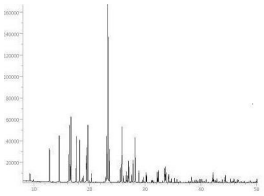
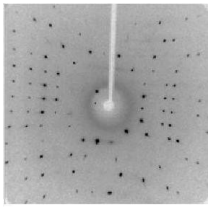
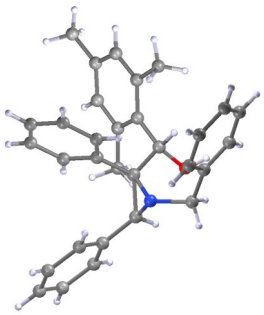
Crystal structure solution (powders and single crystal): theory and practice

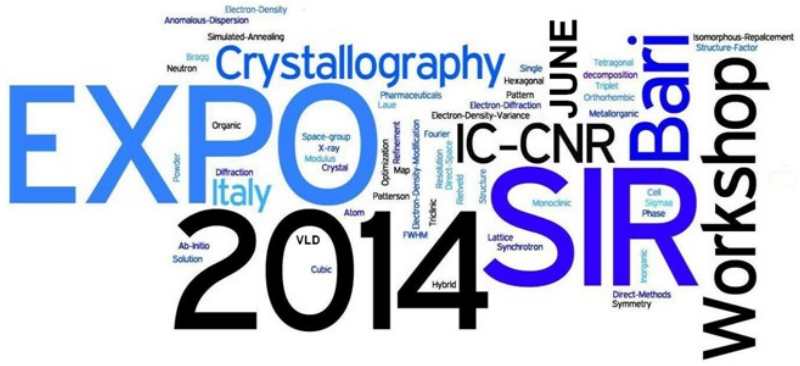






10-13 JUNE 2014

Dipartimento di Scienze della Terra e Geoambientali, University of Bari, Bari, Italy



International EXPO/SIR Workshop

organized by Institute of Crystallography-CNR of Bari

http://www.ba.ic.cnr.it/workshop2014/

The **International EXPO/SIR Workshop** will focus on the latest advances of the crystallographic methods for solving structures by both powder (**Module 1**) and single crystal (**Module 2**) diffraction data.
It will be devoted to the use of the latest versions of **EXPO** and **SIR**.
The workshop will include theoretical and practical sessions. Participants will have the opportunity to personally use **EXPO** and/or **SIR** under the supervision of the authors.

Module 1 (10-11 June)
Crystal structure solution by powder diffraction data

TOPICS

- ✓ Indexation and space group determination
- ✓ Pattern decomposition
- ✓ Phasing *via* Direct Methods
- ✓ Model optimization and Rietveld refinement
- ✓ Direct space methods
- ✓ Computer session

Module 2 (12-13 June)
Crystal structure solution by single crystal data

TOPICS

- ✓ Ab initio phasing by Direct Methods
- ✓ Ab initio phasing by Patterson deconvolution
- ✓ Solving *via* Vive La Difference (VLD)
- ✓ Solving *via* Simulated Annealing
- ✓ Molecular Replacement and automatic refinement/completion
- ✓ Use of the Graphical User Interface
- ✓ Computer session