Open-access Crystallographic Databases (for the teaching of geometric structural crystallography *and much more***)**

Peter Moeck, Physics, Portland State University, ***&*** all other ***Members of International Advisory Board of the Crystallography Open Database (COD)***: Daniel Chateigner, Xiaolong Chen, Marco Ciriotti, Robert T. Downs, Saulius Gražulis, Armel Le Bail, Luca Lutterotti, Yoshitaka Matsushita, Miguel Quirós Olozábal, Hareesh Rajan, Alexandre F.T. Yokochi

Financial support from the Northwest Academic Computing Consortium and Portland State University (to PM) is gratefully acknowledged. The Vilnius development group of the Crystallography Open Database (under the direction of SG) is supported by the Research Council of Lithuania, contract No. MIP-124/2010.

Outline

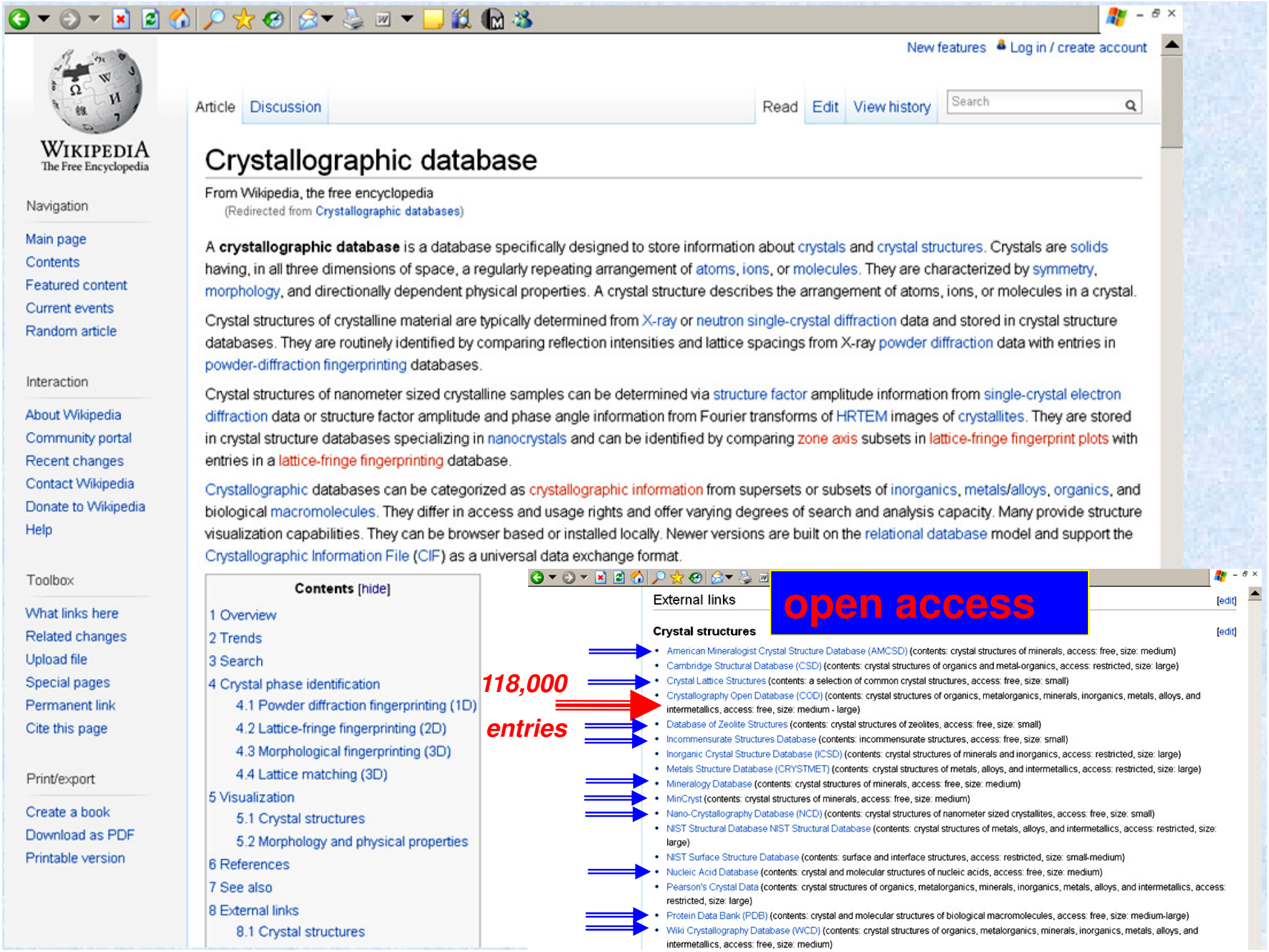
- What kind of crystallographic data are there in open access?

- What might be done with them for teaching purposes?

- What else might be done with some of these data?

- Anybody interested in uploads of data to the COD in the Crystallographic Information File (CIF) format?

- Anybody interested in downloads of CIFs from the COD or American Mineralogist Crystal Structure Database for powder XRD, EBSD, or other purposes?


New features
Log in / create account
Article
Discussion
Read
Edit
View history
Search
WIKIPEDIA
The Free Encyclopedia
Navigation
Main page
Contents
Featured content
Current events
Random article
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Crystallographic database
From Wikipedia, the free encyclopedia
(Redirected from Crystallographic databases)
A crystallographic database is a database specifically designed to store information about crystals and crystal structures. Crystals are solids having, in all three dimensions of space, a regularly repeating arrangement of atoms, ions, or molecules. They are characterized by symmetry, morphology, and directionally dependent physical properties. A crystal structure describes the arrangement of atoms, ions, or molecules in a crystal.
Crystal structures of crystalline material are typically determined from X-ray or neutron single-crystal diffraction data and stored in crystal structure databases. They are routinely identified by comparing reflection intensities and lattice spacings from X-ray powder diffraction data with entries in powder-diffraction fingerprinting databases.
Crystal structures of nanometer sized crystalline samples can be determined via structure factor amplitude information from single-crystal electron diffraction data or structure factor amplitude and phase angle information from Fourier transforms of HRTEM images of crystallites. They are stored in crystal structure databases specializing in nanocrystals and can be identified by comparing zone axis subsets in lattice-fringe fingerprint plots with entries in a lattice-fringe fingerprinting database.
Crystallographic databases can be categorized as crystallographic information from supersets or subsets of inorganics, metals/alloys, organics, and biological macromolecules. They differ in access and usage rights and offer varying degrees of search and analysis capacity. Many provide structure visualization capabilities. They can be browser based or installed locally. Newer versions are built on the relational database model and support the Crystallographic Information File (CIF) as a universal data exchange format.
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4.1 Powder diffraction fingerprinting (1D)
4.2 Lattice-fringe fingerprinting (2D)
4.3 Morphological fingerprinting (3D)
4.4 Lattice matching (3D)
5 Visualization
5.1 Crystal structures
5.2 Morphology and physical properties
6 References
7 See also
8 External links
8.1 Crystal structures
118,000
entries
External links [edit]
open access
Crystal structures [edit]
American Mineralogist Crystal Structure Database (AMCSD) (contents: crystal structures of minerals, access: free, size: medium)
Cambridge Structural Database (CSD) (contents: crystal structures of organics and metal-organics, access: restricted, size: large)
Crystal Lattice Structures (contents: a selection of common crystal structures, access: free, size: small)
Crystallography Open Database (COD) (contents: crystal structures of organics, metalorganics, minerals, inorganics, metals, alloys, and intermetallics, access: free, size: medium - large)
Database of Zeolite Structures (contents: crystal structures of zeolites, access: free, size: small)
Incommensurate Structures Database (contents: incommensurate structures, access: free, size: small)
Inorganic Crystal Structure Database (ICSD) (contents: crystal structures of minerals and inorganics, access: restricted, size: large)
Metals Structure Database (CRYSTMET) (contents: crystal structures of metals, alloys, and intermetallics, access: restricted, size: large)
Mineralogy Database (contents: crystal structures of minerals, access: free, size: medium)
MinCryst (contents: crystal structures of minerals, access: free, size: medium)
Nano-Crystallography Database (NCD) (contents: crystal structures of nanometer sized crystallites, access: free, size: small)
NIST Structural Database NIST Structural Database (contents: crystal structures of metals, alloys, and intermetallics, access: restricted, size: large)
NIST Surface Structure Database (contents: surface and interface structures, access: restricted, size: small-medium)
Nucleic Acid Database (contents: crystal and molecular structures of nucleic acids, access: free, size: medium)
Pearson's Crystal Data (contents: crystal structures of organics, metalorganics, minerals, inorganics, metals, alloys, and intermetallics, access: restricted, size: large)
Protein Data Bank (PDB) (contents: crystal and molecular structures of biological macromolecules, access: free, size: medium-large)
Wiki Crystallography Database (WCD) (contents: crystal structures of organics, metalorganics, minerals, inorganics, metals, alloys, and intermetallics, access: free, size: medium)

- Specifications
- Documentation
- Software
- COMCIFS
- Dictionary definition languages
- CIF dictionaries
- checkCIF

CIF

The International Union of Crystallography is the sponsor of the **Crystallographic Information Framework**, a standard for information interchange in crystallography.

The acronym CIF is used both for the *Crystallographic Information File*, the data exchange standard file format of Hall, Allen & Brown (1991) (see Documentation), and for the *Crystallographic Information Framework*, a broader system of exchange protocols based on data dictionaries and relational rules expressible in different machine-readable manifestations, including, but not restricted to, Crystallographic Information File and XML.

CIF was developed by the IUCr Working Party on Crystallographic Information in an effort sponsored by the IUCr Commission on Crystallographic Data and the IUCr Commission on Journals, and was adopted in 1990 as a standard file structure for the archiving and distribution of crystallographic information. It is now well established and is in regular use for reporting crystal structure determinations to *Acta Crystallographica* and other journals. It is often cited as a model example of integrating data and textual information for data-centric scientific communication. In 2006 the importance of CIF and the value of its accompanying web-based service for the validation of structural data, *checkCIF*, were recognised by the Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP). In their report, the judges 'were impressed with the way in which CIF and checkCIF are easily accessible and have served to make critical crystallographic data more consistently reliable and accessible at all stages of the information chain, from authors, reviewers and editors through to readers and researchers. In doing so, the system takes away the donkeywork from ensuring that the results of scientific research are trustworthy without detracting from the value of human judgement in the research and publication process'.

This part of the IUCr web site provides comprehensive documentation and software resources for users and developers of CIF software.

