Open access crystallographic databases & COD in its 11th year

Peter Moeck[1], Daniel Chateigner[2], Robert T. Downs[3], Saulius Gražulis[4], Armel Le Bail[5], Luca Lutterotti[6], Miguel Quirós[7], & all other members of our International Advisory Board

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Funding: *Research Council of Lithuania, NorthWest Academic Computing Consortium, National Science Foundation, PANalytical, Crystal Impact* ***& our various home institutions***

1. **Motivation:** *the time was right to do this ten years ago, so we did, now we have something quite significant to show for*


nature

www.nature.com/nature Vol 461 | Issue no. 7261 | 10 September 2009

Data's shameful neglect *page 145*

Research cannot flourish if data are not preserved and made accessible. All concerned must act accordingly.

2. **Open access crystallographic databases**

"There is nothing so powerful as an idea whose time has come."

Victor Hugo, 1802 - 1885

3. **Crystallography Open Database in its 11th year**

4. **Efforts by Portland State's Nano-Crystallography Group / future Bicrystallography Open Database**

https://www.dataone.org/

cod.iutcaen.unicaen.fr

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Re: emergency sit... | DataONE

Home | Feeds (J) | Read Mail | Print | Page | Safety

DataONE
Data Observation Network for Earth

Search: DataONE Website | For: crystallography | Go

Conne

"Changing the culture of science from one where publications were viewed as the primary product of the scientific enterprise to one that also equally values data." William Michener (of the DataONE project), in: Nature 461 (2009) 160-163

About | Participate | Resources | Education | Data

Spring 2013 Newsletter

The Spring 2013 issue of DataONENews is now available. Features Include: Report from Bill Michener discussing the recent Whitehouse memo: Increasing Access to the Results of... read more

Tweets

Stephanie Hampton @se_hampton 18 Jun
YAY! MT @carlystrasser: Check out new @DataONEorg 'Coffeehouse'- aggregator for blogs on data mgmt, sharing, preserv. ow.ly/m9Uy2

PressForward @pressfwd 18 Jun
@carlystrasser @dataoneorg @recology_ please get in touch if you'd like to chat! cc: @epistemographer

Patricia Hswe @pmhswe 18 Jun
MT @carlystrasser: Check out new @DataONEorg 'Coffeehouse' - aggregator 4

Compose new Tweet...

Internet

Crystallographic database

From Wikipedia, the free encyclopedia
(Redirected from Crystallographic databases)

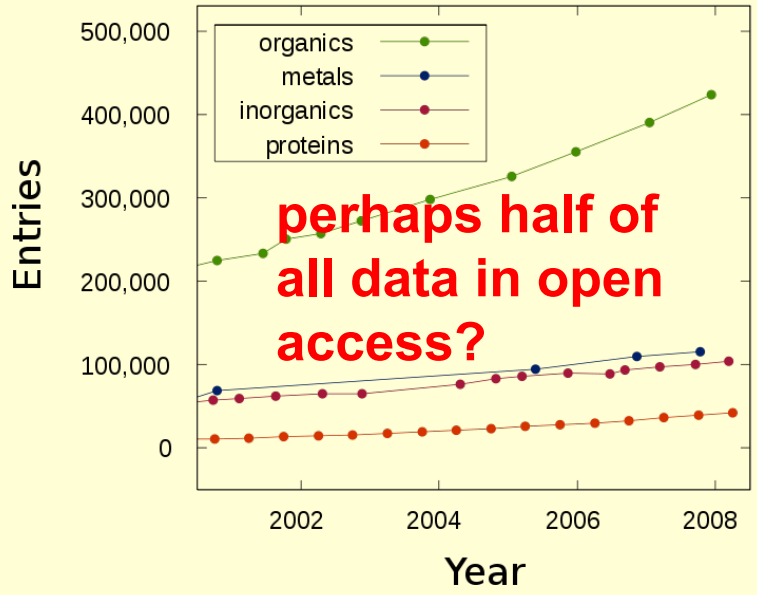
A **crystallographic database** is a database specifically designed to store infor
having, in all three dimensions of space, a regularly repeating arrangement of at
morphology, and directionally dependent physical properties. A crystal structure

Crystal structures of crystalline material are typically determined from X-ray or ne
databases. They are routinely identified by comparing reflection intensities and l
powder-diffraction fingerprinting databases.

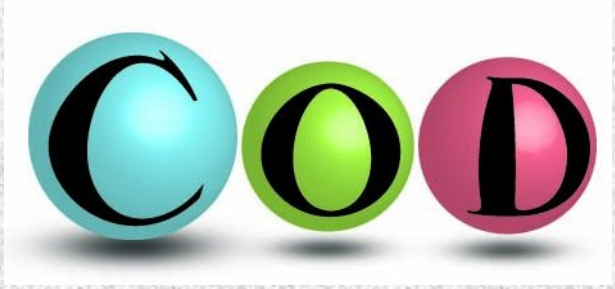
Crystal structures of nanometer sized crystalline samples can be determined via
diffraction data or structure factor amplitude and phase angle information from F
in crystal structure databases specializing in nanocrystals and can be identified b
entries in a lattice-fringe fingerprinting database.

Crystallographic databases can be categorized as crystallographic information f
biological macromolecules. They differ in access and usage rights and offer vary
visualization capabilities. They can be browser based or installed locally. Newer
Crystallographic Information File (CIF) as a universal data exchange format.

Contents [hide]



Crystallography Open Database



http://www.crystallography.net

mirrors worldwide **http://cod.ibt.lt**

http://cod.ensicaen.fr

http://qiserver.ugr.es/cod

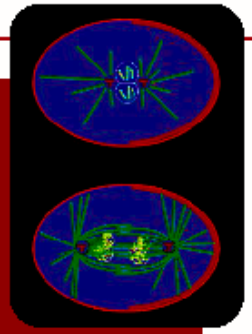
http://nanocrystallography.org

web portal: http://nanocrystallography.net

more than 235,000 entries

NETWATCH

edited by Mitch Leslie



IMAGES

Starring The Cell

Chromosomes caress, tangle, then get wrenched apart as a French torch song plays in "Twisted Sisters," probably the most touching movie ever made about the first division of meiosis. It's also one of the standouts at the Web site of the Bioclips project, sponsored by the French government. The virtual multiplex displays entrants from the last four rounds of the Cinema of the Cell festival. Held annually at the European Life Scientist Organization meeting, the contest lets researchers and students present their educational Web films, which use techniques from traditional animation to stop-motion with Lego blocks. The more than 30 shorts range from "A Day in the Life of a Social Amoeba" to a work about the establishment of cell polarity in nematodes from auteurs at the University of Wisconsin, Madison (above).

