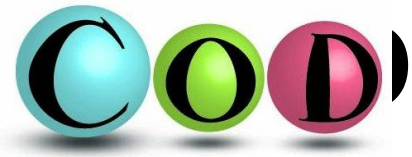
News in Open Databases

COD, PCOD, TCOD, MPOD, FPSM …

D. Chateigner, S. Grazulis, J. Butkus, A. Merkys, A. Daškevič, O. Pérez, G. Pepponi, L. Lutterotti, M. Quirós Olozábal, A. Le Bail, R. Downs, P. Moeck, A.F.T. Yokochi

Association Française de Cristallographie 2013, Bordeaux



- Introduction

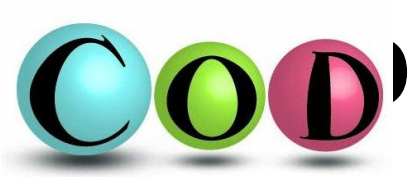
Data uploads at increasing rates. Automated software tools developed to provide consistent, uniform and accurate information:

> **155000** cif files (1/12/2011)

> **235000** cif files (1/06/2013)

- automated structure deposition tools;
- collaboration platform for structure validation and curation;
- improved data quality – uniformity, integrity, and trustworthiness;
- scientific data freely accessible to anyone
- some automated publishers harvesting
- incorporated in 5 industrial major softwares

Deposit your data to COD before publication!



http://www.crystallography.net/

Crystallography Open Database
Validation and Deposition Interface

Select CIF file for check:
/home/saulius/ALL.CIF Browse...

