The OChemDb software

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Why

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A very important step in the solution process of a newly determined crystal structure is the check of the final refined structure model, specifically in terms of bond lengths, bond and torsion angles. This step is fundamental not only for a deep comprehension of the molecular geometry from which a precise understanding of the structure-property relationships of the compound under study can derive, but also for depositing data and publishing the structure solution.

Other

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Its extensive associated software system, which is commercial, provides several user-friendly tools and multiple functions for searching the database, analysing its entries and displaying structures.

Our solution

The Open Chemistry Database (OChemDb) is a new free web portal which has been developed for assisting in the crystal structure determination process by surveying on bond distances, bond angles, torsion angles, atom types and space groups. It uses a suitably designed database of solved crystal structures.

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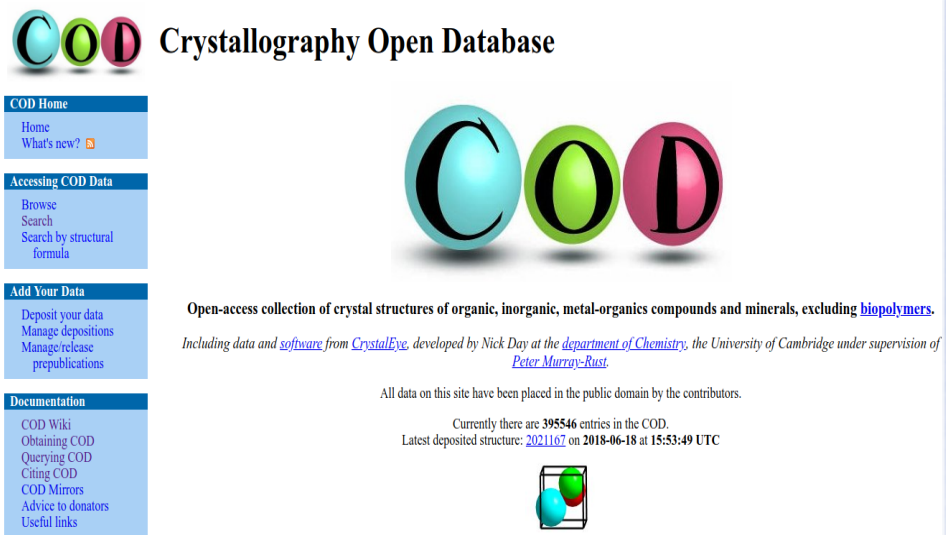
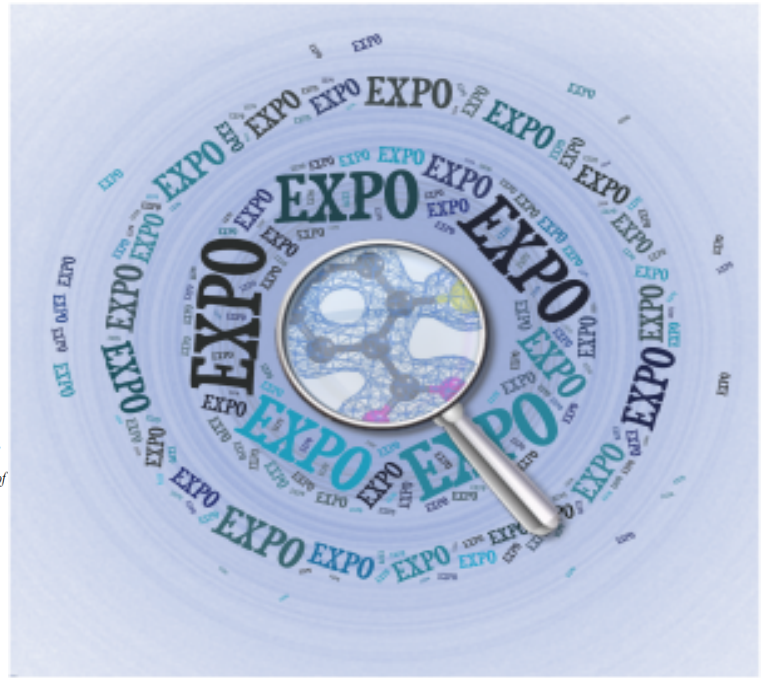
OChemDb is free for academic and non-profit research institutions.