www.bioclips.com

RESOURCES

Where Birds Count

The careful observations of birdwatchers are invaluable to scientists studying avian distribution and abundance. eBird, a recently revamped site from Cornell University's Lab of Ornithology and the National Audubon Society, helps researchers access and analyze birders' tallies. One of the lab's collaborations with birdwatchers (*Science*, 3 June, p. 1402), eBird lets visitors submit their sightings to a database that already has entries from 15,000 people. Researchers can then parse the records, plotting counts for a particular area or species. For instance, you can chart the number of ospreys seen in each week of the year and map the fish-eaters' favorite haunts.

www.ebird.org

COMMUNITY SITE

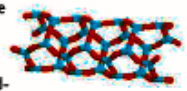
Schizophrenia Symposium

Find out the conclusions of the latest study comparing different antipsychotic drugs, track down a potential collaborator in Italy, or discover what leading schizophrenia researchers have on their minds. You can do all this and more at the Schizophrenia Research Forum, which officially opened this week. Sponsored by the nonprofit National Alliance for Research on Schizophrenia and Depression and the U.S. National Institute of Mental Health, the diverse site is modeled on a meeting place for Alzheimer's researchers (www.alzforum.org). Features include a news section and interviews with scientists such as Robin Murray of the Institute of Psychiatry in London, who helped show that "obstetric events" such as premature birth boost the risk of schizophrenia. Visitors to the Idea Lab can bat around novel notions. Live chats with experts start next month, and a gene database is in the works.

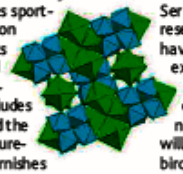
www.schizophreniaforum.org

DATABASE

Free the Crystals!



This site is some crystallographers' answer to open-source software, providing an alternative for chemists and other researchers who can't afford the fees charged by suppliers of crystallographic data. Supervised by an international team of scientists, The Crystallography Open Database houses measurements for some 18,000 molecules, from superconducting materials to antibiotics. Visitors can scan the data, which were contributed by site users, for molecules sporting a specific combination of elements. The results appear as a standard "Crystallographic Information File" that includes atomic coordinates and the source of the measurements. A linked site furnishes predicted structures for more than 1500 compounds, such as boron-containing nanotubes (top image) and fluoroaluminate crystals.



www.crystallography.net

DATABASE

Dinosaur Name Game

Like the ancient beasts themselves, most of the names scientists have coined for dinosaurs over the last 2 centuries are defunct. At the new database TaxonSearch from paleontologist Paul Sereno of the University of Chicago, researchers can uncover which handles have survived and which have gone extinct as experts have refined taxonomies. Unlike other narrower references, the site focuses on taxonomic levels above the genus, and it will cover all archosaurs—the group that comprises dinosaurs and their kin—except for birds and crocodiles. Dig into the listings to find out who first named a group, its official definition, and its chronological range. For example, the name of the clade Ankylosauridae, to which the herbivore *Ankylosaurus* (above) belongs, dates back to 1908. And if a name has died out, you can learn why. Sereno has posted the first batch of 50 records and plans to add about 700 more within the next few weeks.

Send site suggestions to netwatch@aaas.org. Archive: www.sciencemag.org/netwatch

CREDITS (TOP TO BOTTOM): FONG-PHILLIE ANNE GOSS, JOHN WHITE/UNIVERSITY OF WISCONSIN, MADISON; FRANCOIS GOHIER/PHOTO RESEARCHERS INC.; CRYSTALLOGRAPHY OPEN DATABASE

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www.crystallography.net

Crystallography Open Da

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metal-organic compounds and minerals, excluding biopol

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

COD Advisory Board thanks The Research Council of Lithuania for their financial
publication
"Crystallography Open Database (COD): an open-access collection of crystal
platform for world-wide collaboration",
Nucleic Acids Research. (2012) PDF version

We thank Crystal Impact GbR for their financial support of the publicati
"Crystallography Open Database - an open-access collection of crystal str
J. Appl. Crystallogr. (2009) PDF version

Currently there are **235786** entries in the COD.
Latest deposited structure: 7109374 on **2013-05-17** at **12:48:22 UT**

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Hareesh Rajan, Alexandre F.T. Yokochi

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  'y-x,-x,2/3+z'
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  'x-y,-y,2/3-z'
loop
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http://www.crystallography.net/result.php?id=20171%

Results

Result : There are 100 entries in the selection

You can download the COD numbers of the selection as a text file

You can download all files as a single ZIP archive

Searching COD ID like 20171%

COD ID: 2017100	
CIF file HKL data Original IUCr paper	Formula : - C5 H9 N O6 S - Comments : Minkov, Vasily S.; Boldyreva, Elena V. DL-Cysteinium semioxalate Acta Crystallographica Section C 65(5) (2009) o245-o247 Space group :P -1 Cell volume: 443.62 Cell parameters:5.6664; 9.0149; 9.7749; 109.349; 102.282; 100.119;

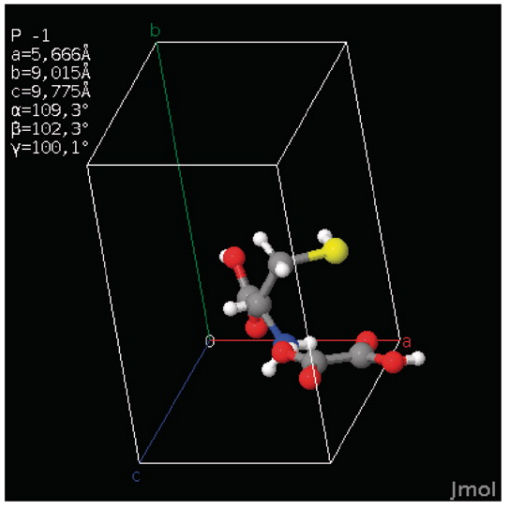
Gražulis S. et al. *Nucl. Acids Res.* 40 (2012) D420-D427, open access

Results | 2017100 - CIF informa...

Information card for 2017100

2017099 << 2017100 >> 2017101

Preview



CIF file

Download 2017100.cif

HKL data file

Download 2017100.hkl

Original IUCr paper

Structure parameters

Common name	DL-cysteinium semioxalate
Chemical name	DL-Cysteinium semioxalate

```
loop_
_refln_index_h
_refln_index_k
_refln_index_l
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_refln_F_squared_meas
_refln_F_squared_sigma
_refln_observed_status
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2 0 0 443.74 483.55 3.27 o
3 0 0 105.70 102.49 1.73 o
4 0 0 109.80 97.14 0.68 o
5 0 0 61.24 59.93 0.88 o
```


Acta Crystallographica Section C

Crystal Structure Communications

Volume 65, Part 5 (May 2009)

organic compounds

html | pdf | cif | 3d view | structure factors | cited in | similar papers

Acta Cryst. (2009). C**65**, o245-o247 [doi:10.1107

DL-Cysteinium semioxalate

V. S. Minkov and E. V. Boldyreva

Abstract: Two chiral counterparts (L- and D-cysteinium are present in the structure of the title compound, C_3H_8 anion ratio. The carboxy group of the cysteinium cation relative to the amino group. The crystal structure is built cysteinium cations are connected to each other not direc semioxalate anions linked to each other *via* O-H...O hydr interesting feature of the crystal structure is the absenc bonds.