Validate

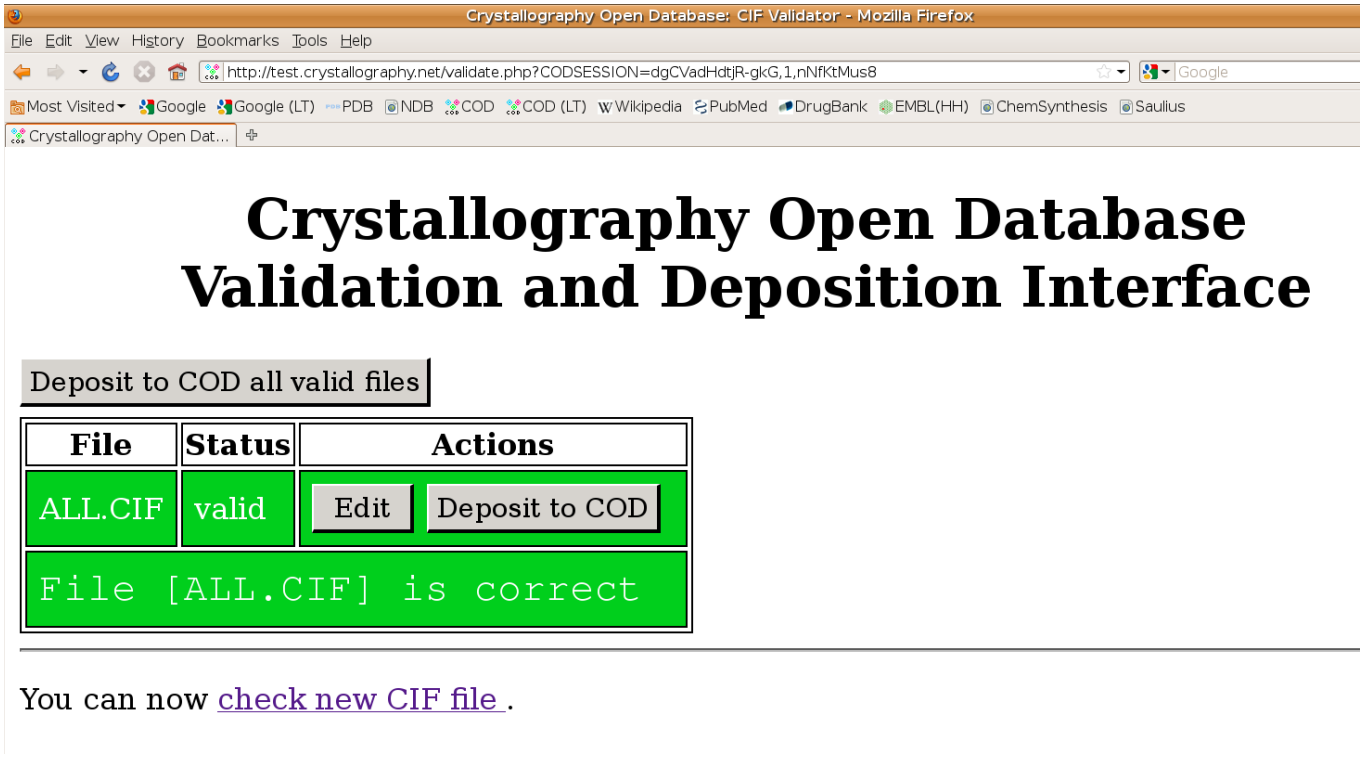
About this Validation Interface

This interface allows you to upload, validate and edit CIF files before submitting them for deposition.

Steps

The process of files deposition, after you have uploaded your data is prettty simple.
First step, after files have been uploaded, is validation. Our scripts performs some validation. Results are displayed to you next to your files.

COD - Automated data deposition



Predicted COD

2011 state: 898.707 SiO_2 entries were added from *ZEFSAII* zeolite predictions and the contributions from *GRINSP* increased to 163.520 (silicates, phosphates, sulfates of Al, Ti, V, Ga, Nb, Zr, or zeolites, fluorides, etc). The PCOD is the first database to attain and offer **more than one million of CIF entries**.

Software : a new *GRINSP* version is now available [3] for parallel computing (for instance using fully the 8 processors of an INTEL core i7).

Other data from other prediction computer programs (*CASTEP*, *CERIUS2*, *CRYSTAL*, *G42*, *GULP*, *USPEX*…) are expected, just send them, please.

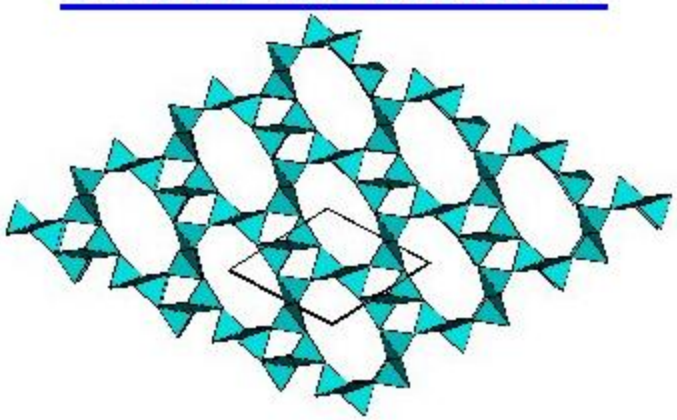
www.crystallography.net/pcod

Predicted Crystallography Open Database

Upload data

or

Search the database



Updated November 2009 : 1.062.771 entries in the PCOD

The largest collection of CIFs in the world

(see the "What is New" page)

Content :

PCOD contains (see the complete list) inorganic compounds (silicates, phosphates, sulfates of Al, Ti, V, Ga, Nb, Zr, zeolites, fluorides, etc) predicted - or enumerated - mainly by ZEFSA II (898.707 SiO_2 entries) or by GRINSP (163.520 entries), or by other programs.