Data source

Crystallography Open Database (COD) includes entries in CIF format. Currently there are more than 412558 entries in the COD. Their number is continually growing.
We generated data (distances, angles, torsions,...) from COD CIF files by using new ad-hoc functions written in EXPO2014.





Implementation

The interactive web interface has been designed with a variety of query options and has made the search efficient by incorporating auto-complete dropdown boxes and graphical tools to draw molecule.

- jQuery, Bootstrap
- Php,Mysql
- OpenBabel, CDK, JSME, JSMOL

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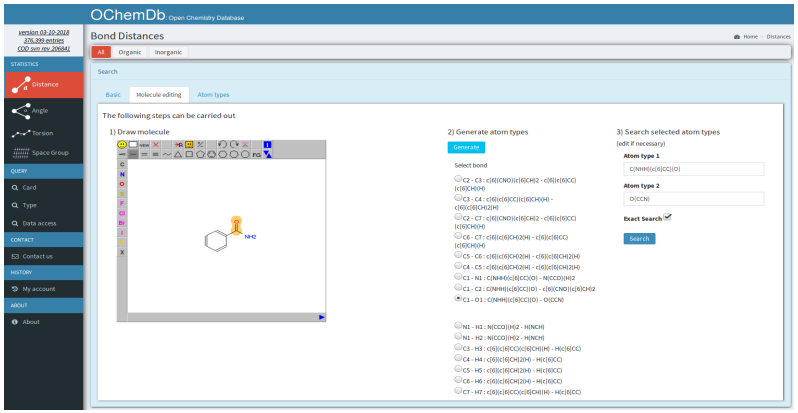
In the first version of OChemDb we have

- 54 millions of bond angle values
- 26 millions of bond distance values
- 5 millions of bond torsion values
- 1 million of atom types

The proposed database will be updated at regular intervals.

OChemDb: Use case



Search for atom type

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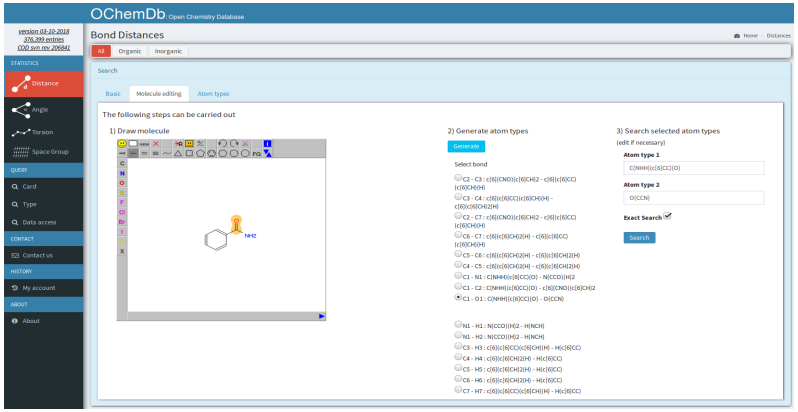
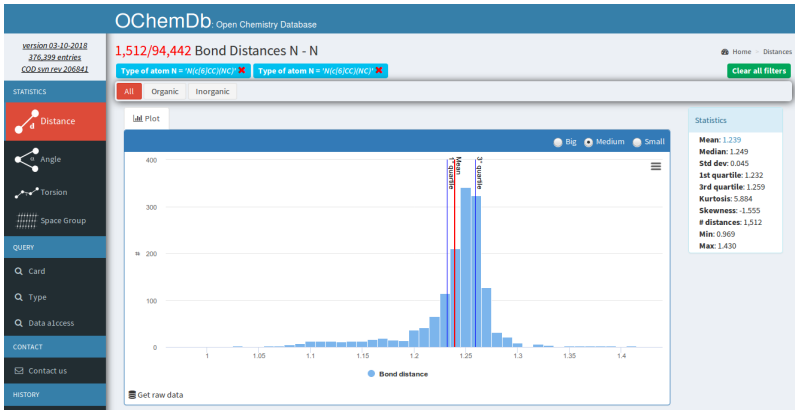
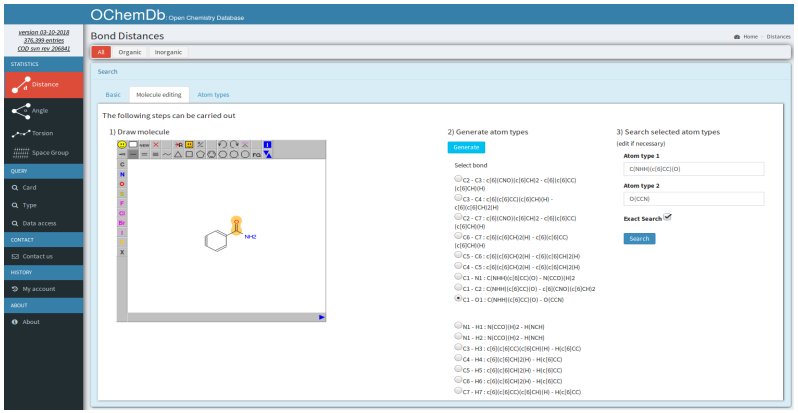