Formula: $C_3H_8NO_2S^+ \cdot C_2HO_4^-$

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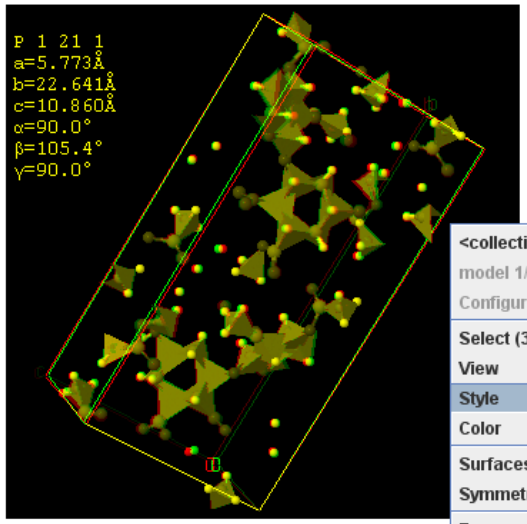
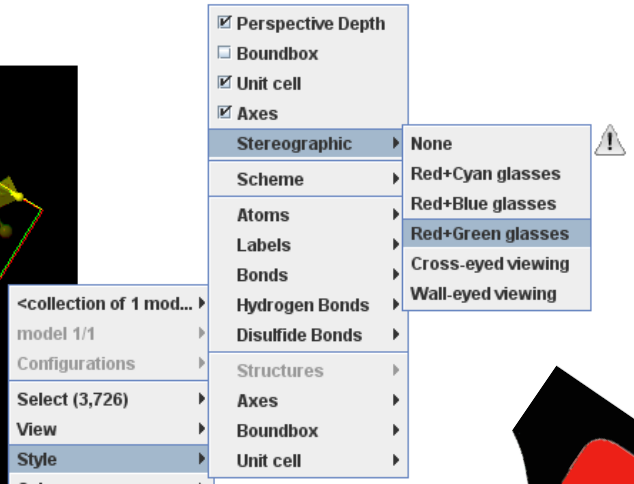
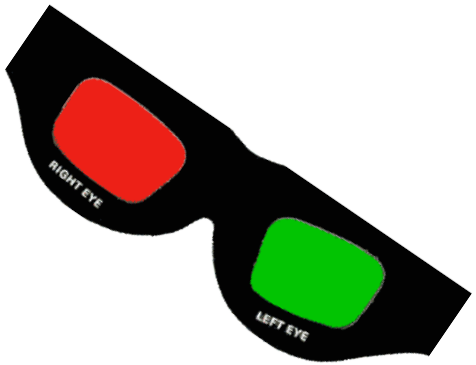
7109374 << **7150000** >> 7150001

Preview







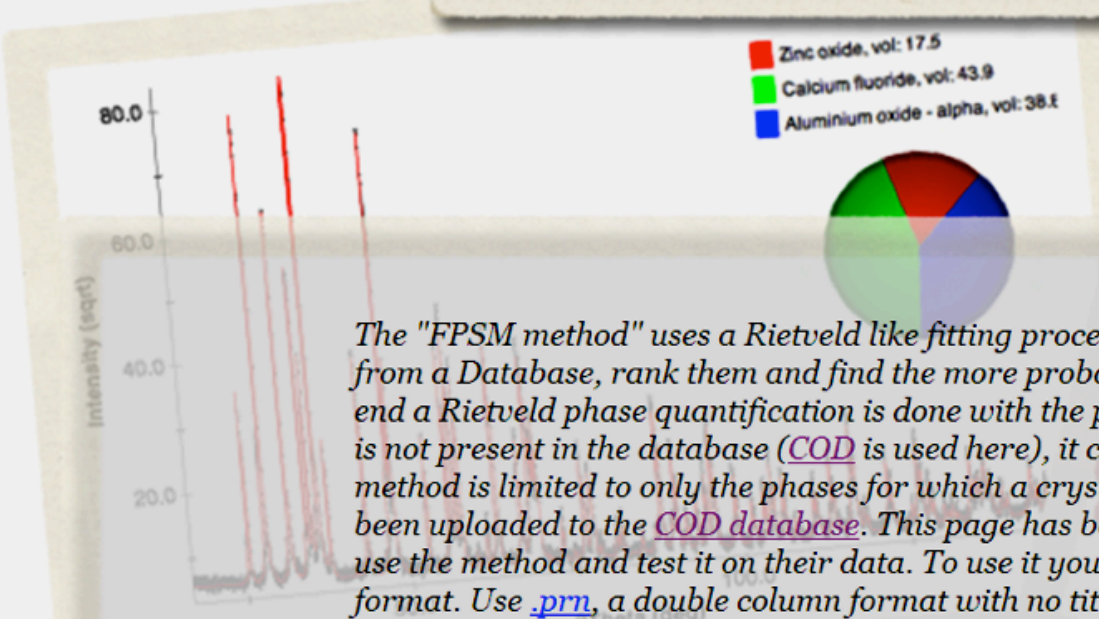
Coordinates 7150000.cif

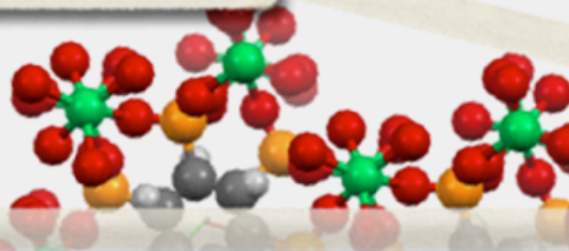
Structure parameters

Formula	31 N O15 -
Calculated formula	31 N O15 -
Title of publication	elated to carba-pyranoses: synthesis of acetylated derivatives of 4-amino-2,4-dideoxy-3-O-(bet carba-pyranose from a D-glucose template.

Full Profile Search Match

by L. Lutterotti using COD





The "FPSM method" uses a Rietveld like fitting procedure to test all possible crystal structures from a Database, rank them and find the more probable in your diffraction pattern. In the end a Rietveld phase quantification is done with the phases identified. Be aware that if a phase is not present in the database (COD is used here), it cannot be found nor quantify; so this method is limited to only the phases for which a crystal structure has been determine and has been uploaded to the COD database. This page has been constructed to permit other people to use the method and test it on their data. To use it you need to upload a datafile in proper format. Use .prn, a double column format with no title line, first column contains the 2theta coordinates (d space for TOF), the second column the intensity (corrected for incident intensity for TOF). You need also to specify some additional instrument characteristics (wavelength, geometry etc.). If the selected instrumental broadening function much the one of your instrument, then a reasonable analysis of crystallite sizes and microstrain is reported.