MPOD
Material Property Open Database

www.materialproperties.org

- Collects, opens access to published material properties data
- Keeping connection to structural information: COD
- New cif-compliant .MPOD files
- Search tool
- Online view of property tensors
- Publication references

Coded Properties

- elastic stiffness and compliance, internal friction
- refractive indices, dielectric permittivity and stiffness
- electrical resistivity, polarisation, coercive field
- thermoelectric power
- heat capacity
- thermal conductivity, diffusivity and expansion
- piezoelectricity, electrostriction, electromechanical coupling
- piezooptic, photoelastic
- superconducting critical fields, penetration and coherence lengths …
- Magnetic transition temperatures

Original published paper serves as reference

Experimental information is given

One mpod file for one publication and one phase

Material Properties Open Database

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properties
submit
documentation
references

Input search parameters

Phase Name: aluminum
Formula contains:
COD code:
Publication author: Submit

Search results:

Found datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000002	1000002.mpod	9008460	None	aluminum	Al	2
1000003	1000003.mpod	9008460	None	aluminum	Al	3
1000093	1000093.mpod	9008460	None	Aluminum	Al N	53
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	54

Datafile info

code	:	1000069
filename	:	1000069.mpod
cod code	:	1010458
phase generic	:	KDP
phase name	:	Mn-doped potassium dihydrogen phosphate
chemical formula	:	
publication	:	37

Property values

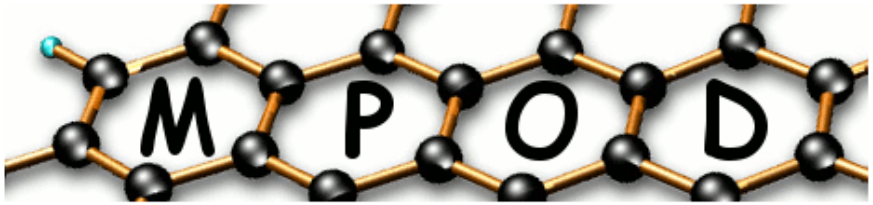
Other experimental conditions/parameters

measurement method [n.a.] : XRD

Properties' values

piezoelectric dij [m.V^-1]

-	-	-	2.3(1)	-	-
-	-	-	-	2.3(1)	-
-	-	-	-	-	47(2)



Material Properties Open Database

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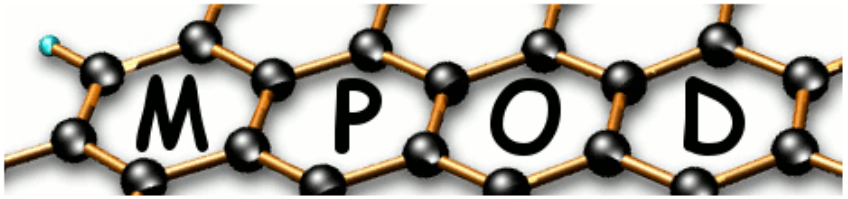
Publication details

title	Anisotropy of the superconducting state parameters and intrinsic pinning in low-level Pr-doped YBa2Cu3O7-d single crystals
authors	Kortyka, A.; Puzniak, R.; Wisniewski, A.; Zehetmayer, M.; Weber, H.W.; Cai, Y.Q.; Yao, X.
journal	Superconductor Science and Technology
year	2010
volume	23
issue	10
first page	None
last page	None
reference	065001
pages number	7

Associated datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000107	1000107.mpod	None	None	YBCO	Y Ba2 Cu3 O6.915	65



Material Properties Open Database

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Property details

tag	_prop_superconducting_critical_field2_Hc2i
name	prop superconducting critical field2 Hc2i
description	_superconducting_critical_field2_Hc2i
tensor dimensions	3
units	T
units detail	tesla