International Tables for Crystallography

Volume G: Definition and exchange of crystallographic data

First online edition (2006)

Edited by S. R. Hall and B. McMahon

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sample pages
purchase
CIF dictionaries

Describes CIF, the data exchange standard of crystallography. Provides: information for scientists who wish to record or use the results of a single-crystal or powder diffraction experiment; the data ontology necessary for designing interoperable

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_atom_site_fract_y
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_atom_site_occupancy
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  O1    O2-    6 c 0.39848(9) 0.31858(9) 0.38307(3) 1.  0 d
  O2    O2-    6 c 0.39674(9) 0.29595(9) 0.87152(3) 1.  0 d
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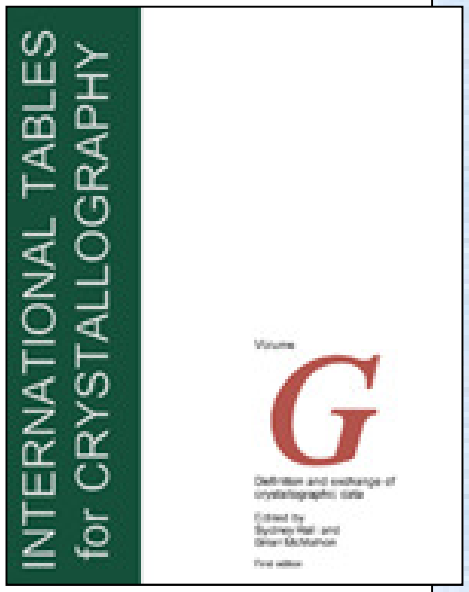

Reciprocal Net

a distributed crystallography network for researchers, students and the general public

- Home
- About Reciprocal Net
- Site Network
- Learn About
  - Common Molecules
  - Crystallography
  - Crystallization
  - Chemistry
- Help

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Learn About:
Common Molecules

Alphabetical List of all Common Molecules in our Collection »
Find Common Molecules »
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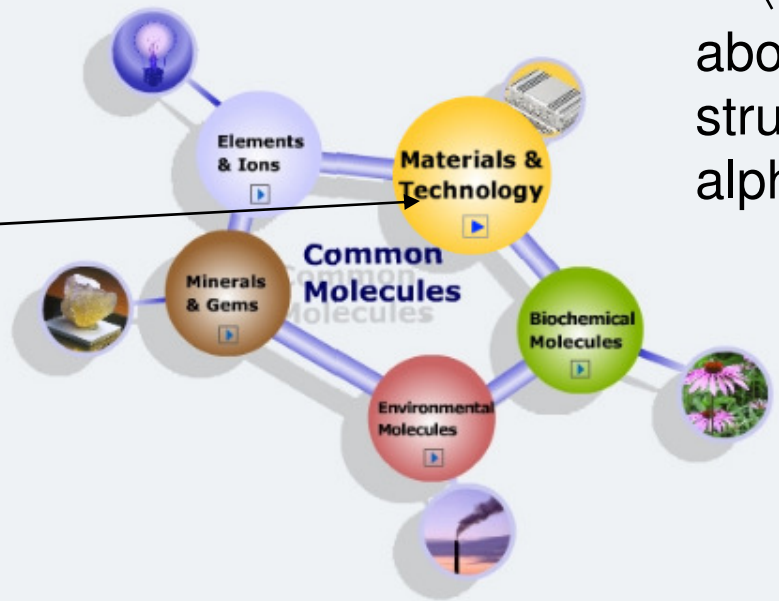
Welcome to the Common Molecules collection, part of the Reciprocal Net project! The molecules in this site are considered common based on their general use or presence in the world in and around us or by the interest they spark because of their fascinating structural properties and innovative applications. We focused on molecules studied in chemistry classrooms of schools and colleges but our growing collection includes also current research results that might be of interest for the general public.

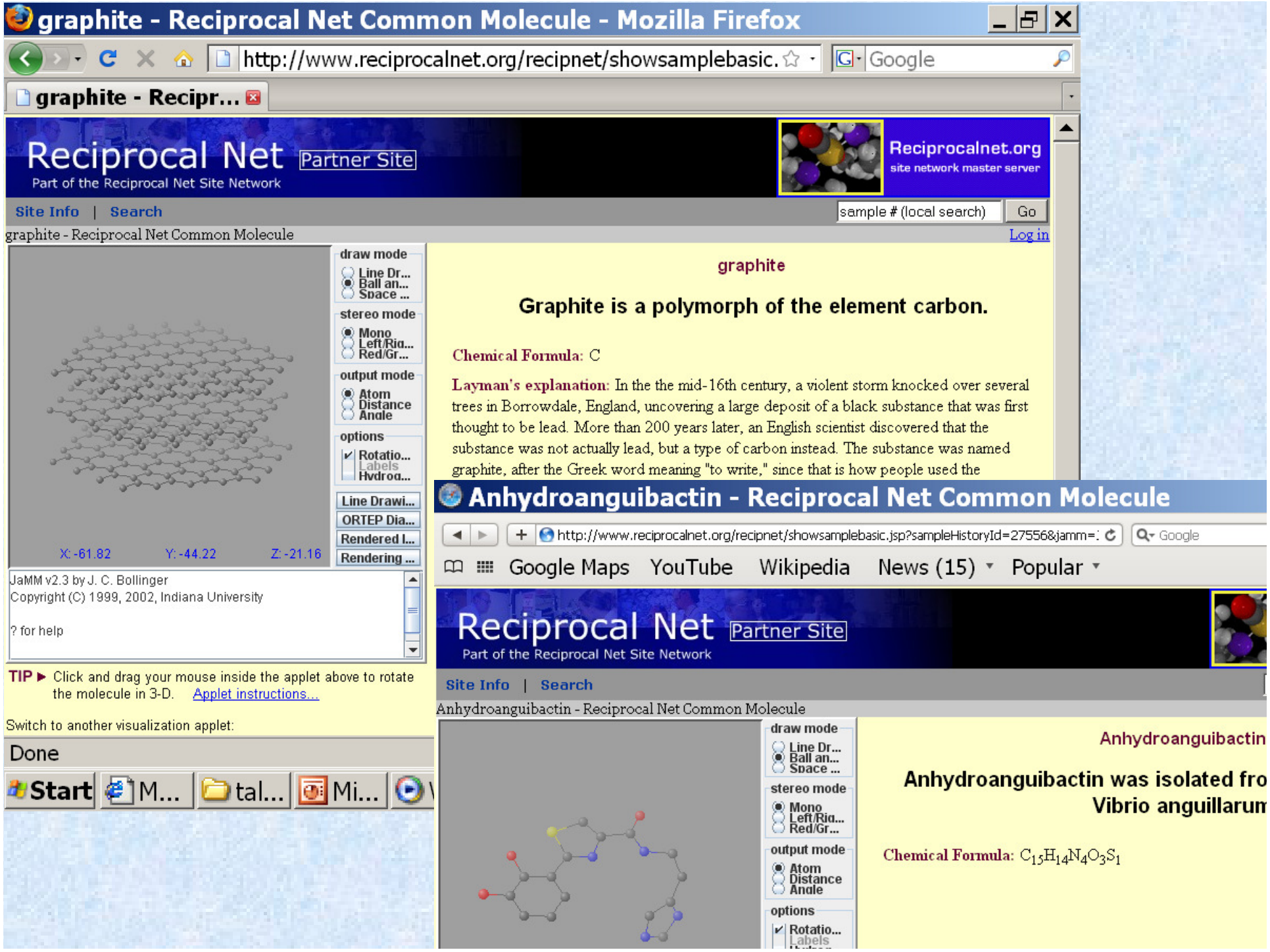
By clicking on a category below, general information on the category and a list of clickable compound classes is given; the latter will lead you to a list on molecules. Individual pages for the molecules can also be reached via an Alphabetical list. The individual molecule pages provide you with some information about the molecule and a java applet (miniJaMM) that allows you to view and rotate the molecule. The applet JaMM2 features advanced option such as 3D viewing, rendering and requesting geometrical parameters. The presented structural data were obtained by using the technique of X-ray crystallography, one of the principal methods for determining the structure of molecules. In cases where no data were available, the most probable structure of a molecule was calculated using molecular mechanics or low level *ab initio* methods.



Elements, Ions and Simple Molecules | Materials and Technology | Biochemical Molecules | Minerals and Gems | Environmental Molecules

130 crystal structures and individual molecules for Materials & Technology, CIF downloadable