See paper: L. Lutterotti, H. Pilliere, C. Fontugne, P. Boullay, D. Chateigner (2013), submitted to J. Appl. Cryst.

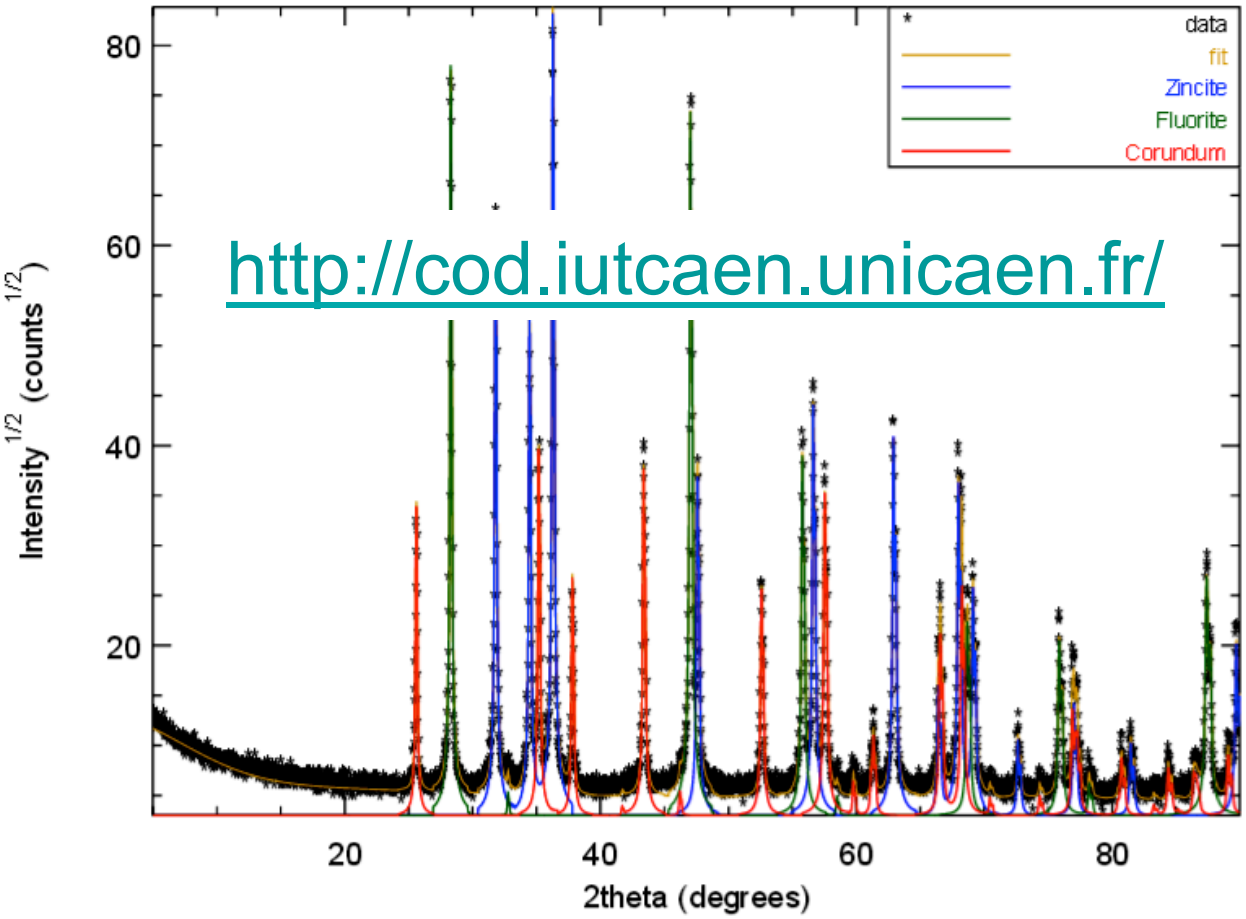
Diffraction pattern and sample composition

Found phases and quantification:

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

Final Rietveld fit



http://cod.iutcaen.unicaen.fr/

34.160	88
34.180	90
34.200	94
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34.240	148
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34.280	219
34.300	313
34.320	449
34.340	580
34.360	858
34.380	1102
34.400	1600
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34.440	2777
34.460	2830
34.480	2766
34.500	2381
34.520	2052
34.540	1697
34.560	1354
34.580	961
34.600	696
34.620	392
34.640	265
34.660	187
34.680	146
34.700	156

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Log in | Upload a file | Validate data | Deposit structures | Finish

Choose deposition type
-- choose one --

Depositor details
Your name:

Your COD password (if you do not have a COD account yet, please type a new password that you remember and we will create an account for you):

Your e-mail address (*it will not be disclosed to 3rd parties*):

Begin deposition

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 pretty simple.
First step, after files have been uploaded, is validation. Our scripts perform some checks to see if all necessary data are present in the submitted file. Results are displayed to you next to your files.
If a file is correct, you can deposit it to COD. After the deposition, COD numbers for the newly deposited structures will be displayed.
If a file is not correct you can edit it file in your browser window and validate it once more.

File formats

Currently we accept two types of files:

- Plain CIF files;
- ZIP archives, which does contain CIF files.

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Theoretical Crystall ×

www.crystallography.net/tcod/

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Open-access collection of theoretically calculated or refi
of organic, inorganic, metal-organic compounds and
biopolymers

All data on this site have been placed in the public domain b

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

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Daniel Chateigner, Xiaolong Chen, Marco Ci
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Hareesh Rajan, Alexandre F.T. Yokochi

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# This file is available in the Crystallography Open Database (COD),
# http://www.crystallography.net/
#
# All data on this site have been placed in the public domain by the
# contributors.
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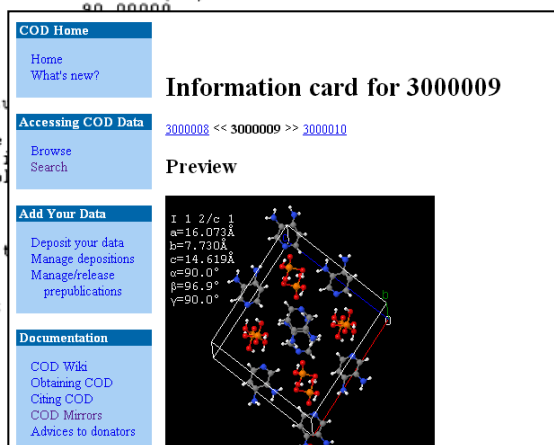
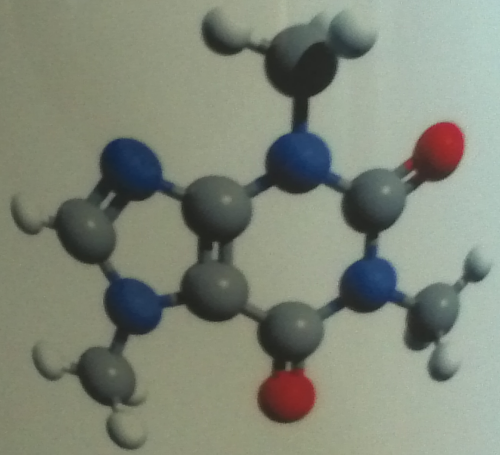


Looking for caffeine?