Search for atom type



N-N distribution

OChemDb: Use case



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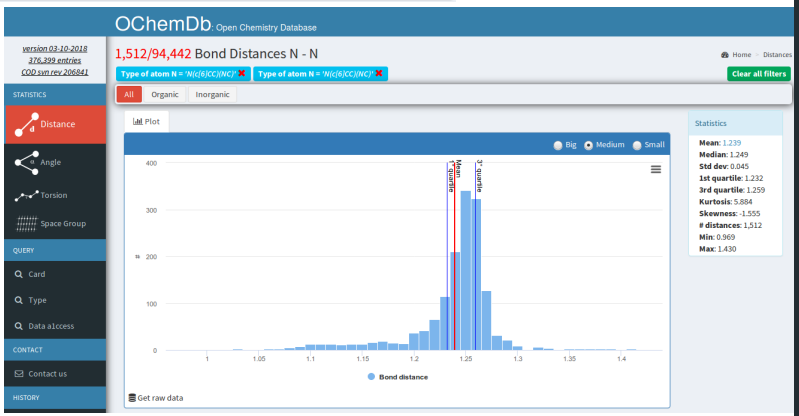

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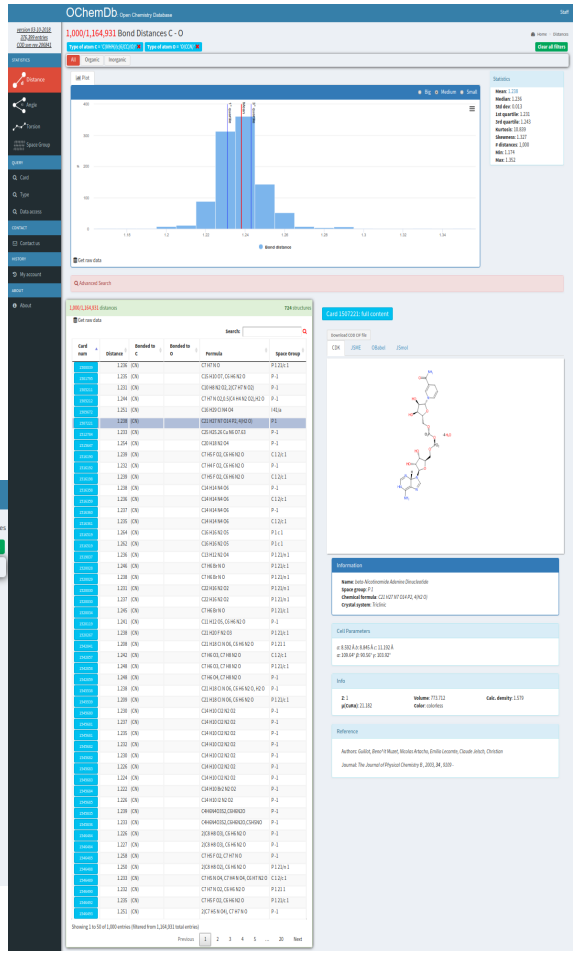

