



EXPO&more International Workshop

Crystallographic Software for Powder Diffraction Data

30 September - 3 October 2019

Organized by the Institute of Crystallography (IC) - CNR Bari, Italy

Starting with EXPO

Aurelia Falcicchio, Bari, 30 September 2019

EXPO2014 is a program devoted to structure solution of powder diffraction data



Main Functions

EXPO2014 PROGRAM

Indexing

An automatic peak search routine generates a list of "d" values corresponding to the experimental peaks. The values are processed for providing the cell parameters

Space group determination

A list of all the possible extinction symbols compatible with the reflections in the experimental pattern is provided. The extinction groups are ranked according to their probability values. The list of the corresponding compatible space groups is given

Estimation of integrated intensities

The program uses the Le Bail algorithm and combines it with a least squares procedure minimizing the difference between observed and calculated pattern

Structure solution by direct methods

DM are able to estimate phases directly from the structure factor amplitudes. The inverse Fourier transform of the structure factors gives the electron density map from which the model can be obtained

Real space techniques

An alternative approach to DM, based on real space techniques, has been introduced in EXPO2014

Structure model optimization

The obtained structure model is optimized and completed *via* an automatic structure model optimization procedure

Rietveld refinement

Structure model refinement by Rietveld method is available

Crystal structure visualization

EXPO2014 includes a viewer for 3D crystal structure visualization. This viewer is a modified version of Jav program to visualize structural models and electron density maps.

Registration and download

EXPO2014 is distributed free of charge for academic, scientific, educational, non commercial users.

Enter the following URL in a browser:

<http://www.ba.ic.cnr.it/softwareic/expo/expo2014-download/>

Click on 'Register' and enter your personal data

After registration you will receive an e-mail confirmation and you will be allowed to the download

System requirements



Windows 32-bit or 64-bit: Windows 10, Windows 8, Windows 7, Vista, XP, File *.exe



Mac OS X: OS X 10.10 (Yosemite), OS X 10.9 (Mavericks), OS X 10.8 (Mountain Lion), Mac OS X 10.7 (Lion), , Mac OS X 10.6 (Snow Leopard), Mac OS X 10.5 (Leopard). File *.dmg



GNU/Linux: Ubuntu 14.04 LTS, Ubuntu 15.04, Fedora 22 File *.deb, *.rpm, *.tar.gz

Technical details

❖ Program built using
OpenGL and GTK
libraries

❖ Program written in
Fortran and C++

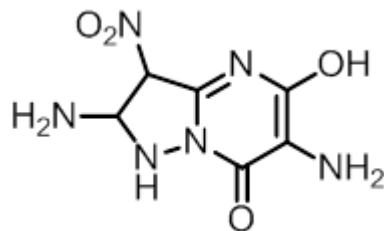
❖ Licensed under terms
of a Licence
Agreement



