refinement of the structure model. It is written in Fortran95 and C++ and it runs on different platforms (Windows, Linux, Mac OS X). EXPO is free of charge for no profit institutions. Its last version, EXPO2008, includes innovative computing procedures providing more reliable results in short time. Supported by a graphic interface powerful and easy to handle, it is highly automatic and user friendly to users non-expert in crystallography also. The main steps of EXPO2008 are: a) cell parameters determination; b) space group identification; c) extraction of the integrated intensities from the experimental profile; d) application of Direct Methods for solving the phase problem and providing the electron density map chemically interpreted; e) optimization of the map by using procedure combining Fourier transform calculations and weighted least squares; f) solution of organic structures by adopting two direct space alternative strategies: 1) the information provided by Direct Methods is combined with a Simulated Annealing procedure for reducing the number of degrees of freedom (this choice may be conveniently applied when the Direct Methods map is meaningful and the number of freedom degrees is quite large); 2) the Simulated Annealing algorithm is applied without any connection with the Direct Methods solution process; g) structure refinement by Rietveld method. EXPO2008 is able to solve quite difficult structures (structures up to 70 non-hydrogen atoms in the asymmetric unit have been successfully studied). Applications to pharmaceutical compounds will be shown.

[1] A. Altomare, R. Caliendo, M. Camalli, C. Cuocci, C. Giacovazzo, A.G.G. Moliterni, R. Rizzi, *J. Appl. Cryst.* **37** (2004) 1025-1028.