about 250 more structures over alphabetical list


graphite - Reciprocal Net Common Molecule - Mozilla Firefox
http://www.reciprocalnet.org/recipnet/showsamplebasic.
Google
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Reciprocal Net
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graphite - Reciprocal Net Common Molecule
Log in
draw mode
Line Dr...
Ball an...
Space ...
stereo mode
Mono
Left/Rig...
Red/Gr...
output mode
Atom
Distance
Angle
options
Rotatio...
Labels
Hydrog...
Line Drawi...
ORTEP Dia...
Rendered I...
Rendering ...
X: -61.82
Y: -44.22
Z: -21.16
graphite
Graphite is a polymorph of the element carbon.
Chemical Formula: C
Layman's explanation: In the the mid-16th century, a violent storm knocked over several trees in Borrowdale, England, uncovering a large deposit of a black substance that was first thought to be lead. More than 200 years later, an English scientist discovered that the substance was not actually lead, but a type of carbon instead. The substance was named graphite, after the Greek word meaning "to write," since that is how people used the
JaMM v2.3 by J. C. Bollinger
Copyright (C) 1999, 2002, Indiana University
? for help
TIP ▶ Click and drag your mouse inside the applet above to rotate the molecule in 3-D. Applet instructions...
Switch to another visualization applet:
Done
Start
Anhydroanguibactin - Reciprocal Net Common Molecule
http://www.reciprocalnet.org/recipnet/showsamplebasic.jsp?sampleHistoryId=27556&jamm=
Google
Google Maps
YouTube
Wikipedia
News (15)
Popular
Reciprocal Net
Partner Site
Part of the Reciprocal Net Site Network
Site Info | Search
Anhydroanguibactin - Reciprocal Net Common Molecule
draw mode
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Ball an...
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stereo mode
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Left/Rig...
Red/Gr...
output mode
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options
Rotatio...
Labels
Anhydroanguibactin
Anhydroanguibactin was isolated fro
Vibrio anguillarum
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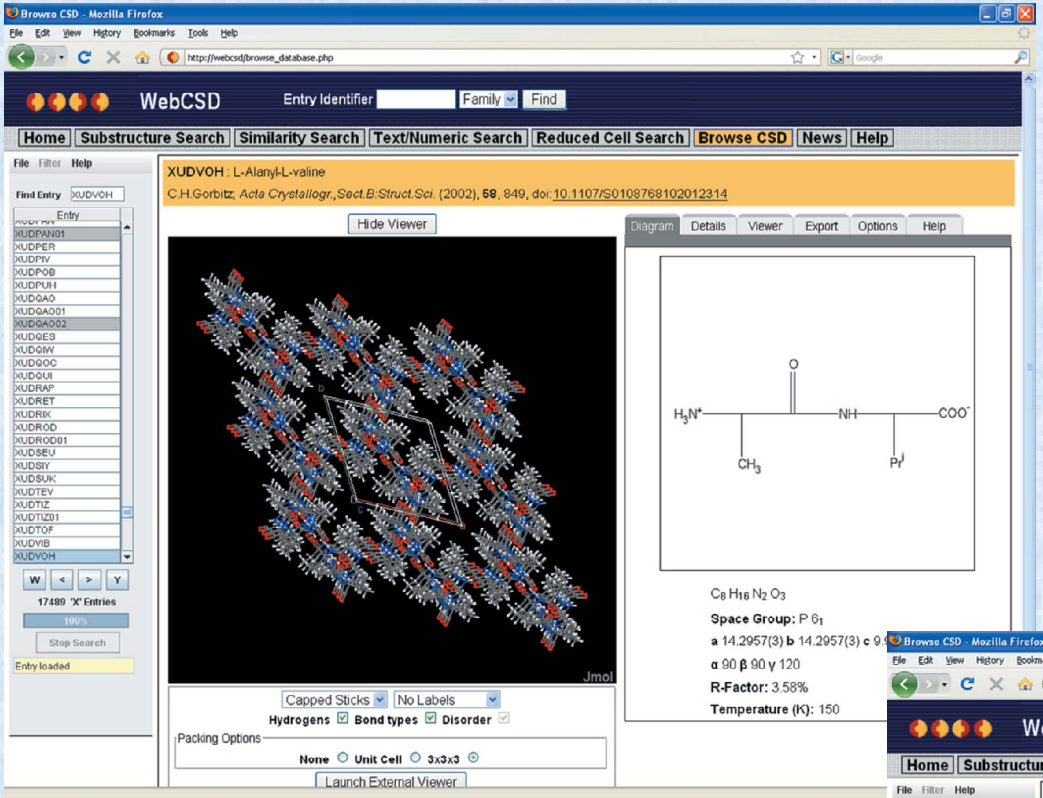
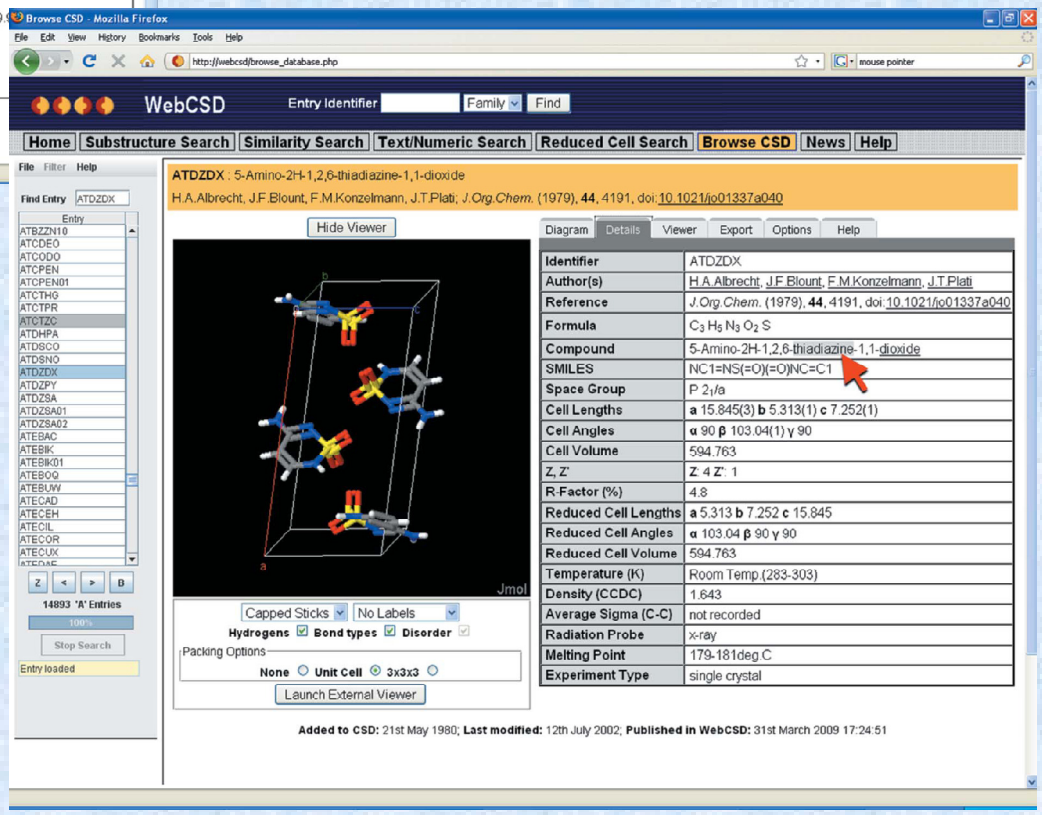


500 CIFs of important organics can be displayed and downloaded

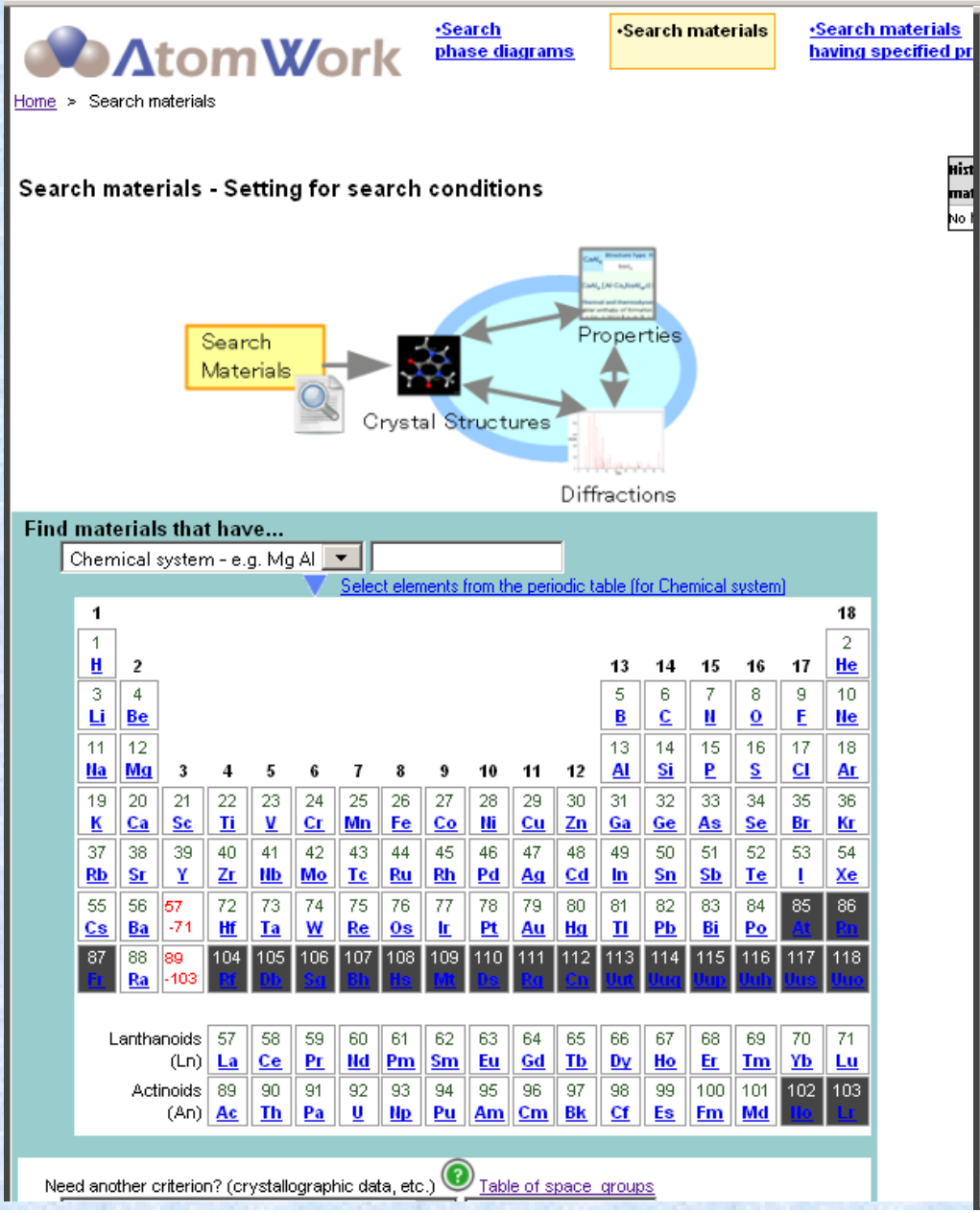


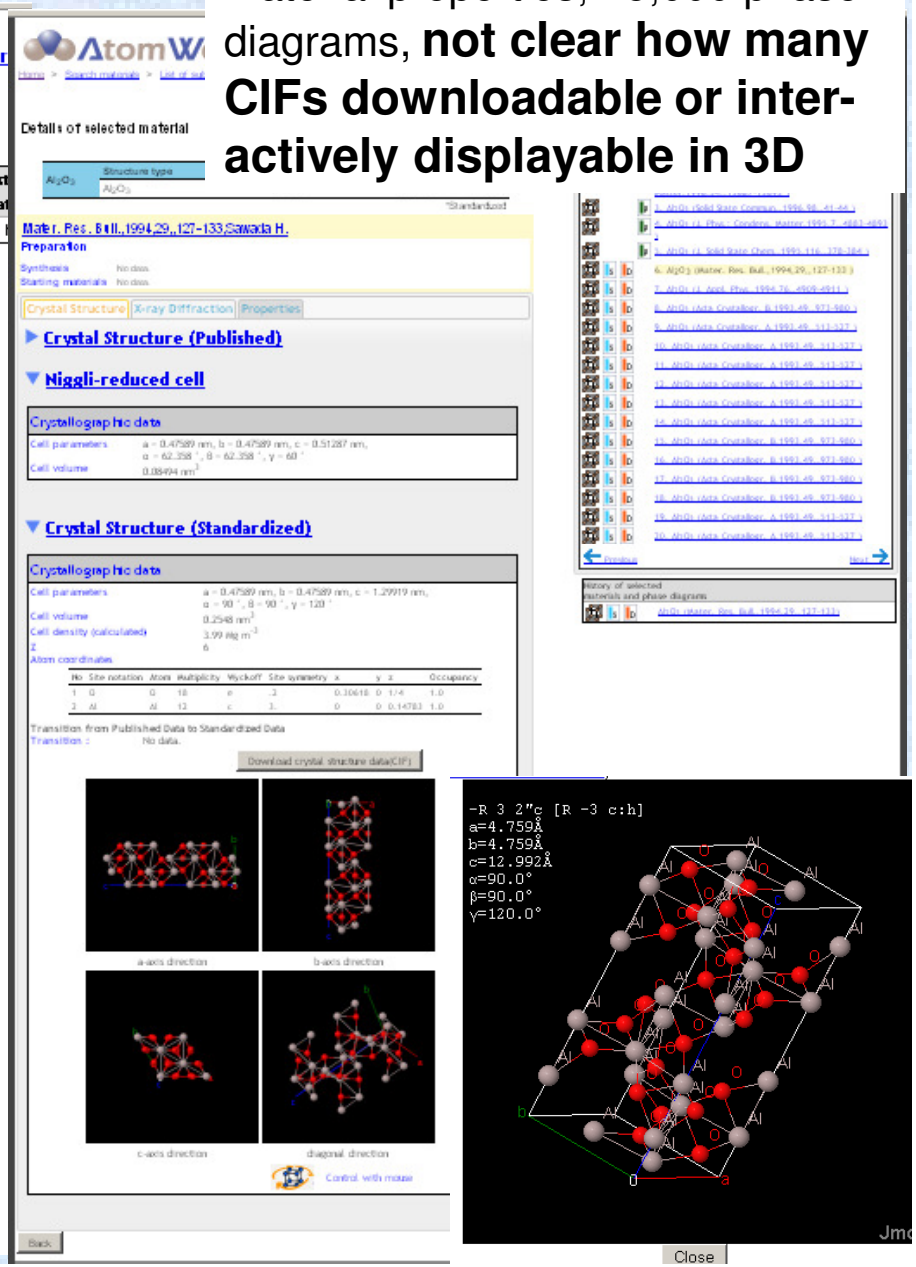
Ian R. Thomas et al., WebCSD: the online portal to the Cambridge Structural Database, *J. Appl. Cryst.* **43** (2010) 362–366