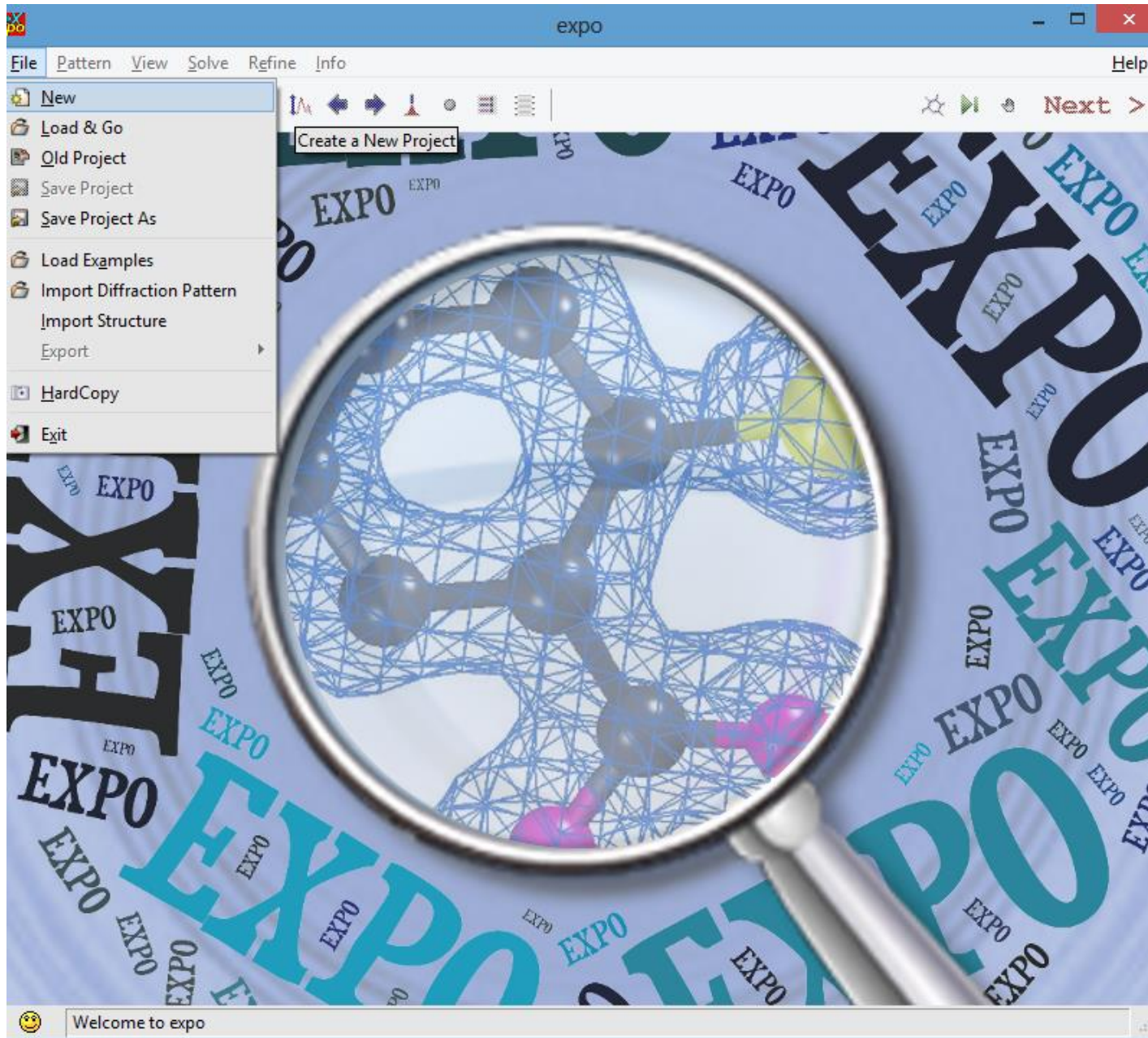
How to run EXPO2014

- ◆ by graphic interface
- ◆ *via an ASCII input file*

**An example: EXPO2014 default run on
 $C_6H_8N_6O_5$ (*and2*) structure**



by graphic interface

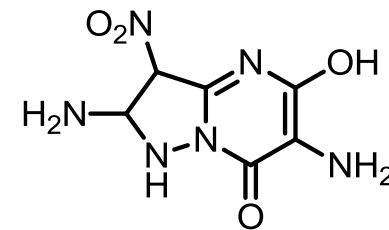


by graphic interface (Import Diffraction Pattern)