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And it's FREE!

http://nanocrystallography.net

All good open access crystallography resources, e.g. space group drawings, …

Portland State UNIVERSITY

Interactive Databases

Crystallography Open Database [Mirror, modified search interface and Jmol displays] Search and view

Wiki Crystallography Database Search and view

Educational subset of COD Search and view

Nano-Crystallography Database Search and view

Crystal Morphology Database Search and view

Bicrystallography Open Database

searchable collection of CIFs for all kinds of simulations and visualizations of grain boundaries

to be derived from user inputs and freely modifiable at the atomic level

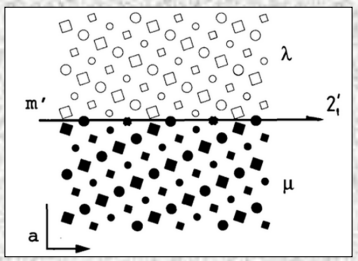
Several crystallography databases are offered for browsing. You can search the databases, downl and display the contained Crystallographic Information Files (CIFs), view 3D models of the encode crystal structures and morphologies.

We also provide the North American mirror of the Crystallography Open Database (COD). This is the

Bicrystallography Open Database

"… disclose generic relations between different interfaces, specify crystallographically equivalent variants of an interface and classify line defects in interfaces. The symmetry of a bicrystal imposes constraints on tensor properties of the bicrystal interface, provides classification of the interfacial vibrational modes, discloses possible interfacial transitions etc."

V. Janovec, Th. Hahn and H. Klapper, Twinning and domain structures, International Tables for Crystallography (2006), Vol. D, ch. 3.2, pp. 377-392.



No textbook, only a few original papers and book chapters

diamond, Σ = 5 (310)/[001] 36.9° tilt boundary, viewed down [001], **black white (two color) layer group *p2$_1$'am'***

R. C. Pond and J. P. Hirth, in Ehrenreich, H., *Solid State Physics: Advances in Research and Applications*, Volume 47, 1994, pp. 287-365

CeO_2 Σ = 5 (310)/[001] 36.9° tilt boundary, dichromatic complex has 3 atoms per lattice point of dichromatic pattern I4/mm' m'

two color layer group ***c2'mc'*** - *a genuine back-white group, polar physical properties can exist*

p2'mm' - *polar physical properties cannot exist*

p2$_1$'mn' - *polar physical properties can exist*

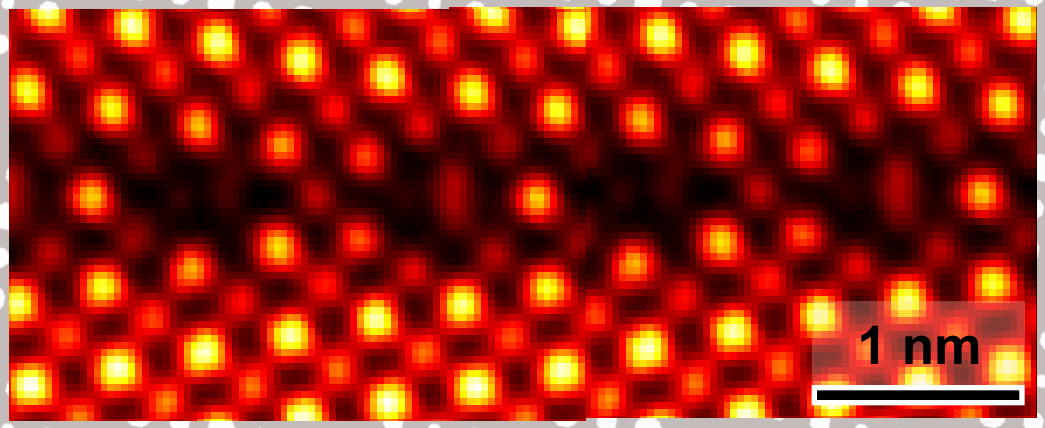
two color layer group ***c2'mm'*** – *a gray group, polar physical properties cannot exist*

CeO_2 Σ = 5 (120)/[001] 53.1° tilt boundary viewed down [001]

another "idea whose time has come"

primitive cubic lattice, 5 atoms per lattice point of dichromatic pattern P4/mm' m', zero rigid body shift and expansion for simplicity

Aberration-corrected translation-symmetry averaged STEM Z-contrast, H. Yang et al., Phil. Mag. 2012, 1-11, iFirst Article.



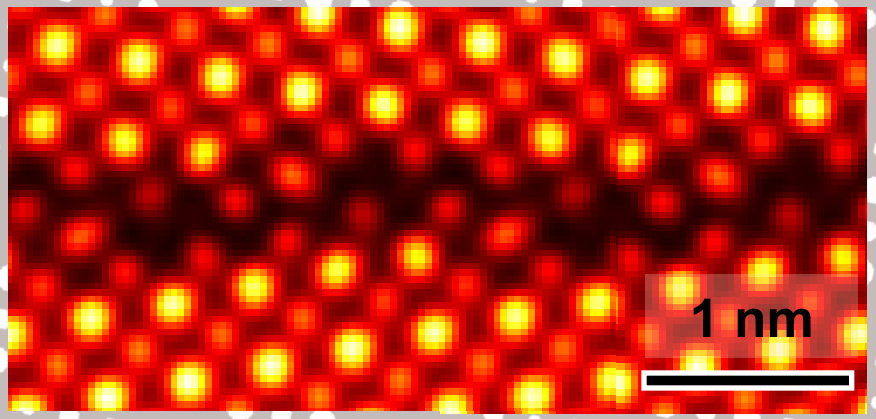
both mixed O and Ti as well as Sr columns are located at interface

Frieze Group *11m*

$SrTiO_3$ Σ = 13a, (510)/[001], 22.6° tilt boundary in [001] projection, sectioned at ½ [510], large disks Sr columns, medium disks pure O columns, small disks mixed O and Ti columns

primitive cubic lattice, 5 atoms per lattice point of dichromatic pattern P4/mm’m’, zero rigid body shift and expansion for simplicity

Aberration-corrected translation-symmetry averaged STEM Z-contrast, H. Yang et al., Phil. Mag. 2012, 1-11, iFirst Article.