http://crystdb.nims.go.jp/index_en.htm

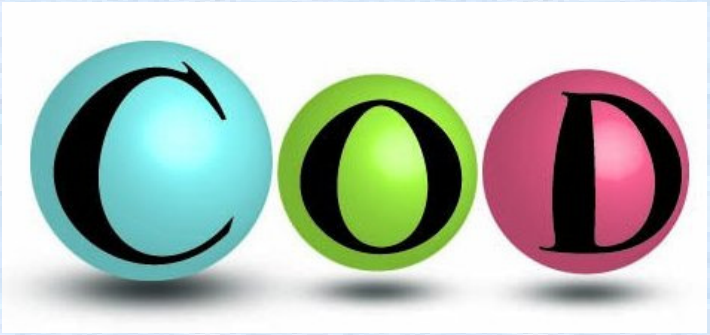
National Institute for Materials Science, Tsukuba, Japan

former? **Linus Pauling File,** 82,000 crystal structures, 55,000 material properties, 15,000 phase diagrams, **not clear how many CIFs downloadable or interactively displayable in 3D**





probably all useful crystallographic data for teaching already in open access



http://cod.ibt.lt

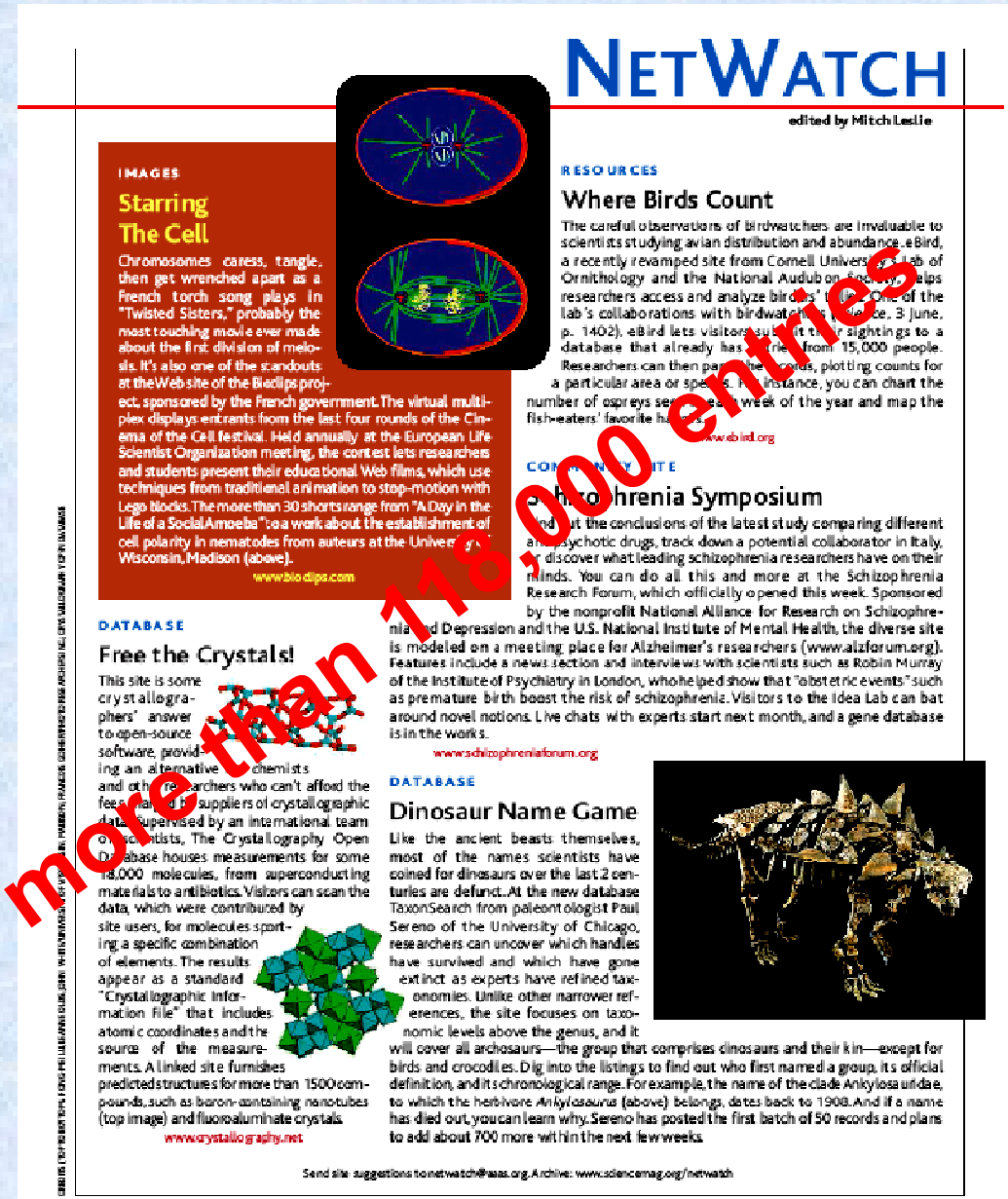
mirrors worldwide

www.crystallography.net
cod.ensicaen.fr
nanocrystallography.org
jcod.nanocrystallography.net
cod.nanocrystallography.net/cod

web portal

http://nanocrystallography.net

now more than 118,000 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 Biodips 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.biodips.com

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

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' lists. 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 tallies from 15,000 people. Researchers can then peruse the counts, plotting counts for a particular area or species. For instance, you can chart the number of ospreys seen 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

Dinosaur Name Game

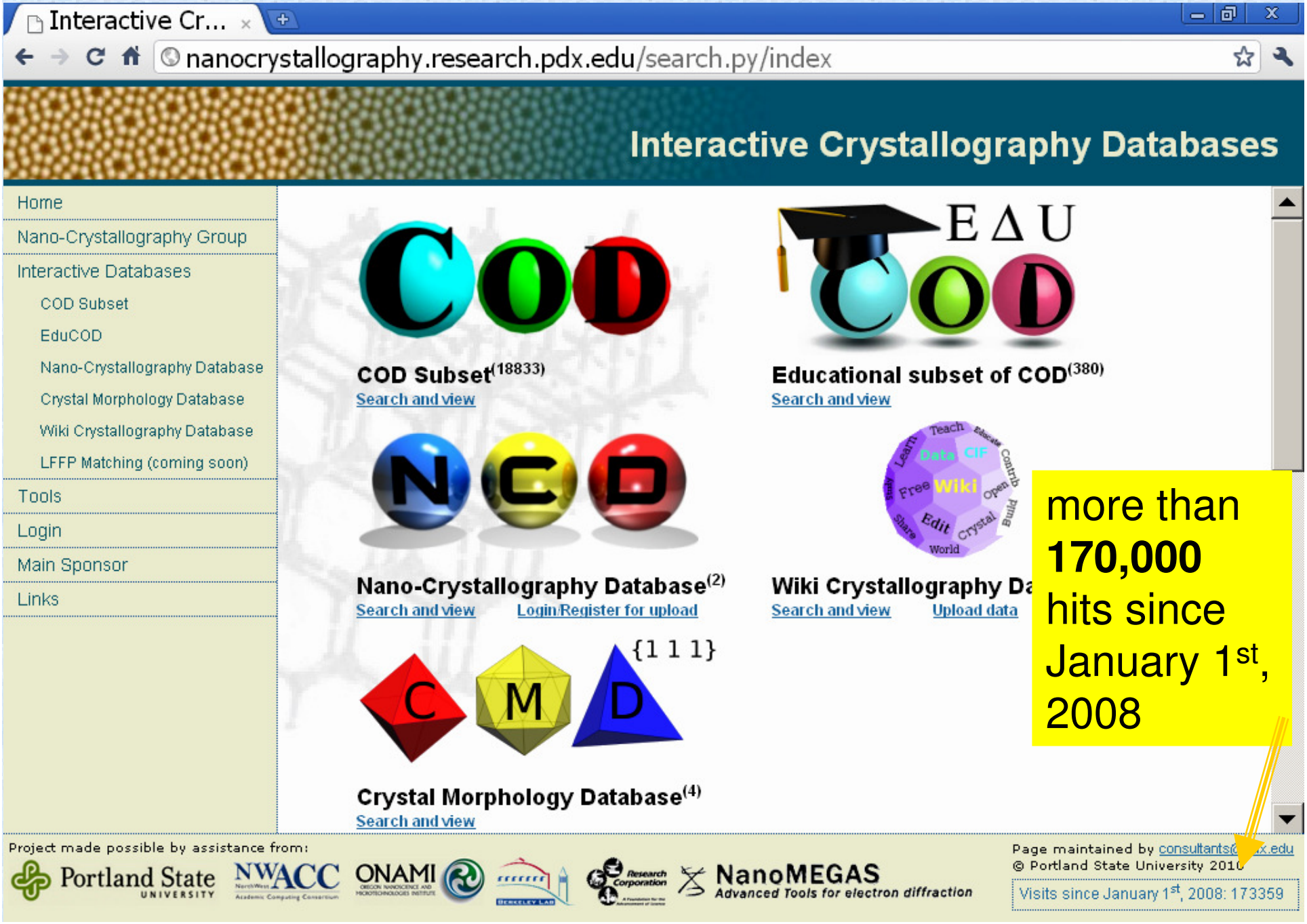
Like the ancient beasts themselves, most of the names scientists have coined for dinosaurs over the last 2 centuries are defunct. At the new database TaxonSearch from paleontologist Paul Sereno of the University of Chicago, researchers can uncover which handles have survived and which have gone extinct 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.