Full results list

How to access to our software

- Connect to *http://www.ba.ic.cnr.it/softwareic*

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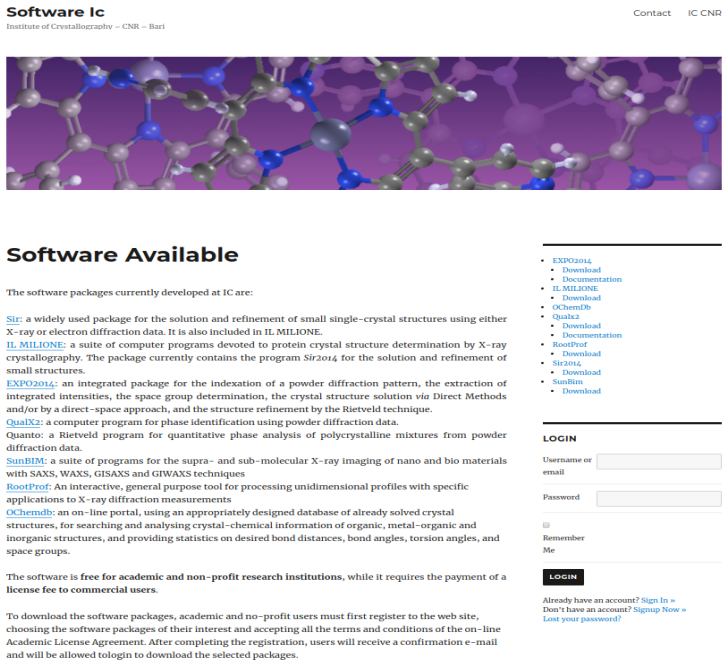
After your registration, you will be allowed to use our software at .*http://www.ba.ic.cnr.it/ochemdb*



Software Ic
Institute of Crystallography – CNR – Bari

Contact IC CNR

Software Available

The software packages currently developed at IC are:

- Sir: a widely used package for the solution and refinement of small single-crystal structures using either X-ray or electron diffraction data. It is also included in IL MILIONE.
- IL MILIONE: a suite of computer programs devoted to protein crystal structure determination by X-ray crystallography. The package currently contains the program *Sir2014* for the solution and refinement of small structures.
- EXPO2014: an integrated package for the indexation of a powder diffraction pattern, the extraction of integrated intensities, the space group determination, the crystal structure solution *via* Direct Methods and/or by a direct-space approach, and the structure refinement by the Rietveld technique.
- QualX2: a computer program for phase identification using powder diffraction data.
- Quanto: a Rietveld program for quantitative phase analysis of polycrystalline mixtures from powder diffraction data.
- SunBIM: a suite of programs for the supra- and sub-molecular X-ray imaging of nano and bio materials with SAXS, WAXS, GISAXS and GIWAXS techniques
- RootProf: An interactive, general purpose tool for processing unidimensional profiles with specific applications to X-ray diffraction measurements
- OChemdb: an on-line portal, using an appropriately designed database of already solved crystal structures, for searching and analysing crystal-chemical information of organic, metal-organic and inorganic structures, and providing statistics on desired bond distances, bond angles, torsion angles, and space groups.

The software is **free for academic and non-profit research institutions**, while it requires the payment of a **license fee to commercial users**.

To download the software packages, academic and no-profit users must first register to the web site, choosing the software packages of their interest and accepting all the terms and conditions of the on-line Academic License Agreement. After completing the registration, users will receive a confirmation e-mail and will be allowed tologin to download the selected packages.

- EXPO2014
  - Download
  - Documentation
- IL MILIONE
  - Download
- OChemDb
- QualX2
  - Download
  - Documentation
- RootProf
  - Download
- Sir2014
  - Download
- SunBim
  - Download

LOGIN

Username or email

Password

Remember Me

LOGIN

Already have an account? Sign In »
Don't have an account? Signup Now »
Lost your password?