only pure O columns are located at interface

Frieze Group *p11g*

$SrTiO_3$ Σ = 13a, (510)/[001], 22.6° tilt boundary in [001] projection, sectioned at ¼ [510], large disks Sr columns, medium disks pure O columns, small disks mixed O and Ti columns

Summary

Open access crystallographic databases, combined some 350,000 – 400,000 entries

COD in it's 11th year, more than 235,000 entries

http://journals.iucr.org/j/issues/2009/04/00/kk5039/kk5039.pdf 38 quotes in web of science, June 11, 2013

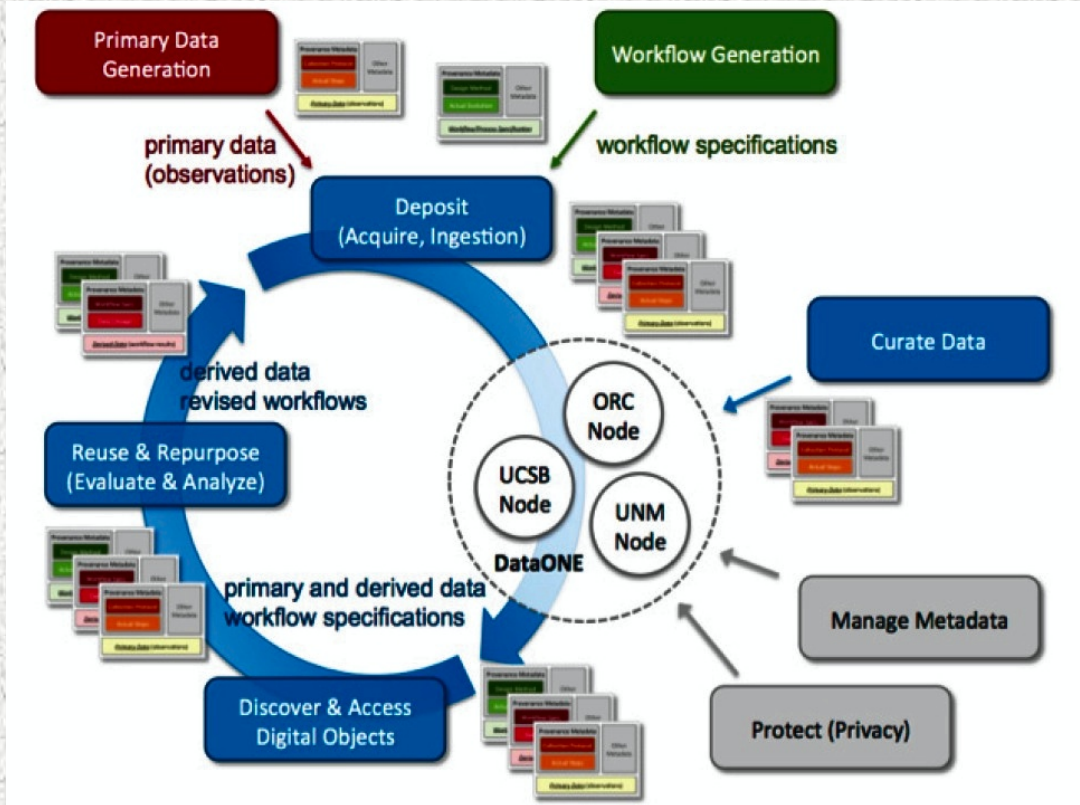
http://nar.oxfordjournals.org/content/40/D1/D420.full.pdf+html 2 quotes in web of science, 2683 downloads from the Nucleic Acids Research website, June 11, 2013

TCOD in it's first few months, 96 entries

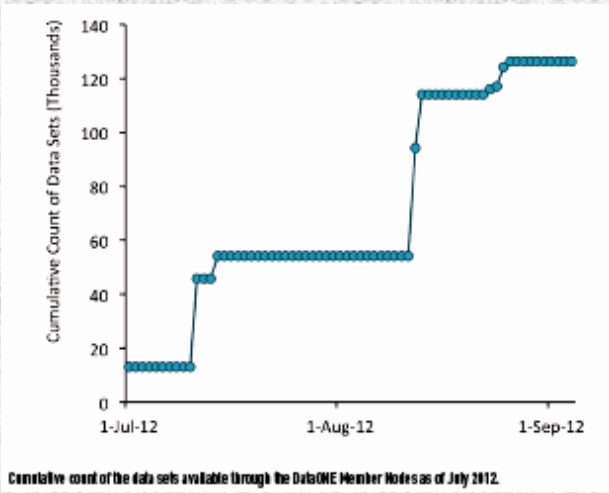
Open access crystallography resource portal, nanocrystallography.net

Plans for Bicrystallography Open Database

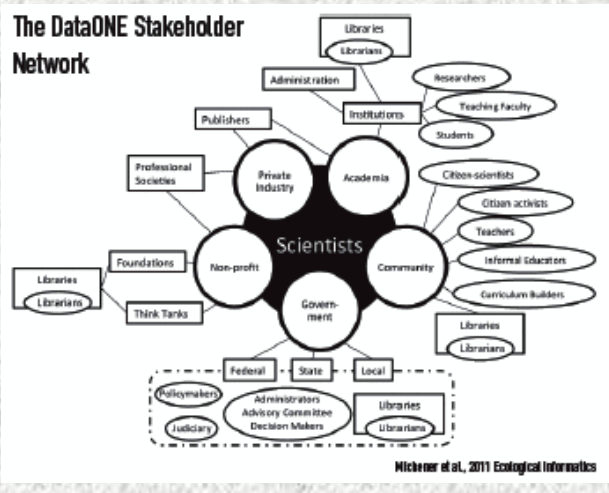
We are also for collaborations, but open access crystallographic data and web sites are not going to go away.



Lifecycle of data incorporating primary data, derived data, and workflow artifacts with corresponding provenance metadata for quality assessment.



Cumulative count of the data sets available through the DataONE Member Nodes as of July 2012.



Michener et al., 2011 Ecological Informatics

www.dataONE.org

DataONE NEWS

About CNI

- Membership
- CNI Collaborations
- Staff
- Steering Committee
- CNI Awards
- History

About CNI

Home / About CNI

http://www.cni.org/

The Coalition for Networked Information (CNI) is an organization dedicated to supporting the transformative promise of digital information technology for the advancement of scholarly communication and the enrichment of intellectual productivity. Some 200 institutions representing higher education, publishing, information technology, scholarly and professional organizations, foundations, and libraries and library organizations make up CNI's members; CNI is entirely funded through membership dues. Semi-annual membership meetings bring together representatives of CNI's constituencies to discuss ongoing and new projects, and to plan for future initiatives.

CNI is based in Washington, DC and led by Executive Director Clifford A. Lynch and Associate Executive Director Joan K. Lippincott.