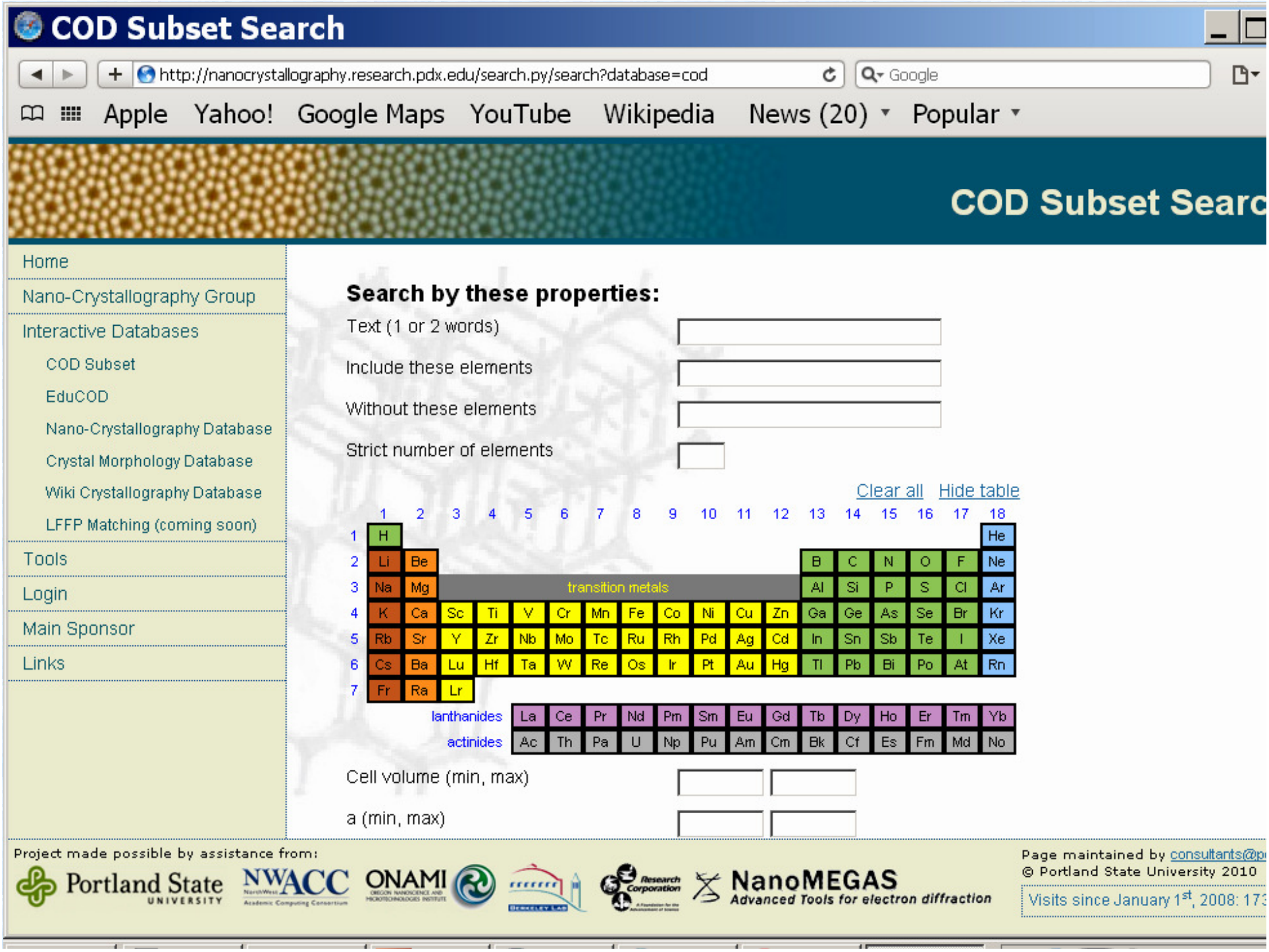
Send site suggestions to netwatch@aaas.org. Archive: www.sciencemag.org/netwatch

www.sciencemag.org SCIENCE VOL 310 28 OCTOBER 2005 597

Published by AAAS

http://nanocrystallography.research.pdx.edu/CIF-searchable

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Google
Apple Yahoo! Google Maps YouTube Wikipedia News (20) Popular
COD Subset Searc
Home
Nano-Crystallography Group
Interactive Databases
COD Subset
EduCOD
Nano-Crystallography Database
Crystal Morphology Database
Wiki Crystallography Database
LFFP Matching (coming soon)
Tools
Login
Main Sponsor
Links
Search by these properties:
Text (1 or 2 words)
Include these elements
Without these elements
Strict number of elements
Clear all
Hide table
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
H He
Li Be B C N O F Ne
Na Mg transition metals Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Lr
lanthanides La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
actinides Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No
Cell volume (min, max)
a (min, max)
Project made possible by assistance from:
Portland State UNIVERSITY
NWACC
ONAMI
Research Corporation
NanoMEGAS
Advanced Tools for electron diffraction
Page maintained by consultants@p
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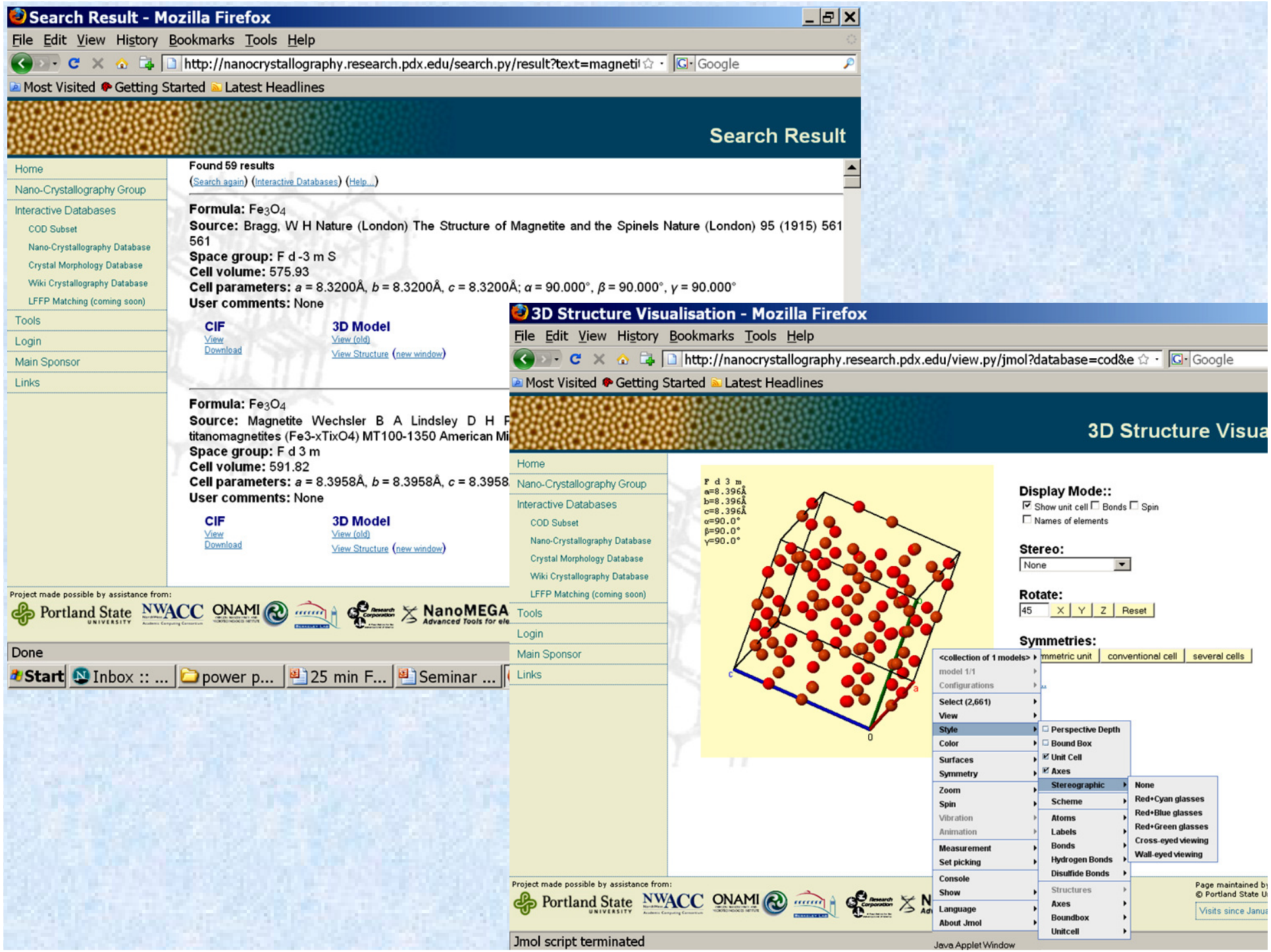
Visits since January 1st, 2008: 173


