CRYSTALLOGRAPHY OPEN DATABASE) and PCOD (PREDI

COD Advisory Board :

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INTRODUCTION

The COD was created in March 2003 and was built on the PDB model of open access on the Internet. It is intended that this database [1] consists of any small or medium crystal structure (inorganic, organic, organometallic). Currently (2008) the total entry number is >70000, including ~10000 entries from the American Mineralogist Crystal Structure Database (AMCSD) [2], all the IUCr data and CIF files donations from a few laboratories in Europe or from individuals. The distribution is made through an Apache/MYSQL/PHP system that takes queries on chemistry, ranges of cell parameters, volumes, etc, as well as combinations of fields, and can download or upload CIF files.

WHO NEEDS COD ?

Petition text for Open Data in Crystallography:

« It is requested that CSD, ICSD, CRYSTMET and ICDD provide a light version of their content (crystal data or powder patterns) at no cost on the Web. A light version consists of the complete database that is fully searchable on the Web by crystal parameters and references and returns the CIFs. It would not consist of the other value-added possibilities produced by these companies, which would stay inside of the toll versions - unless, of course, they want to give more... The principle defended here is that the atomic positions in natural or synthetic crystal samples of our Universe are not copyrightable. »

OPEN DATA

and

Crystallography Databases

Open access on the Web :

PDB (proteins)
NDB (nucleic acids)
AMCSD (minerals)

Toll databases :

CSD (organic, organometallic)
ICSD (inorganic, minerals)
CRYSTMET (metals, intermetallics)
ICDD (powder patterns)

SEARCH the COD

The COD wishes to offer minimal and simple search possibilities, allowing you :

to verify if the structure you intend to solve is not already solved,

to find models or fragments for solving your current problem,

to make a correct job if an editor asks you to review a manuscript.

PETITION RESULTS

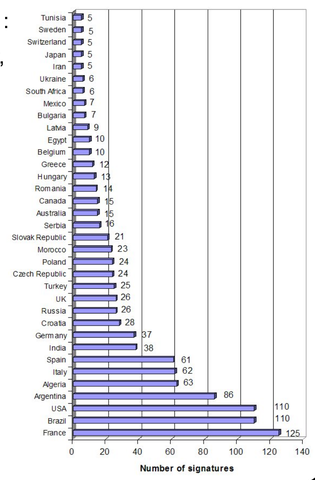
Between May and June 2005, included :

1150 YES signatures for the above text, 4 NO, from 78 countries

Including the signature of one Nobel Laureate (Richard J. Roberts, supporting PubChem as well)

35 countries with more than 5 signatures, representing 1054 signatures are listed on the graph :

For understanding their motivations, read the texts sent by the signers at: http://www.crystallography.net/petition/ You can continue to sign (but not in August due to a scheduled university shutdown).



POSITION of ASSOCIATIONS

Letters from the COD to :

IUCr (International Union of Crystallography), ACS (American Chemical Society), RSC (Royal Society of Chemistry)

asking them for the permission to download systematically the CIF files available at their Web sites,

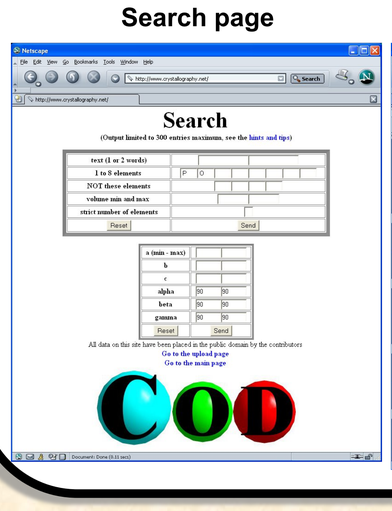
have not obtained positive answer yet.

Do letters from petitioners will be more convincing ?

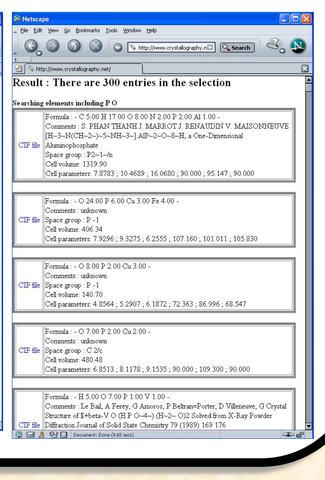
Karimat El-Sayed, Egypt:
"Egypt is a developing country and we cannot have the regular crystallographic databases which we really need in our work, accordingly, if the crystallographic community allows us to have it on line, it will be a big achievement for the third world countries."

SEARCH OPTIONS

Search page



Results



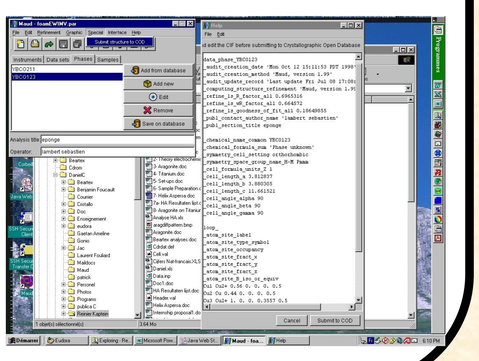
DONATE your CIFs

The positions of atoms in samples of our universe (natural of synthetic) are NOT COPYRIGHTABLE.