Distance

A chemical bond distance between two elements can be sought in the database by selecting and evaluating all the crystal structures that contain it.

The search can be optionally limited to organic or inorganic structures.

Angle

The function of the OChemDb ‘Angle’ main page is to search for bond angles.
A table makes available all the bond angles identified and stored in the database (the current number is 29 770), each one specified by the three bonded atomic species which form it.

The bond-angle search is organized in away similar to the bond-distance search.
The basic survey requires that the triad of bonded atoms is specified and/or their first neighbours and/or their numbers of oxidation and/or the minimum- and maximum-angle values.

The result of the search is a list which contains all the values of the required bond angle present in the database and, for each angle value(A), the number of the corresponding database card (NA), the first-order neighbours bonded to the three atoms involved in the angle (B), the chemical formula (F) and the space group

Torsion

The OChemDb ‘Torsion’ main page can be used for investigating free torsion angles contained in the database.
A table containing all the torsions in the database (the current number is 636) is shown and the graphic and computational tools supporting the ’Angle’ page are valid here too.
The search options and the output of results are organized similarly to the case of bond distances and angles.

In the torsion distribution, the mean value is evaluated byusing the von Mises function (von Mises, 1918), suitable to describe circular variables.
Since the sign of torsion is relevant only for a small percentage of structures, we plot the absolute values to give a more interpretable representation (particularly when the multi-modal case occurs)

Space group

The OChemDb ‘Space Group’ main page is practical for searching space groups.
The frequency in the OChemDb database of each of the 230 space groups is plotted and rankedin a table.
The number of database crystal structures corre-sponding to each of the seven crystal systems (trigonal hexagonal and trigonal rhombohedral are separated) is also given
It is possible to execute a search under the restraining condition of organic or inorganic compounds. Moreover, an additional filter can be applied to select only the chiral spacegroups.

Card

The function of the OChemDb Card main page is to search for a card in the database by supplying its identifying seven-digit number.

When the card is found, its content is shown: graphical visualization of both the crystal structure by JSmol and the structural formula by JSME, general information depending on the corresponding COD CIF content, and all bond distances, bond angles and torsions in the crystal structure.

Statistics on bond distances, angles and torsions can be graphically acquired by searching ina general way or specified by the current atom types

Type

This tool is operative for two actions:

(i) editing and searching for a specified atom type and

(ii) drawing a molecular model by JSME, generating the atom type for each atom in the model and searching for one of the types.

The exact atom type is sought in the database.

Other pages

Data access

The user can select this option to retrieve information on bulk data generated by OChemDb.
The RESTful architectural style has been adopted for implementing data access.
In the current version, only a subset of the overall database information can be queried