Search Result - Mozilla Firefox
File Edit View History Bookmarks Tools Help
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Google
Most Visited Getting Started Latest Headlines
Search Result
Home
Nano-Crystallography Group
Interactive Databases
COD Subset
Nano-Crystallography Database
Crystal Morphology Database
Wiki Crystallography Database
LFFP Matching (coming soon)
Tools
Login
Main Sponsor
Links
Found 59 results
(Search again) (Interactive Databases) (Help...)
Formula: Fe3O4
Source: Bragg, W H Nature (London) The Structure of Magnetite and the Spinels Nature (London) 95 (1915) 561
561
Space group: F d -3 m S
Cell volume: 575.93
Cell parameters: a = 8.3200Å, b = 8.3200Å, c = 8.3200Å; α = 90.000°, β = 90.000°, γ = 90.000°
User comments: None
CIF
View
Download
3D Model
View (old)
View Structure (new window)
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titanomagnetites (Fe3-xTixO4) MT100-1350 American Mi
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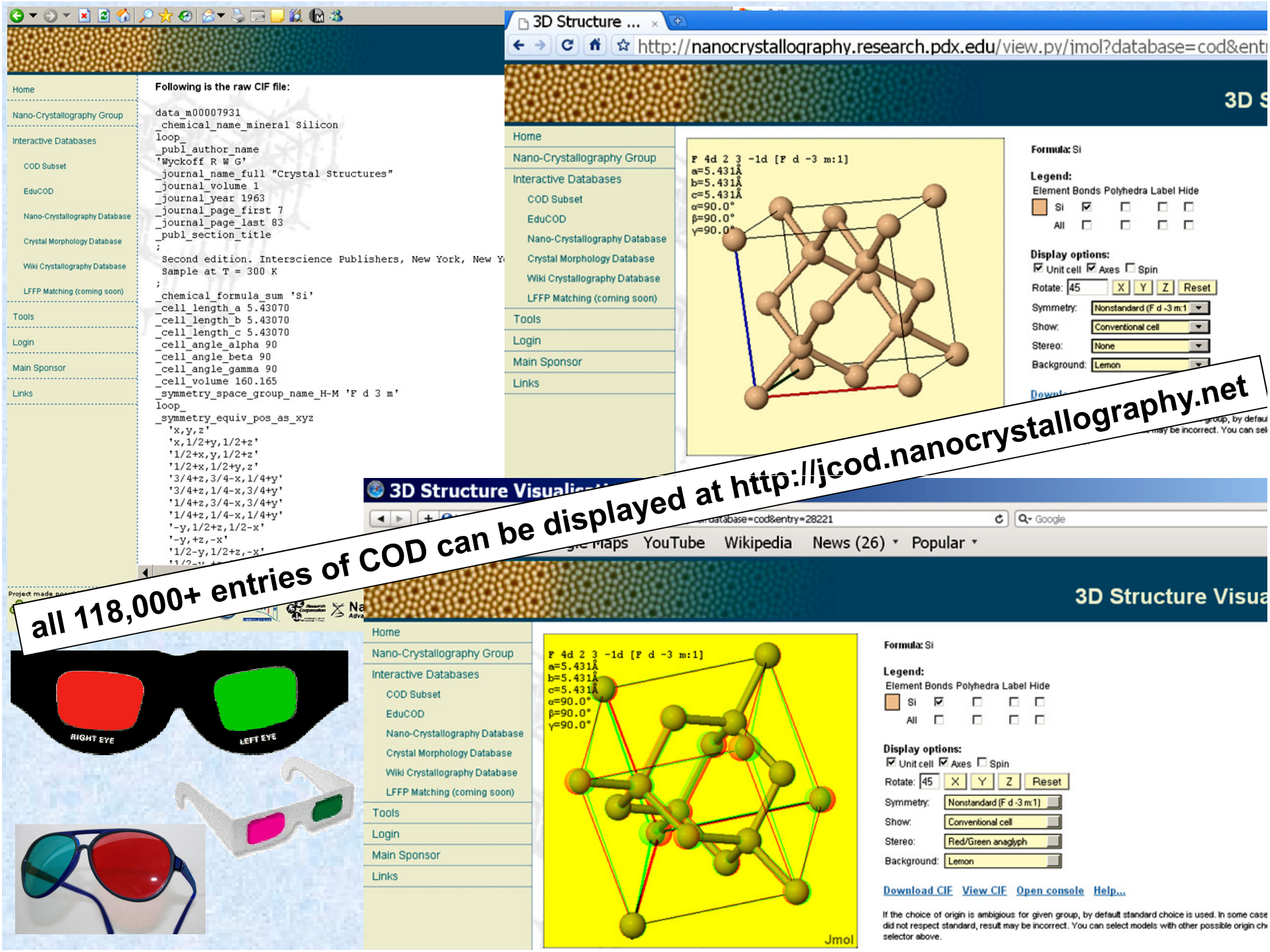
Project made possible by assistance from:
Portland State
NWACC
ONAMI
NanoMEGA
Done
Start
Inbox :: ...
power p...
25 min F...
Seminar ...
3D Structure Visualisation - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://nanocrystallography.research.pdx.edu/view.py/jmol?database=cod&e
Google
Most Visited Getting Started Latest Headlines
3D Structure Visua
Home
Nano-Crystallography Group
Interactive Databases
COD Subset
Nano-Crystallography Database
Crystal Morphology Database
Wiki Crystallography Database
LFFP Matching (coming soon)
Tools
Login
Main Sponsor
Links
F d 3 m
a=8.396Å
b=8.396Å
c=8.396Å
α=90.0°
β=90.0°
γ=90.0°
Display Mode::
Show unit cell Bonds Spin
Names of elements
Stereo:
None
Rotate:
45 X Y Z Reset
Symmetries:
mmetric unit conventional cell several cells
<collection of 1 models>
model 1/1
Configurations
Select (2,661)
View
Style
Color
Surfaces
Symmetry
Zoom
Spin
Vibration
Animation
Measurement
Set picking
Console
Show
Language
About Jmol
Perspective Depth
Bound Box
Unit Cell
Axes
Stereographic
Scheme
Atoms
Labels
Bonds
Hydrogen Bonds
Disulfide Bonds
Structures
Axes
Boundbox
Unitcell
None
Red+Cyan glasses
Red+Blue glasses
Red+Green glasses
Cross-eyed viewing
Wall-eyed viewing
Project made possible by assistance from:
Portland State
NWACC
ONAMI
Page maintained by
© Portland State U
Visits since Janu
Jmol script terminated
Java Applet Window


Home
Nano-Crystallography Group
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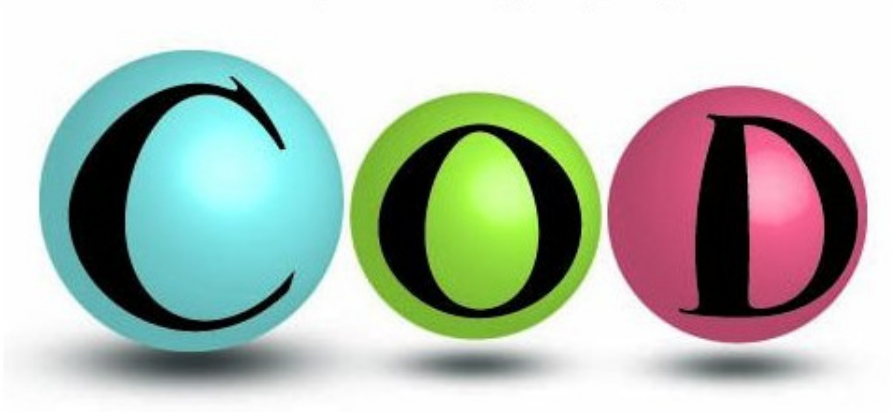
COD Subset
EduCOD
Nano-Crystallography Database
Crystal Morphology Database
Wiki Crystallography Database
LFFP Matching (coming soon)
Tools
Login
Main Sponsor
Links
Following is the raw CIF file:
data_m00007931
_chemical_name_mineral Silicon
loop_
_publ_author_name
'Wyckoff R W G'
_journal_name_full "Crystal Structures"
_journal_volume 1
_journal_year 1963
_journal_page_first 7
_journal_page_last 83
_publ_section_title
;
Second edition. Interscience Publishers, New York, New Y
Sample at T = 300 K
;
_chemical_formula_sum 'Si'
_cell_length_a 5.43070
_cell_length_b 5.43070
_cell_length_c 5.43070
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 90
_cell_volume 160.165
_symmetry_space_group_name_H-M 'F d 3 m'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'x,1/2+y,1/2+z'
'1/2+x,y,1/2+z'
'1/2+x,1/2+y,z'
'3/4+z,3/4-x,1/4+y'
'3/4+z,1/4-x,3/4+y'
'1/4+z,3/4-x,3/4+y'
'1/4+z,1/4-x,1/4+y'
'-y,1/2+z,1/2-x'
'-y,+z,-x'
'1/2-y,1/2+z,-x'
3D Structure ...
http://nanocrystallography.research.pdx.edu/view.py/jmol?database=cod&entr
3D S
F 4d 2 3 -1d [F d -3 m:1]
a=5.431Å
b=5.431Å
c=5.431Å
α=90.0°
β=90.0°
γ=90.0°
Formula: Si
Legend:
Element Bonds Polyhedra Label Hide
Si
All
Display options:
Unit cell Axes Spin
Rotate: 45 X Y Z Reset
Symmetry: Nonstandard (F d -3 m:1
Show: Conventional cell
Stereo: None
Background: Lemon
all 118,000+ entries of COD can be displayed at http://cod.nanocrystallography.net
3D Structure Visualis
database=cod&entry=28221
Google
Maps YouTube Wikipedia News (26) Popular
3D Structure Visua
RIGHT EYE
LEFT EYE
Stereo: Red/Green anaglyph
Jmol
Download CIF View CIF Open console Help...
If the choice of origin is ambigious for given group, by default standard choice is used. In some case
did not respect standard, result may be incorrect. You can select models with other possible origin ch
selector above.

http://www.crystallography.net/

Crystallography ...

www.crystallography.net



Crystallography Open Database

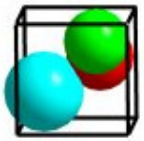
Deposit your data (NEW!)

or

Upload data

or

Search the database



View the Petition for Open Data in Crystallography

Call to Volunteers

See also the **PCOD** : Predicted Crystallography Open Database

More on the COD project : **what's new**

Recent open access paper regarding COD development was published in Journal of Applied Crystallography. PDF and HTML versions are available.

COD Advisory Board thanks Crystal Impact GbR for their financial support of this paper publication.

cif applications

Journal of
Applied
Crystallography

ISSN 0021-8898

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Accepted 4 May 2009

This article is dedicated to Michael Berndt.

Crystallography Open Database – an open-access collection of crystal structures

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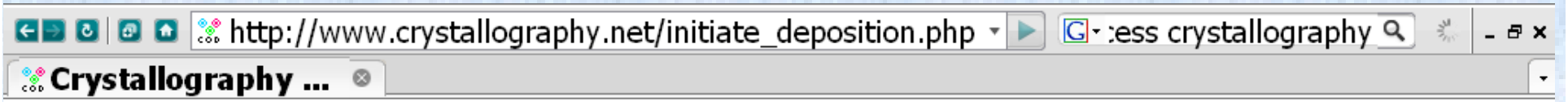
The Crystallography Open Database (COD), which is a project that aims to gather all available inorganic, metal–organic and small organic molecule structural data in one database, is described. The database adopts an open-access model. The COD currently contains ~80 000 entries in crystallographic information file format, with nearly full coverage of the International Union of Crystallography publications, and is growing in size and quality.



Crystallography Open Database
Validation and Deposition Interface

Choose deposition type

Personal communication to COD

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.