Associated datafiles

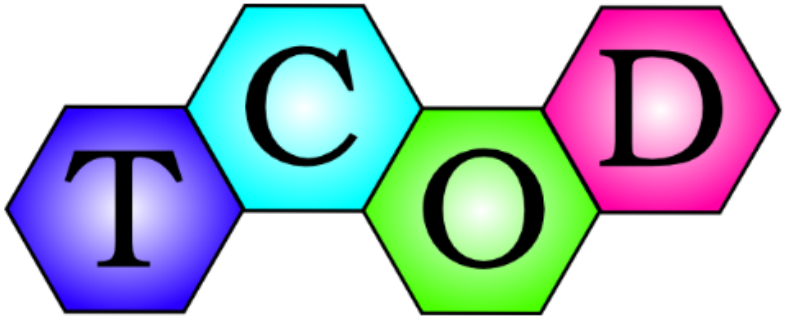
code	filename	cod code	phase generic	phase name	chemical formula	publication
1000097	1000097.mpod	9088326	None	LiFeAs	Li Fe As	56
1000102	1000102.mpod	None	?	iron arsenide	Ba Fe2 As1.3 P0.7	60
1000107	1000107.mpod	None	None	YBCO	Y Ba2 Cu3 O6.915	65
1000108	1000108.mpod	None	None	YBCO	Y Ba2 Cu3 O6.973	65
1000109	1000109.mpod	None	None	Pr-YBCO	Y0.992 Pr0.008 Ba2 Cu3 O6.934	65

TCOD
Theoretical COD

www.crystallography.net/tcod

- Extending COD to numerically refined structures
- DFT, MD, first-principles … optimized
- launched May 2013

Theoretical Crystallography Open Database



Open-access collection of theoretically calculated or refined crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers

All data on this site have been placed in the public domain by the contributors.

Currently there are **96** entries in the TCOD.
Latest deposited structure: 20000096 on **2013-05-09** at **11:48:25 UTC**

CIFs Donators

COD Home

Home
What's new?

Accessing COD Data

Browse
Search

Add Your Data

Deposit your data
Manage depositions
Manage/release prepublications

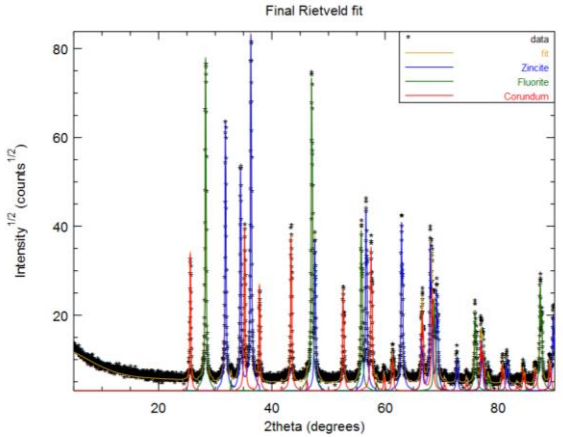
Documentation

COD Wiki
Obtaining COD
Citing COD
COD Mirrors
Advices to donators

FPSM
Full-Profile Search-Match

cod.iutcaen.unicaen.fr

- Identify and quantify phases from powder diffraction patterns
- x-ray, neutron or electron patterns



Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9004178	Zincite	20.5148	29.1683	1893.8	4.76139e-08
1000043	Fluorite	42.3438	33.7285	2154.45	0.00036731
9007498	Corundum	37.1414	37.1032	1941.94	0.000229095

Final Rietveld analysis, Rw: 0.154707, GofF: 1.90021

Acknowledgments

- Vilnius COD development group: Research Council of Lithuania, contract No. MIP-124/2010
- all CIF donators, listed on our Web page, numerous anonymous volunteers who help to collect data and keep COD running
- Commercial supporters for donation (hardware and financial support)
- Xmat project “Combination of X-Ray diffraction and X-Ray Fluorescence techniques in material science”, supported by the Provincia Autonoma di Trento and the European Union in the framework of the Marie Curie COFUND program
- Conseil Régional de Basse-Normandie and FEDER: Chaire d’Excellence L. Lutterotti