Our current Program Plan is available online. The Program Plan is a snapshot of our plans and priorities for the year as of early November. It includes some background information about CNI and its collaborative activities, and discusses program initiatives planned for the year (July 1-June 30).

For announcements about the CNI community, subscribe to CNI-ANNOUNCE or point your news reader to CNI News.

More information is available about the history of CNI. See also Key Benefits of CNI Membership and the Membership FAQ.

Last updated: Thursday, December 13th, 2012

Browse By Topic

The Topics pages organize some material, produced by CNI staff and/or hosted on our website, around a few themes that have been important to CNI's work in recent years. Each topic page includes a brief description of that subject, as well as links to some representative materials in that area. Please note that **topic page lists are not comprehensive**, and, in most cases, they are primarily representative of CNI's most recent activity.

Topics

Scholarly Note-Taking On The Web

Michael Buckland (UC Berkeley) & Ryan Shaw (UNC Chapel Hill) explore how current Web technology can aid scholarly editing projects by making research notes available through Web publication, as one example. Their presentation was made at CNI's recent spring 2013 member meeting in San Antonio, TX.

About CNI

Latest News

CNI at ALA Annual in Chicago
JUNE 13, 2013

Reminder: Open Repositories 2013
JUNE 12, 2013

The Library in 2020, edited by Joe Janes, and my chapter on the Public Library
JUNE 11, 2013

1st European MOOCs & Libraries Conf — London, July 12, 2013
JUNE 10, 2013

Read all news

Upcoming Events

Jul 8, 2013 - Jul 12, 2013
Open Repositories (OR) 2013

Ebooks In 2013

CNI director Cliff Lynch provides an overall assessment in "Ebooks in 2013: Promises Broken, Promises Kept, and Faustian Bargains"

Quick Links

CNI Meetings

Cliff Lynch: Talks & Interviews

Publications by CNI Staff

Members

Event Calendar

Videos & Podcasts

JOURNAL OF CHEMICAL INFORMATION AND MODELING

EDITORIAL

pubs.acs.org/jcim

J. Chem. Inf. Model. 2011, 51, 3029–3029

Data-Driven High-Throughput Prediction of the 3-D Structure of Small Molecules: Review and Progress. A Response to the Letter by the Cambridge Crystallographic Data Centre

PierreBaldi*

Department of Computer Science, University of California, Irvine, Irvine, California 92697-3435, United States

Published: November 22, 2011

ultimately for advancing our understanding of the data they are meant to interpret. Accurate prediction of 3-D structures is central to chemistry and drug discovery; thus, any restrictions in this area impact not only the scientists that are involved but ultimately all the tax payers.

As history shows, those who stand in the way of democracy and scientific progress end up losing over the long run. The reactionary attitude of the CCDC staff has started to backfire by energizing academic laboratories around the world to find alternative solutions around the CCDC. There are already several efforts (e.g., Crystallography Open Database[3] and CrystalEye[4]) to produce large, freely available databases of crystallographic structures using the same main source as the CSD—publicly available data. Furthermore, quantum mechanical methods have now reached the level of

(3) Gražulis, S.; Chateigner, D.; Downs, R. T.; Yokochi, A. F. T.; Quirós, M.; Lutterotti, L.; Manakova, E.; Butkus, J.; Moeck, P.; Le Bail, A. Crystallography Open Database: An open-access collection of crystal structures. *J. Appl. Crystallogr.* **2009**, *42* (4), 726–729.

"There is nothing so powerful as an idea whose time has come." Victor Hugo

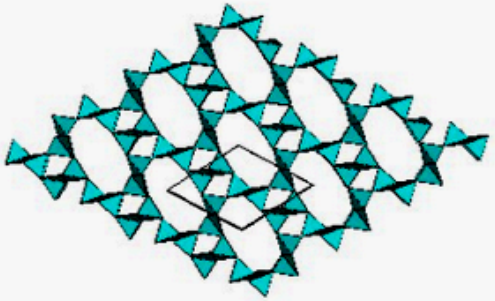
www.crystallography.net/pcod/index.html

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.

http://www.mwdeem.rice.edu/zefsaII/

http://sdpd.univ-lemans.fr/grinsp/index.html

Derived product :

The P2D2 (Predicted Powder Diffraction Database) contains all powder patterns calculated from the PCOD, assembled in a system allowing for search-match (by EVA from Bruker).

All data on this site have been placed in the public domain by the contributors
Have also a look at the COD containing really observed crystal structures.

http://www.crystallography.net/pcod/P2D2/EVA/index.html

paulingfile.com

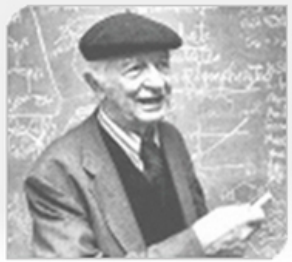
PAULING FILE

"The best way to have a good idea is to have lots of ideas." Linus Pauling

home | scope | phase diagrams | crystal structures | physical properties | products | about us

contents

phase diagrams + crystal structures + physical properties
together in the world largest database for inorganic compounds



Dear Dr. Villars: 27 August 1993

It is surely fine that you are starting a very large scale project to extend the database to cover all non-organic solid state materials. Also, it is fine that you want to call it the PAULING'S FILE.

This letter can serve as my permission.

Sincerely,

Linus Pauling

ded in many products ►► PAULING FILE ► Inorganic Materials Database containing ur

now at: http://crystdb.nims.go.jp/index_en.html

Enter AtomWork

The use of "MatNavi" is free.
(Free of charge)
All you need to do is register.

- Register
- Forgot your Password ?
- Update registration
- Close your account

AtomWork

- Outline
- Disclaimer
- System Requirements

MatNavi

- Basic Properties
- Polymer Database
- Inorganic Material Database
- Computational Electronic Structure Database
- Neutron Transmutation Database
- Interfacial Thermal Conductance Database
- Diffusion Database
- Superconducting Material Database

Inorganic Material Database (AtomWork)

Outline

The Inorganic Material Database aims to cover all basic crystal structure, x-ray diffraction, property and phase diagram data of inorganic and metallic materials from main literature sources.

You have three choices to search data:
1. "Search material" - Search materials by specifying chemical system, chemical formula, substance name, structure type (prototype), Pearson symbol or space group number.
2. "Search Materials having specified property" - Search materials by specifying property.
3. "Search phase diagrams" - Search phase diagrams by specifying chemical system.

As of July 1, 2010, the list of registered data had reached 82,000 crystal structures, 55,000 material properties and 15,000 phase diagrams.

Disclaimer

- National Institute for Materials Science (NIMS) holds the copyright of this database system.
- No reproduction, republication or distribution to third parties of any content is permitted without written permission of NIMS.
- NIMS takes no responsibility for any damage incurred by the user as a result of using this database system.