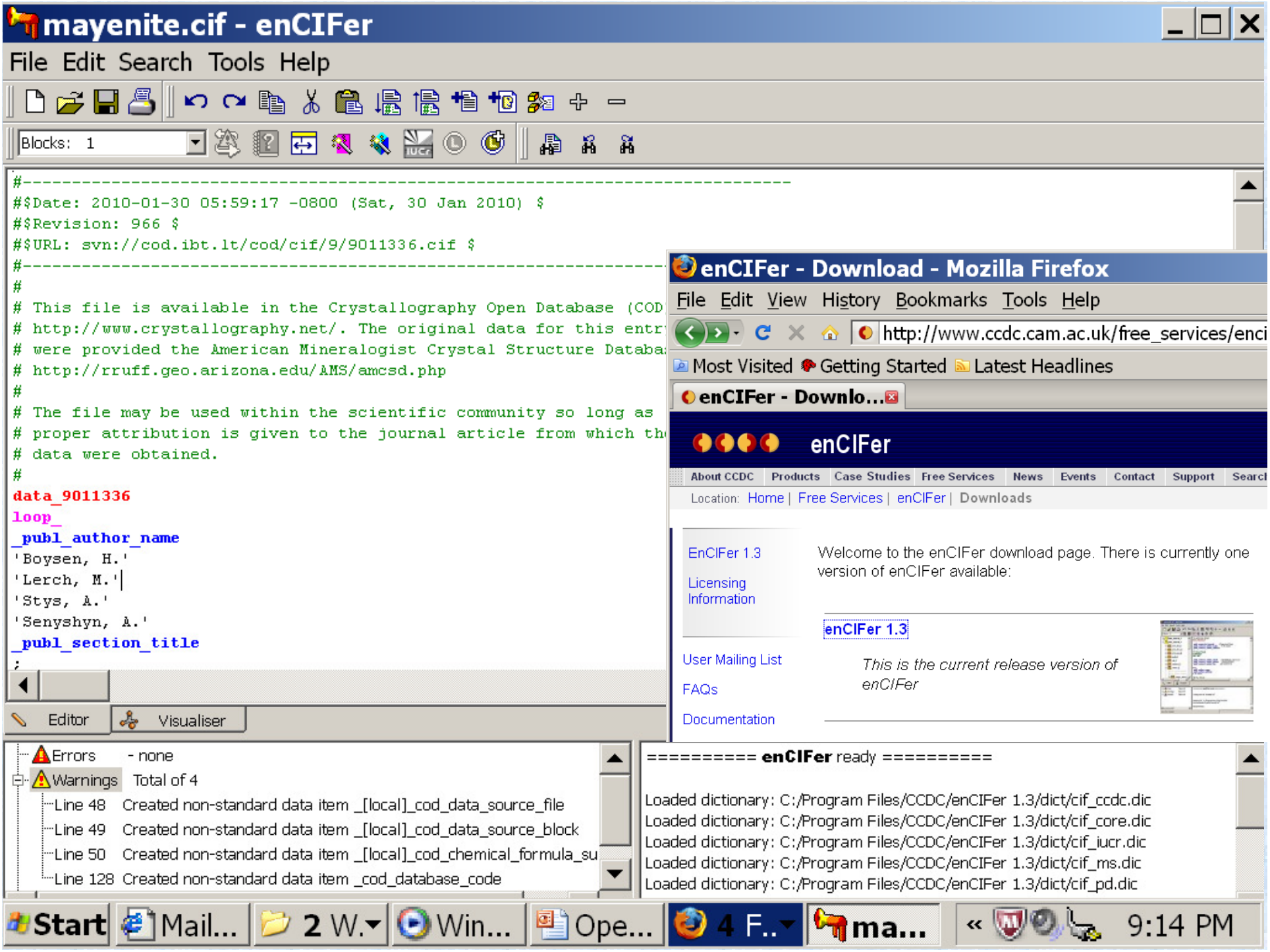
Steps

The process of files deposition, after you have uploaded your data is prettty simple.
First step, after files have been uploaded, is validation. Our scripts performs 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.


mayenite.cif - enCIFer
File Edit Search Tools Help
Blocks: 1
#$Date: 2010-01-30 05:59:17 -0800 (Sat, 30 Jan 2010) $
#$Revision: 966 $
#$URL: svn://cod.ibt.lt/cod/cif/9/9011336.cif $
This file is available in the Crystallography Open Database (COD
http://www.crystallography.net/. The original data for this entr
were provided the American Mineralogist Crystal Structure Databa
http://rruff.geo.arizona.edu/AMS/amcsd.php
The file may be used within the scientific community so long as
proper attribution is given to the journal article from which th
data were obtained.
data_9011336
loop_
_publ_author_name
'Boysen, H.'
'Lerch, M.'
'Stys, A.'
'Senyshyn, A.'
_publ_section_title
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Editor
Visualiser
Errors - none
Warnings Total of 4
Line 48 Created non-standard data item _[local]_cod_data_source_file
Line 49 Created non-standard data item _[local]_cod_data_source_block
Line 50 Created non-standard data item _[local]_cod_chemical_formula_su
Line 128 Created non-standard data item _cod_database_code
enCIFer - Download - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://www.ccdc.cam.ac.uk/free_services/enci
Most Visited Getting Started Latest Headlines
enCIFer - Downlo...
enCIFer
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Location: Home | Free Services | enCIFer | Downloads
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FAQs
Documentation
Welcome to the enCIFer download page. There is currently one version of enCIFer available:
enCIFer 1.3
This is the current release version of enCIFer
========== enCIFer ready ==========
Loaded dictionary: C:/Program Files/CCDC/enCIFer 1.3/dict/cif_ccdc.dic
Loaded dictionary: C:/Program Files/CCDC/enCIFer 1.3/dict/cif_core.dic
Loaded dictionary: C:/Program Files/CCDC/enCIFer 1.3/dict/cif_iucr.dic
Loaded dictionary: C:/Program Files/CCDC/enCIFer 1.3/dict/cif_ms.dic
Loaded dictionary: C:/Program Files/CCDC/enCIFer 1.3/dict/cif_pd.dic
Start
Mail...
2 W.
Win...
Ope...
4 F..
ma...
9:14 PM

Rigaku

Now COD is available for PDXL: Integrated Powder X-ray Diffraction Software!

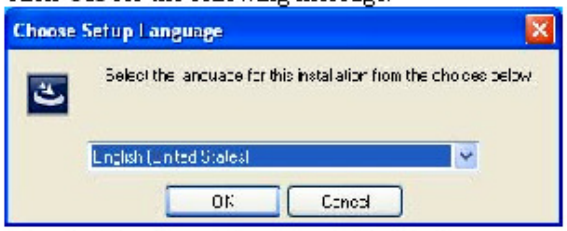
If you own PDXL, COD can be used along with phase identification in PDXL after installing the index file of COD which Rigaku provides. Please install it according to the following procedure.

NOTE: For any publications, including academic papers, presentations at conferences, etc. in which you report the results of phase identification, Rietveld analysis, etc. obtained using COD in PDXL, please make reference to:

> **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. Cryst.*, 2009, 42, 726-729.**

Installation:

1. Download the installer PDXLCODsetup.exe (778MB).
   

2. Execute it.
3. Click **OK** for the following message.
   

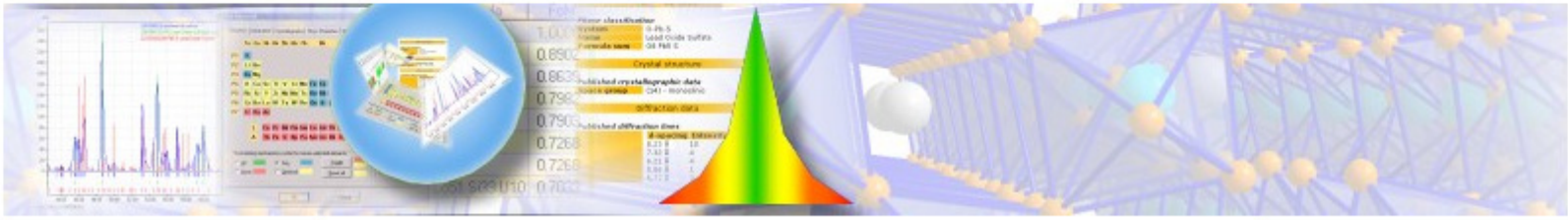
4. Wizard dialog box will appear. Click **Next**.
   

Match! - Phas...

www.crystalimpact.com/match/Default.htm

CRYSTAL IMPACT

About us | Diamond | Endeavour | Match! | Pearson's CD



About Match!

Function list...
Brochure...
References...

Get Match!

Order Now

Demo Version

Evaluate Match! with a time-limited demo version **free-of-charge**.

Reference Patterns

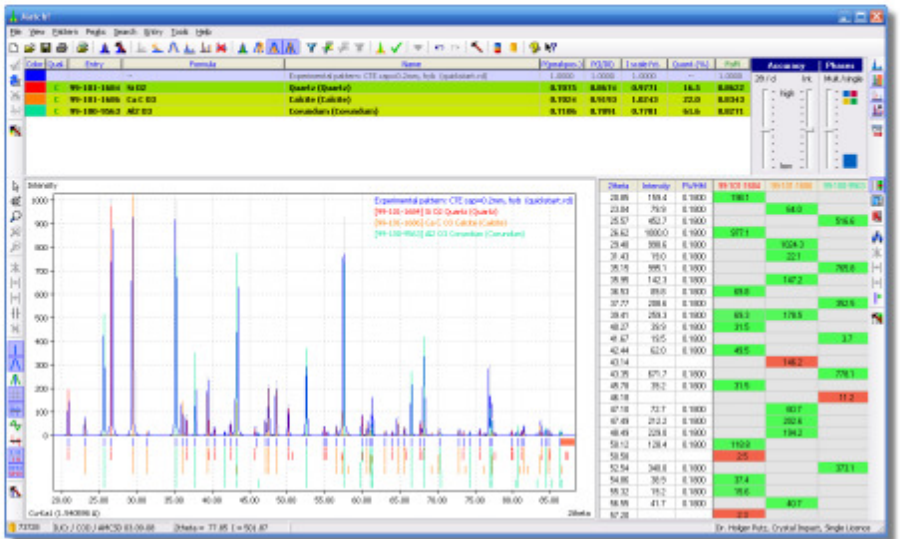
Download reference patterns calculated from the COD **free-of-charge**.

Support

Updates...
Tips & Tricks...
Known bugs...
Frequently Asked Questions...

Match!
Phase Identification from Powder Diffraction

Match! is an easy-to-use software for phase identification from powder diffraction data, which has become a daily task in material scientists work. Match! compares the powder diffraction pattern of your sample to a database containing reference patterns in order to identify the phases which are present. Single as well as multiple phases can be identified based on both peak data and raw (profile) data.
As reference database, you can apply the included **free-of-charge COD database** and/or **ICSD/Retrieve** (if you have a valid licence), use any **ICDD PDF** product, and/or create a user database based on your own diffraction patterns. The user database patterns can be edited manually, imported from peak files, calculated from crystal structure data (e.g. CIF files), or imported from your colleague's user database.
A list of Match!'s most prominent features can be found here.



Version 2 Preview

Jul 22, 2010
Get a detailed preview of **the best Match! you have ever seen!**
The upcoming new **version 2** will run not only on MS Windows but also on Mac OS X and Linux and offer a lot of new features. Read more...

Match! News

July 15, 2010
A **new Match! version 1.10a** has become available in which several bugs have been fixed. More...