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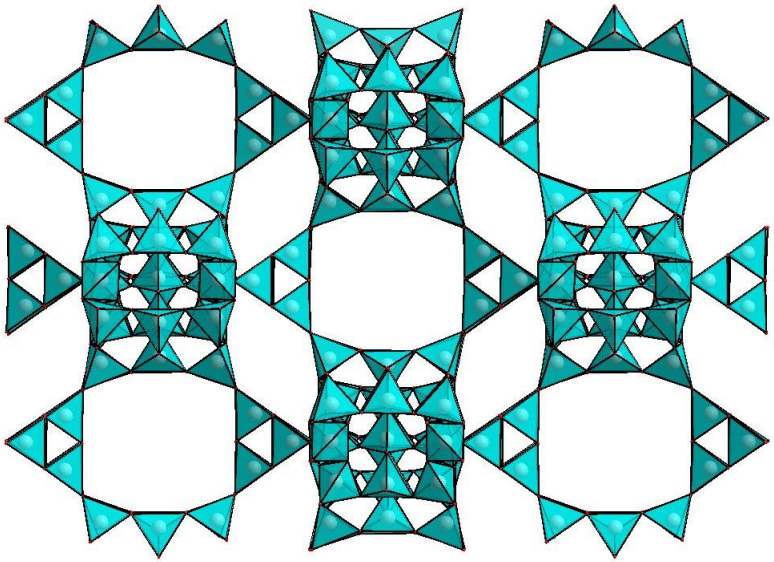
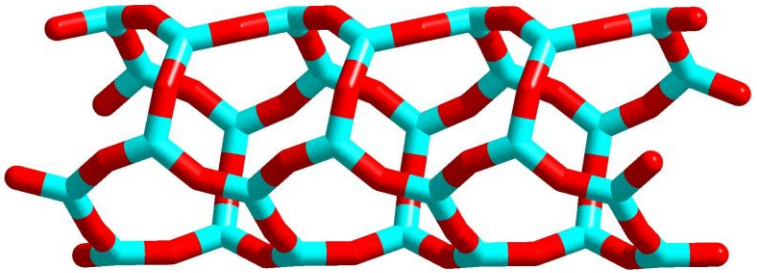
pij 12 -0.32(5)
pij 13 -0.32(5)
pij 21 -0.32(5)
pij 22 0.12(5)
pij 23 -0.32(5)
pij 31 -0.32(5)
pij 32 -0.32(5)
pij 33 0.12(5)
```

VIRTUAL MODELS in PCOD

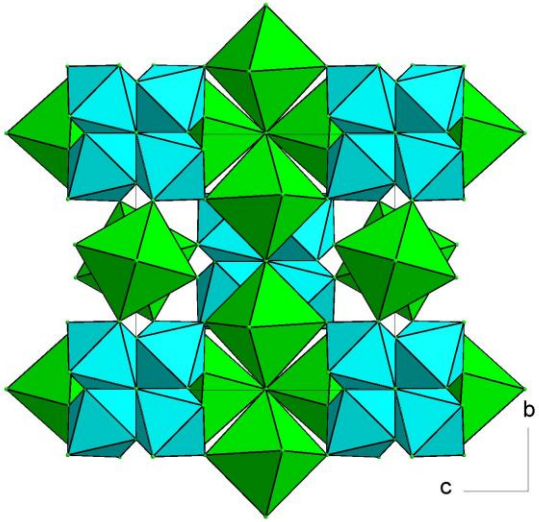
Zeolites



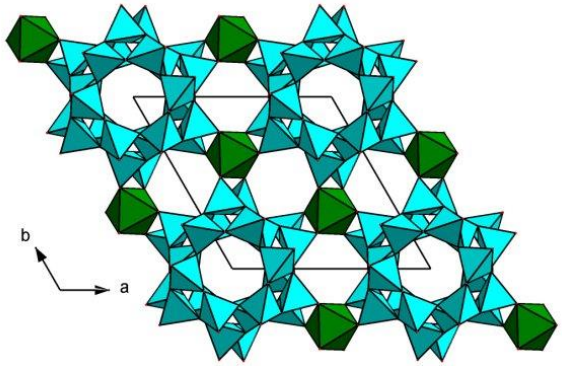
B_2O_3 nanotubes



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

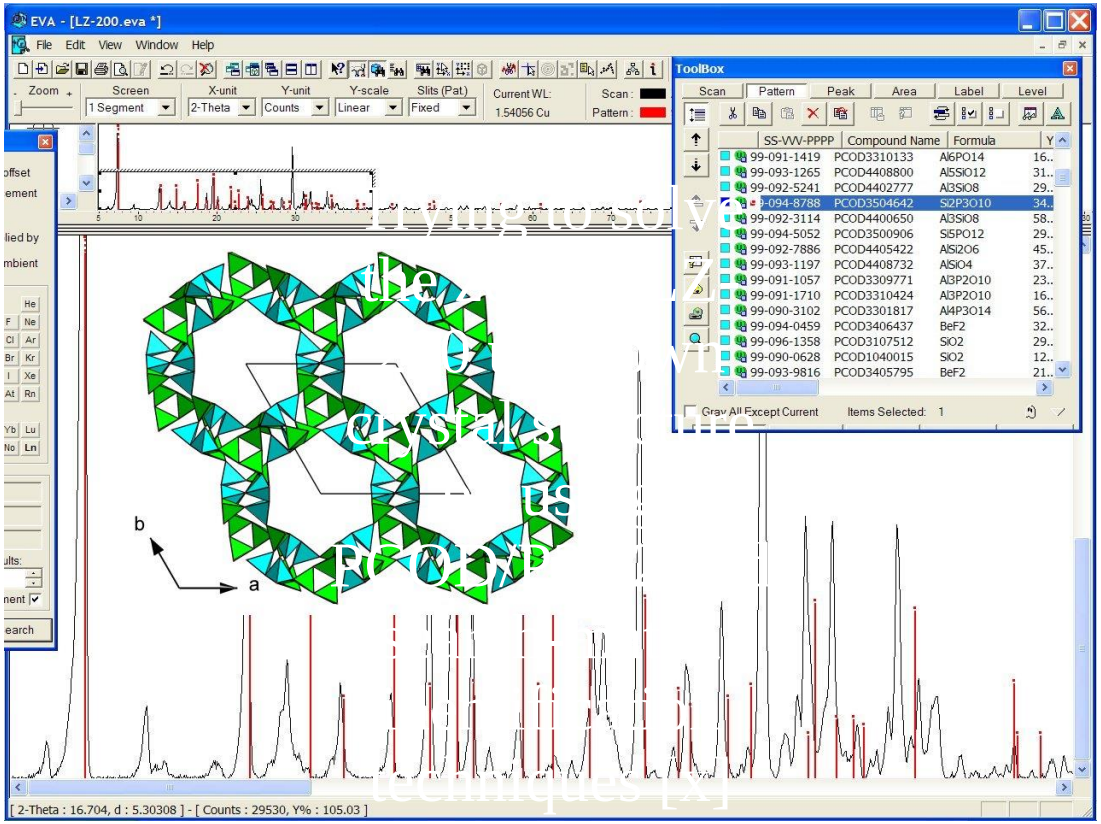


Titanosilicates



PCOD Powder P2D2

All powder patterns (> 1 million) were calculated and gathered in the P2D2 (Predicted Powder Diffraction Database [4]), they can be used for search-match purposes with *EVA* (Bruker), *Highscore* (Panalytical) and more soon.



Coding

- Uses a Starfile syntax: developed for the Crystallographic Information Files (CIF)
- Structural information in the CORE CIF dictionary
- New dictionary for properties in Dictionary Definition Language DDL1
- Some tricks were adopted to adapt vs Starfile syntax
- Units are univocally define in the dictionary itself
- Experimental conditions (temperature, pressure, …) are inserted
- All non-zero components explicitly written
- Diagonally symmetric components not repeated