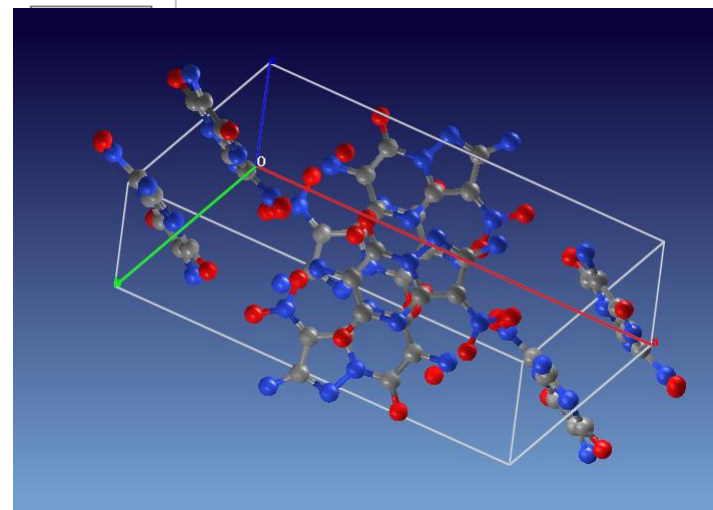
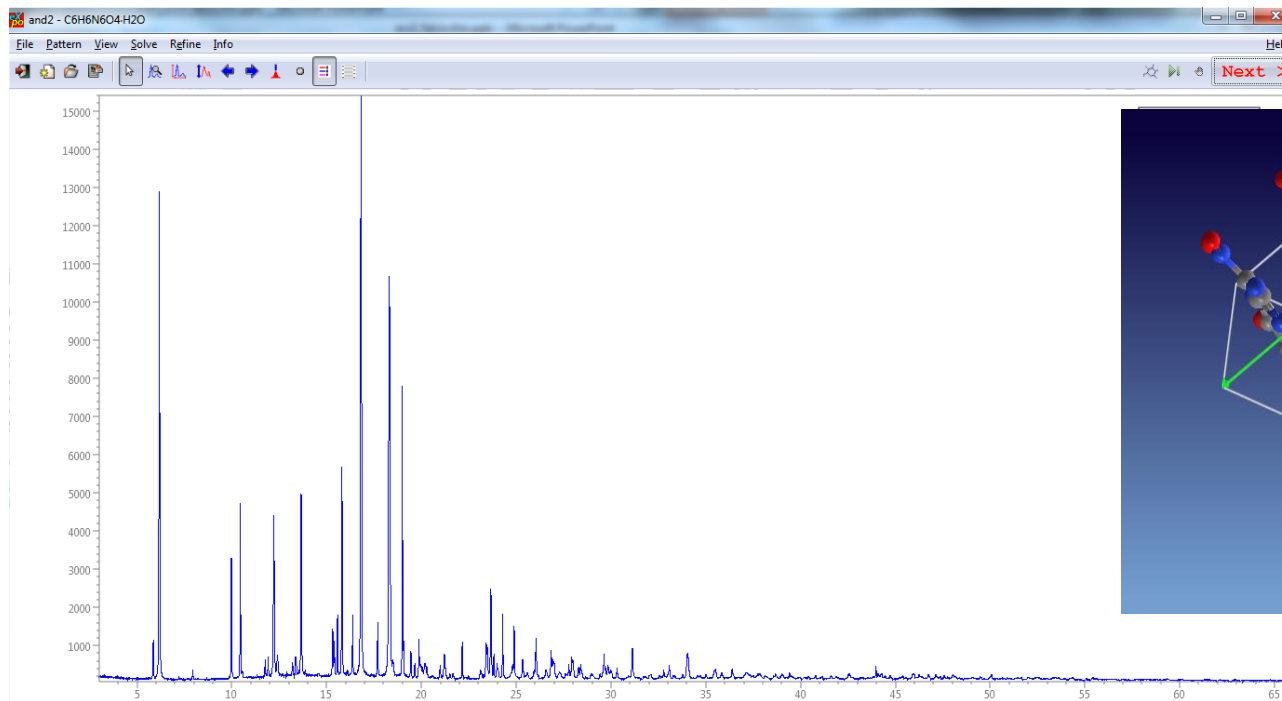


via an ASCII input file (.exp)

```
%structure and2  
%job and2  
%data  
pattern and2.pow  
wave 0.950436  
synchrotron  
%ntreor  
%continue
```



EXPO2014



EXPO2014

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FOR ANY:

- Suggestions
- Bug Reports
- Future requests
- Help

<http://www.ba.ic.cnr.it/contact>