Computational methodologies for the characterization of polycrystalline materials in software developed by the Institute of Crystallography

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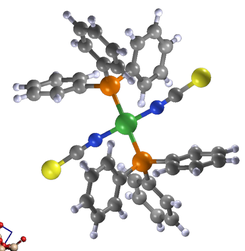
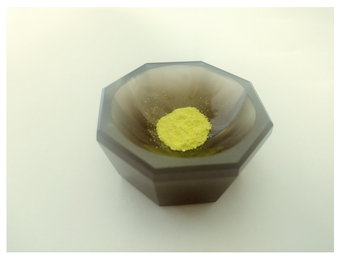
htttp://www.ba.ic.cnr.it/softwareic/

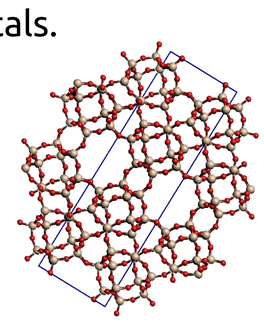
A polycrystalline material or 'powder' is an ensemble of several randomly oriented crystallites



The size of the elementary crystals is of the order of micrometer.
Microcrystalline compounds cannot be singled out to be characterized in the same way as single crystals.

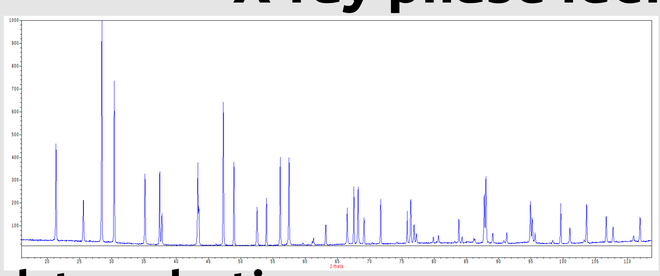


Chemical matter, drugs, minerals, heritage manufacts can be available or can be reduced in the form of crystalline powders.



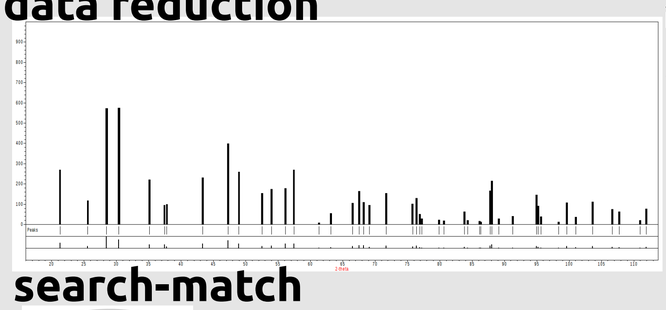
The study of powder is often a challenging task.

X-ray phase identification in a powder mixture: Qualitative Analysis



An X-ray powder diffraction pattern is characterized by a unique distribution of both positions and intensities of Bragg peaks. Each individual crystalline compound has its own "fingerprint", which enables the utilization of powder diffraction data in crystal phase identification.

data reduction



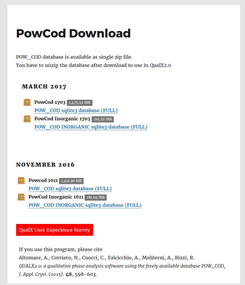
A digitized representation of powder data is quite compact and is especially convenient for comparison with other patterns, provided a suitable database is available.

search-match

Powder diffraction databases (e.g PDF[2], POW_COD) find substantial use in simple identification of crystalline compounds.

POW_COD database

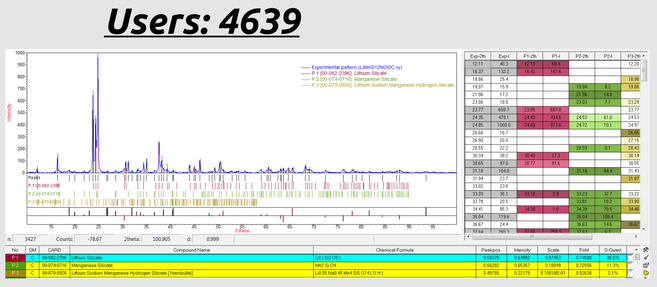
Downloads: 1059
Users: 1039



QUALX2.0 **and** ***POW_COD*** **database are software tools developed by IC for phase identification.[1]**