It is up to you to send your CIFs to the COD, if you consider that the access to the Knowledge has to be open for academic research.

A crystallography program like MAUD can send directly CIFs to the COD :

Why not to modify your own computer program as well (SHELX, SIR, Rietveld, etc) in order to send automatically the final CIF to the COD through the Internet ?

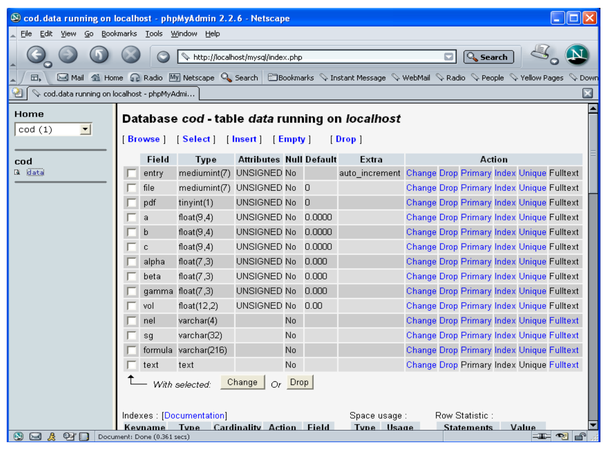


GET the COD TOOLS

EasyPHP (Apache server, MySQL, PHP scripts)

You can download the complete database and make it run on your PC.

You can reuse the complete system and create your lab CIF repository.

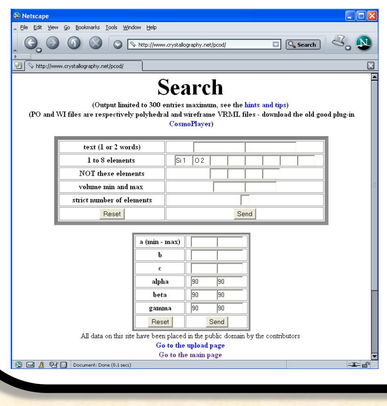


PCOD

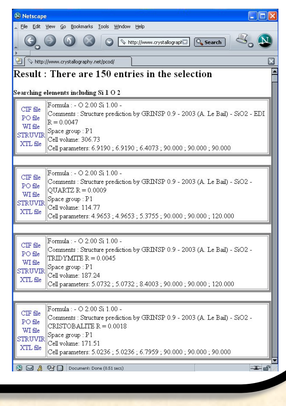
The PCOD, created in December 2003, is a COD subset of crystal structures predicted by the GRINSP computer program [3] . It is growing fast and already contains > 110000 CIF files corresponding to M_2X_3, MX_2, M_2X_5, MX_3 or $M_aM'_bX_c$ formulations (X = O, F; M/M' = B, Na, Si, Al, P, Ca, V, Fe, Re, Zr, etc), including hypothetical zeolites and other binary compounds with N-connected 3D frameworks of M atoms (N = 3, 4, 5, 6) as well as ternary compounds with mixed M/M' frameworks. The PCOD is open for search, download and upload of predicted crystal structures (coming from any prediction computer program, inorganic or small and medium organic molecules).

SEARCHING PCOD

Search page

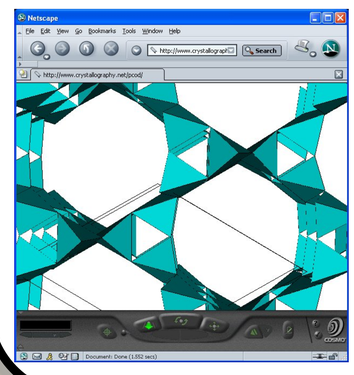


Results

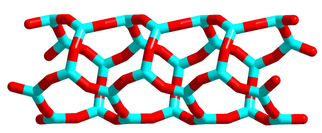


VIRTUAL MODELS in PCOD

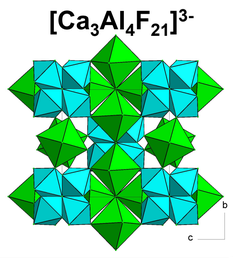
Zeolite



B_2O_3 nanotubes



$[Ca_3Al_4F_{21}]^{3-}$



DONATORS/SPONSORS

Laboratories :

CRISMAT

IPMC institut de physique de la matière condensée

Laboratoire des Oxydes et Fluorures

Thanks to them and to individuals sending CIFs !

CONCLUSION

Continue to sign the petition
(IUCr asked to the COD to obtain letters from people interested)
http://www.crystallography.net/petition/

Waiting for an improbable positive answer from CSD, ICSD, CRYSTMET, ICDD, continue to send your CIFs to the COD (and PCOD)
http://www.crystallography.net/

THANK YOU !

REFERENCES

[1] http://www.crystallography.net/
[2] http://www.geo.arizona.edu/AMS/amcsd.php
[3] http://www.cristal.org/grinsp/

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