July 12, 2010
A **new release of the COD reference database** (now containing more than **107,000 entries!**) has become available for download from here.

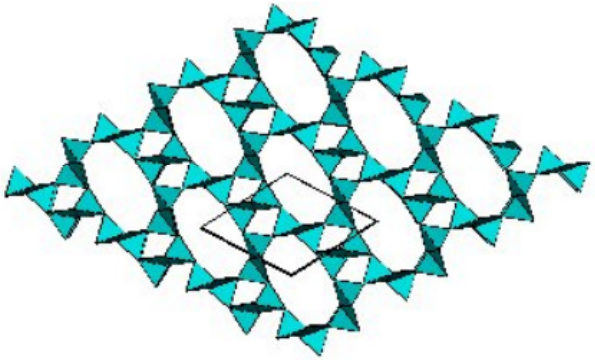
May 6, 2008
A **Match! tutorial in Spanish language** has become available, thanks to the efforts of **Prof. Santiago Rodríguez Almenar**. You can

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.

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).

Installing the P2D2-1 in EVA - Windows Internet Explorer

http://sdpd.univ-lemans.fr/cod/pcod/P2D2/EVA/index.html

Fichier Edition Affichage Favoris Outils ?

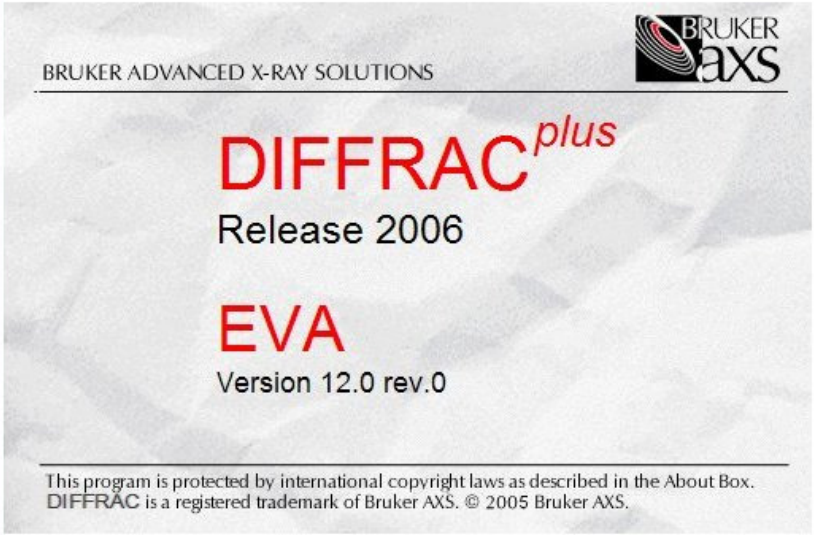
Installing the P2D2-1 in EVA

Installing the P2D2 in EVA

A. Le Bail - March 2008

Installation

0 - The DIFFRAC*Plus* 2006 version is necessary



Installing the P2D2-1 in EVA - Windows Internet Explorer

http://sdpd.univ-lemans.fr/cod/pcod/P2D2/EVA/index

Live Search

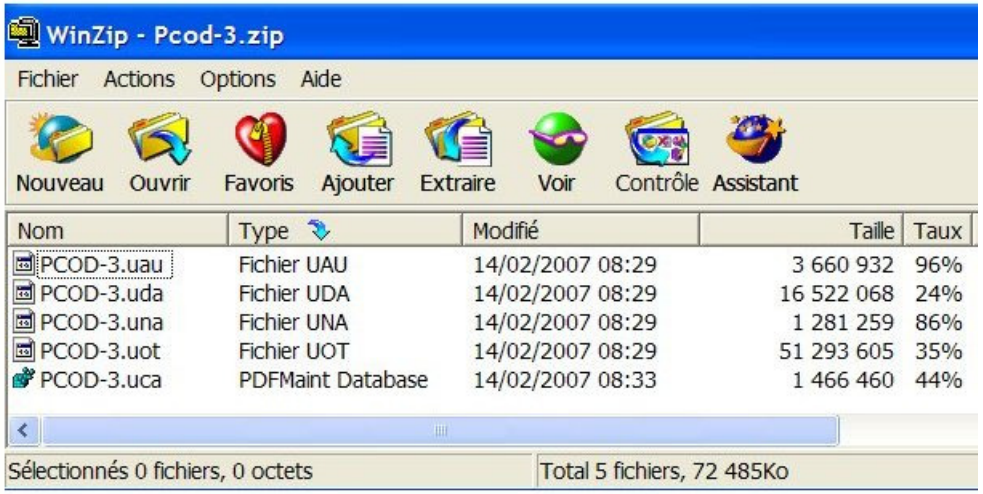
Fichier Edition Affichage Favoris Outils ?

Installing the P2D2-1 in EVA

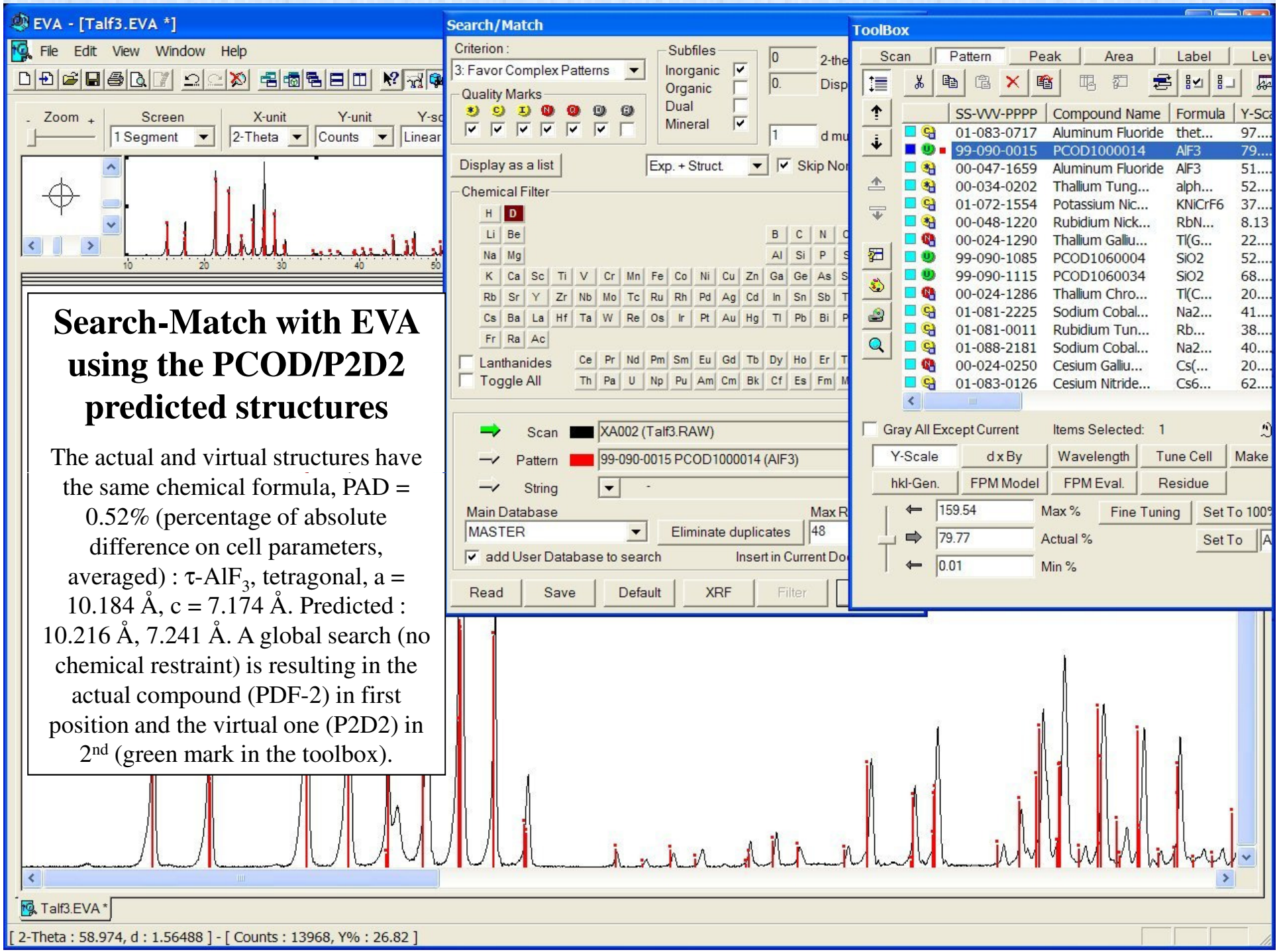
1- Download the binary files compressed into (72 Mo)

2- Unzip the 5 subfiles into the directory where is Eva.exe, generally at :

C:\DiffPlus

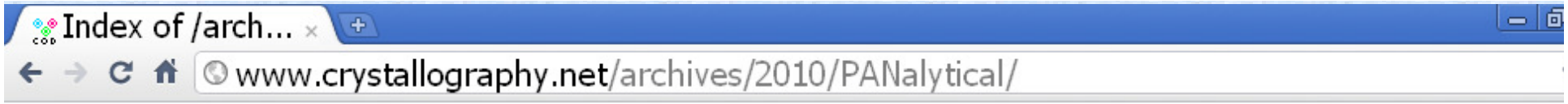


3- Start EVA, go to the settings, declare the PCOD-3.uca as being the U



Search-Match with EVA using the PCOD/P2D2 predicted structures

The actual and virtual structures have the same chemical formula, PAD = 0.52% (percentage of absolute difference on cell parameters, averaged) : τ-AlF_3, tetragonal, a = 10.184 Å, c = 7.174 Å. Predicted : 10.216 Å, 7.241 Å. A global search (no chemical restraint) is resulting in the actual compound (PDF-2) in first position and the virtual one (P2D2) in 2nd (green mark in the toolbox).



Index of /archives/2010/PANalytical

Name	Last modified	Size	Description
Parent Directory		-	
AmMin_April2010_4HS.zip	27-Apr-2010 08:31	39M	
AmMin_Jan2010_4HS.zip	04-Feb-2010 09:44	38M	
AmMin_Mar2010_4HS.zip	26-Feb-2010 14:17	38M	
COD_April2010_4HS.zip	27-Apr-2010 08:57	659M	
COD_Jan2010_4HS.zip	04-Feb-2010 16:16	618M	
COD_Mar2010_4HS.zip	26-Feb-2010 15:14	618M	
PANalytical.txt	03-Jun-2010 14:02	1.3K	
README.txt	03-Jun-2010 14:02	1.3K	
md5sum.dat	03-Jun-2010 14:05	490	
sha1sum.dat	03-Jun-2010 14:05	562	
wget-log	28-May-2010 08:58	62K	
wget-log.1	28-May-2010 09:31	1.0M	