About AtomWork data

AtomWork data part is a collaboration among: National Institute for Materials Science (NIMS), Tsukuba, Japan, Materials Phases Data System (MPDS), Vitznau, Switzerland, and Japan Science Technology Corporation (JST), Tokyo, Japan.

Copyright? What copyright?

- Copyright covers works of authorship (novels, verse, sci. papers, computer programs)
- Copyright covers **only** the expression of the ideas
- Copyright **does not** cover:
  - Ideas
  - (scientific) facts
  - Simple forms (i.e. ones that do not contain individual's "trace of the hand")

Scène à faire *(French for "scene to be made" … In the U.S. it also refers to a principle in copyright law in which certain elements of a creative work are held to be not protected when they are mandated by or customary to the genre.* ***quoted from Wikipedia***

Idea-expression divide*,* ***quoted from Wikipedia***

… courts have recognized that there are particular ideas that can be expressed intelligibly only in one or a limited number of ways. The French name for this doctrine is Scènes à faire. Therefore even the expression in these circumstances is unprotected, or extremely limited to verbatim copying only. This is true in the United Kingdom and most Commonwealth countries. In the United States this is known as the merger doctrine, because the expression is considered to be inextricably merged with the idea. United States courts are divided on whether merger constitutes a defense to infringement or prevents copyrightability in the first place, but it is often pleaded as an affirmative defense to copyright infringement.

COD copyright policy

- Include data:
  - _atom_site_fract_x 0.333
- Exclude potentially copyrighted text:
  - _publication_text
    ;
    Introduction

    We have solved ...
    ;

What Does Copyright Protect?

What does copyright protect?
Copyright, a form of intellectual property law, protects original works of authorship including literary, dramatic, musical, and artistic works, such as poetry, novels, movies, songs, computer software, and architecture. Copyright does not protect facts, ideas, systems, or methods of operation, although it may protect the way these things are expressed. See Circular 1, *Copyright Basics*, section "What Works Are Protected."

Copyright
United States Copyright Office

Copyright Basics

assignation of domain names through accredited registers.

How do I protect my recipe?
A mere listing of ingredients is not protected under copyright law. accompanied by substantial literary expression in the form of an collection of recipes as in a cookbook, there may be a basis for c ingredients to a recipe that you do not wish to be revealed, you s because applications and deposit copies are public records. See F

Can I copyright the name of my band?
No. Names are not protected by copyright law. Some names ma U.S. Patent & Trademark Office, 800-786-9199, for further info

How do I copyright a name, title, slogan, or logo?

What Is Not Protected by Copyright?

Several categories of material are generally not eligible for federal copyright protection. These include among others:

- works that have not been fixed in a tangible form of expression (for example, choreographic works that have not been notated or recorded, or improvisational speeches or performances that have not been written or recorded)
- titles, names, short phrases, and slogans; familiar symbols or designs; mere variations of typographic ornamentation, lettering, or coloring; mere listings of ingredients or contents
- ideas, procedures, methods, systems, processes, concepts, principles, discoveries, or devices, as distinguished from a description, explanation, or illustration

United States

quoted from Wikipedia

Uncreative collections of facts are outside of Congressional authority under the Copyright Clause (Article I, § 8, cl. 8) of the United States Constitution, therefore ***no database right exists in the United States.*** *Originality is the sine qua non* of copyright in the United States (see Feist Publications v. Rural Telephone Service**). This has not stopped database owners lobbying for the introduction of such a right, but so far bills to introduce it in the U.S. have been prevented by the successful lobbying of research libraries, consumer groups and firms who benefit from the free use of factual information.*

**** Sine qua non, Latin, refers to an indispensable and essential action, condition, or ingredient. It was originally a Latin legal term for "[a condition] without which it could not be," or "but for..." or "without which [there is] nothing".***

***** Feist Publications, Inc., v. Rural Telephone Service Co.***, 499 U.S. 340 (1991), commonly called ***Feist v. Rural***, is an important United States Supreme Court case establishing that information alone without a minimum of original creativity cannot be protected by copyright. In the case appealed, Feist had copied information from Rural's telephone listings to include in its own, after Rural had refused to license the information. Rural sued for copyright infringement. The Court ruled that information contained in Rural's phone directory was not copyrightable and that therefore no infringement existed.

*A **database right** is considered to be a property right, comparable to but distinct from copyright, that exists to recognise the investment that is made in compiling a database, even when this does not involve the 'creative' aspect that is reflected by copyright.*

quoted from Wikipedia

Sui generis database right for member states of the European Union

Copyright protection is not available for databases which aim to be "complete", that is where the entries are selected by objective criteria: these are covered by sui generis database rights. While copyright protects the creativity of an author, database rights specifically protect the "qualitatively and/or quantitatively substantial investment in either the obtaining, verification or presentation of the contents".*

Database rights are held in the first instance by the person or corporation which made the substantial investment, so long as the person is a national or domiciliary of a Member State or the corporation is formed according to the laws of a Member State and has its registered office or principal place of business within the European Union.

Article 11(3) provides for the negotiation of treaties to ensure reciprocal treatment outside the EU: as of 2006, no such treaty exists.

***Sui generis** Latin phrase, meaning "of its own kind/genus" and hence "unique in its characteristics".*

Re: Crystallographic data copyrights
From: Eben Moglen <moglen@columbia.edu>
Date: Sun, 04 May 2003 09:02:21 -0400 I will have to be brief. If you need to follow up, let me know.

I assume US law governs throughout; an inaccurate but necessary assumption here. If you extract only the actual coordinate data you have no copyright liability. One cannot copyright facts, only the expression incident to factual reporting. This principle was recognized by the US Supreme Court in 1915 with respect to news reports sent by telegraph. The idea/expression distinction has been held by the Supreme Court to prevent assertion of copyright over telephone white pages, where there is no originality in the concept of alphabetic organization of data. More complex forms of association or organization of data might give rise to claims.
You should move quickly. Proposals for database protection in the US and Europe will close up vast areas of human knowledge within the next decade. Make this data free soon, or you risk losing the chance. How to license your data so that everyone is compelled to make free their improvements or accessions to it is another subject.
Best regards.
--
Eben Moglen *voice:* 212-854-8382 212-854-8382 FREE
Professor of Law *fax: 212-854-7946* *moglen@columbia.edu*
Columbia Law School, 435 West 116th Street, NYC 10027
General Counsel, Free Software Foundation
http://moglen.law.columbia.edu/

Somebody who reads Wikipedia is "rather in the position of a visitor to a public restroom," says Mr. McHenry, Britannica's former editor. "It may be obviously dirty, so that he knows to exercise great care, or it may seem fairly clean, so that he may be lulled into a false sense of security. What he certainly does not know is who has used the facilities before him."
One wonders whether people like Mr. McHenry would prefer there to be no public lavatories at all.

The Economist, Vol. 379, April 22, 2006, pp. 14–15