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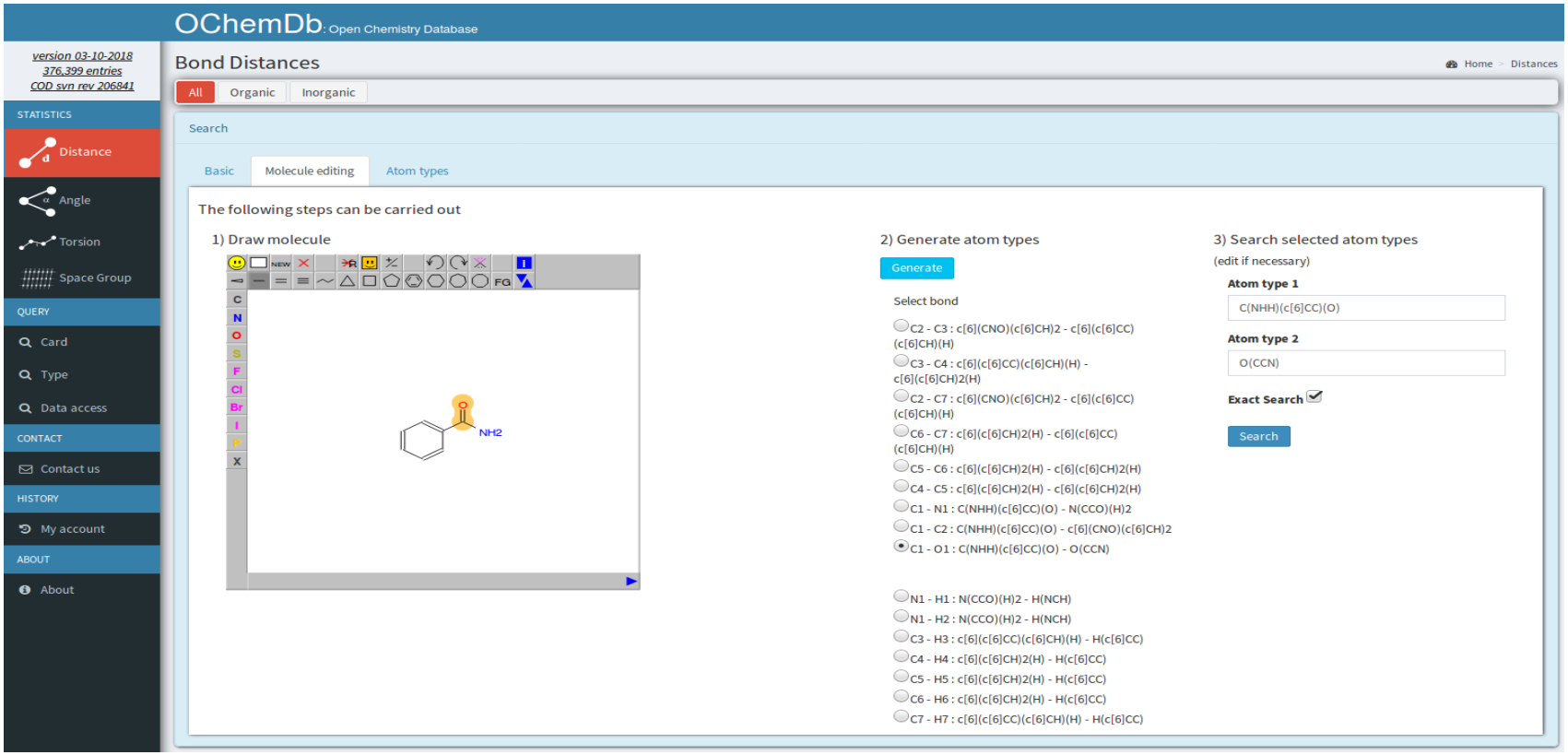
My account

The last 30 pages visited by each registered OChemDb user are stored and made available in a personal account

Example 1: benzamide derivatives



?page = stat_distances&el1 = C&el2 = O&intorno1level2 = C(NHH)(c[6]CC)(O)&intorno2level2 = O(CCN)

Example 2: K2SO4 (potassium sulphate)

We used the ‘Basic’ search by choosing K (potassium) as Atom 1 and O (oxygen) as Atom 2 and, allowing a detailed searching, we specified the first neighbours of K (O) and O (S).

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The first ranked database card number 1000049 corresponds to the potassium sulphate structure with K-O bond different distances in the unit cell

Final remarks

- OChemDb is free for academic use and is available at http://www.ba.ic.cnr.it/ochemdb/ after registration.
- OChemDb, easy to use, requires only a web browser and an internet connection. Every device (mobile or desktop) and every operating system is able to use OChemDb by accessing to its web page.
- The system is in progress and the authors would like to encourage interested Users to join their effort and to provide suggestions.

References

Latest pubblished articles

- *EXPO2013: a kit of tools for phasing crystal structures from powder data*
  A Altomare, C Cuocci, C Giacovazzo, A Moliterni, R Rizzi, N Corriero, A Falcicchio
  Journal of Applied Crystallography **46** (4), 1231 – 1235
- *QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD*
  A Altomare, N Corriero, C Cuocci, A Falcicchio, A Moliterni, R Rizzi
  Journal of Applied Crystallography **48** (2), 598 – 603
- *OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information*
  A Altomare, N Corriero, C Cuocci, A Falcicchio, A Moliterni, R Rizzi
  Journal of Applied Crystallography **51** (4) 1229 – 1236

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Thank you for your attention