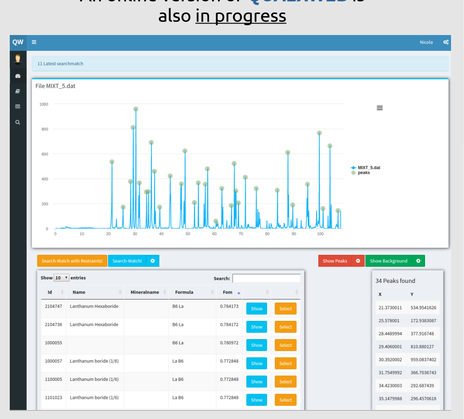
QUALX2.0 software

Downloads: 5090
Users: 4639



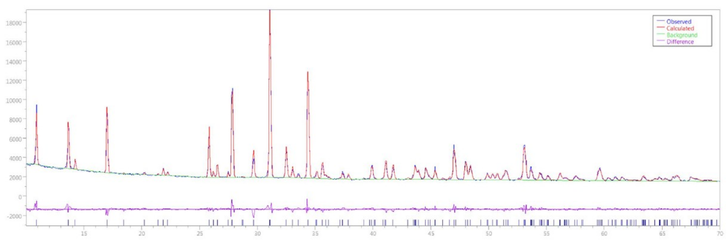
XRPD pattern and qualitative analysis by ***QUALX2.0*** for sample Li_6MnSi_s[3]

An online version of ***QUALXWEB*** is also in progress



Crystal Structure Determination by X-ray powder diffraction

X-ray diffraction is undoubtedly the most important and powerful methodology for elucidation of crystal structures, widely adopted in several scientific fields and technological applications: solid-state chemistry, pharmaceutical, materials science, mineralogy, cultural heritage, ...
A detailed description of the molecular structure is fundamental for understanding the structure-property relationships.

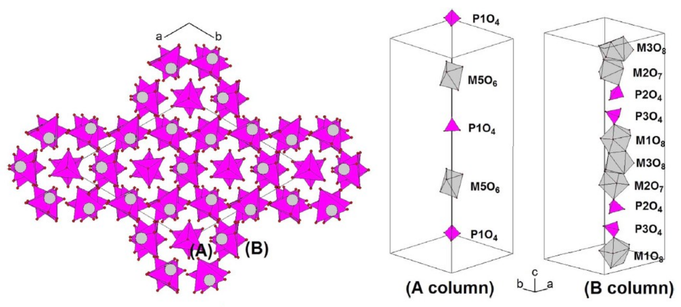


Final Rietveld plot of $Ca_9Dy(PO_4)_7$

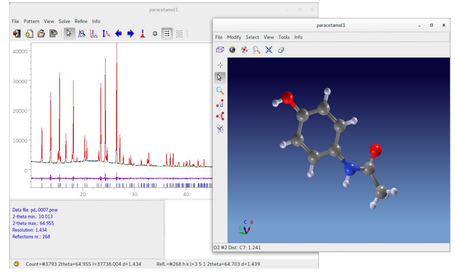
- Diffraction profile reduction
- Cell parameters
- Space group
- Direct methods
- Direct space method
- Fourier transform
- Electron density modification
- Structure model optimization
- Rietveld refinement
- …

EXPO2014 software

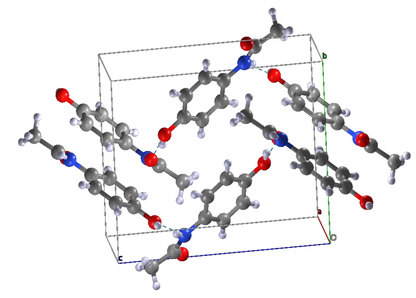
Downloads: 5568
Users: 5734



Structure of $Ca_9RE(PO_4)_7$ phosphates[5]



Crystal structure determination of paracetamol by ***EXPO2014*** software developed by IC.[4]



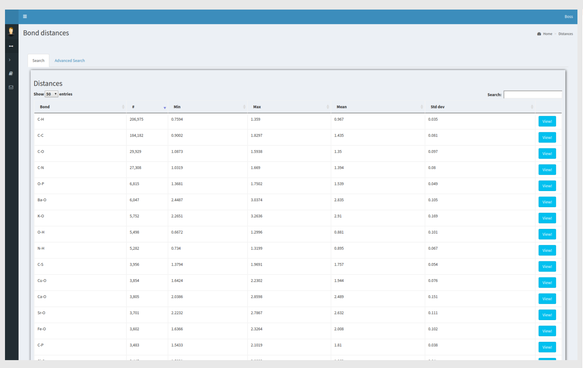
Crystal structure of paracetamol $C_8H_9NO_2$ form I

OChemDb: Open Chemistry Database

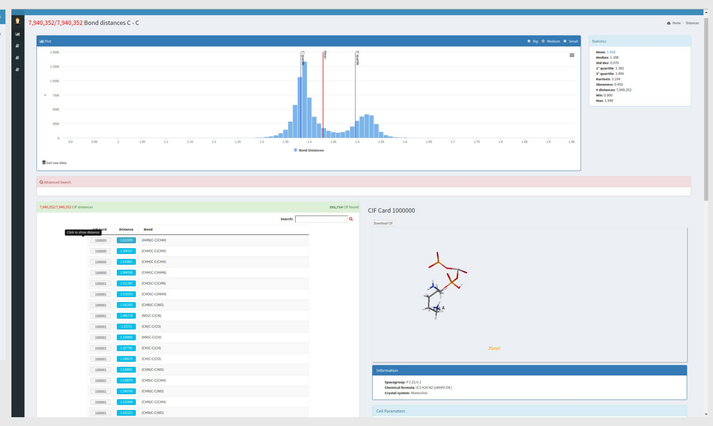
Work in progress

A database dedicated to collect, to make available by statistical tools and to manage crystal chemical information coming from the CIF files contained in the Crystallography Open database (COD)[6]. ***OChemDb*** can be used for searching and analyzing crystal-chemical information (bond distance, bond angle,space group, ...) of structures already solved, to be used for different scientific purposes.

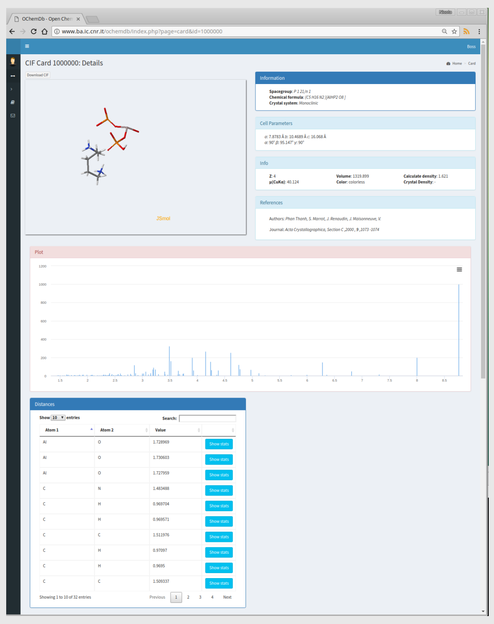
Bond distances to be investigated



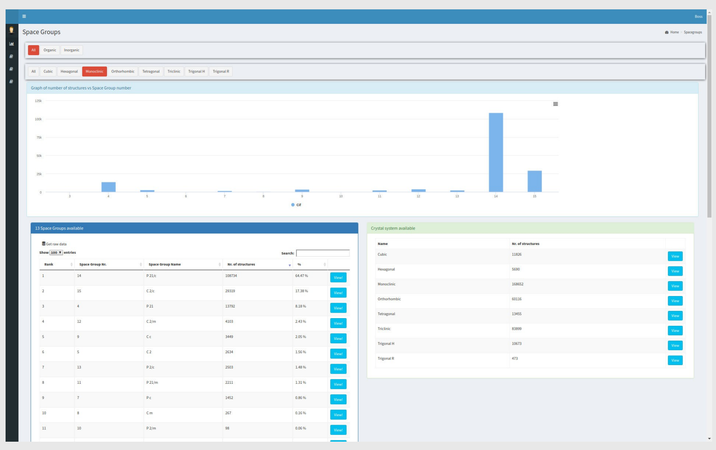
Details about C-C bond distances



Information contained in a CIF file



Stored CIF files of monoclinic structures



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6. Grazulis, S., Chateigner, D., Downs, R. T., Yokochi, A. T., Quiros, M., Lutterotti, L., Manakova, E., Butkus, J., Moeck, P. & Le Bail, A. (2009) "Crystallography Open Database – an open-access collection of crystal structures", J. Appl. Cryst. 42, 726-729.