3D Printing & Open Access Databases for Crystallographic College Education

Peter Moeck
Portland State University, pmoeck@pdx.edu

Jennifer Stone-Sundberg
Portland State University

Trevor J. Snyder
3d Systems Corporation

Werner Kaminsky
University of Washington - Seattle Campus

Saulius Gražulis
Institute of Biotechnology, Vilnius, Lithuania

See next page for additional authors

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Authors
Peter Moeck, Jennifer Stone-Sundberg, Trevor J. Snyder, Werner Kaminsky, Saulius Grazulis, and International Advisory Board of the Crystallography Open Database

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3D printing & open access databases for crystallographic college education

Peter Moeck¹, Jennifer Stone-Sundberg¹,², Trevor J. Snyder³,¹, Werner Kaminsky⁴, Saulius Gražulis⁵, and all members of the International Advisory Board of the Crystallography Open Database

¹ Nano-Crystallography Group, Department of Physics, Portland State University, Portland/Oregon
² Crystal Solutions, LLC, Portland/Oregon
³ 3D Systems Corporation, Wilsonville/Oregon
⁴ Department of Chemistry, University of Washington at Seattle
⁵ Institute of Biotechnology, Vilnius University, Vilnius, Lithuania

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Outline

1. Wikipedia entry and Crystallography Open Database (COD) in its 12th year

2. Supporting efforts at Portland State University in their 11th year

3. Converting Crystallographic Information Files (CIF) to 3D printing files (STL, VRML) – a few models to pass around, a selection of materials to print in from Quickparts.com

4. News from the 3D printing of crystallographic models community

5. Plans for Bicrystallography Open Database

6. Summary
Crystallographic database

A crystallographic database is a database specifically designed to store information about crystal lattices, in all three dimensions of space, a regularly repeating arrangement of atoms or molecules with long-range directional dependence. A crystal structure is a crystallographic database.

Crystallographic databases are typically determined from X-ray or neutron diffraction data. They are also identified by comparison of reflection intensities and 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 full crystal structure databases specializing in nanocrystals and can be identified in entries of a lattice-fringe fingerprinting database.

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

Advisory Board
Daniel Chateigner, Xiaolong Chen, Marco Ciriotti, Robert T. Downs, Saulius Gražulis, Werner Kaminsky, Armel Le Bail, Luca Lutterotti, Yoshitaka Matsushita, Peter Moeck, Peter Murray-Rust, Miguel Quiróz Olozábal, Hareesh Rajan, Alexandre F.T. Yokochi

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

as of Aug. 8, 11:20 am: 293,109 entries

NetWatch
edited by Mitch Leslie

Where Birds Count
The careful observation of birdwatchers is 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 copies seen in each week of the year and map the Ist-exotic-fauna haunts.

Schizophrenia Symposium
Find out the conclusions of the latest study comparing different and psychotropic drugs, track down a potential collaborator in Italy, or discover what led the Schizophrenia Research Association to adopt a new name. 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.

Dinosaur Name Game
Like the ancient beasts themselves, most of the names scientists have coined for dinosaurs over the last 2 centuries are derived from Latin names, and since many scientific names have been chosen by various researchers, some scientists believe that scientists need to be more careful when naming these species. As one way to address the issue, a researcher at the University of Chicago has created a new game that asks players to match the scientific name of a species with its common name. The game is designed to help players develop a better understanding of the scientific names used for dinosaurs and how they are used to classify different species. The game also includes a feature that allows players to vote on the accuracy of the name matches, which can help improve the accuracy of the names used for these species. The game is currently available online at www.sciensig.net and is free to play. The game aims to educate players about the importance of scientific names in the study of dinosaurs and to help them develop a better understanding of the taxonomic relationships between different species.
Neutron and x-ray structure refinements between 15 and 1083 K of piezoelectric gallium arsenate, GaAsO₄: temperature and pressure behavior compared with other α-quartz materials

Philippot, E'; Armand, P'; Yot, P'; Cambon, O'; Goiffon, A'; McIntyre, G J'; Bordet, P'

Journal of Solid State Chemistry
JSSCBI
146
1999
114
123
4.9940(1)
4.9940(1)
11.3871(4)
90
90
120
245.9
3
P 31 2 1
152
trigonal

Ga³⁺ 3.000
As⁵⁺ 5.000
### COD ID: 2017100

**Formula:** C5 H9 N O6 S -
**Comments:** Minkov, Vasily S.; Boldyreva, Elena V.

#### Acta Crystallographica Section C

**Crystal Structure Communications**

**Volume 65, Part 5 (May 2009)**

**organic compounds**

**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\(_3\)H\(_7\)N\(_2\)O\(_4\). The carboxylic group of the cysteinium cation, relative to the amino group. The crystal structure is built from cysteinium cations are connected to each other not direct semioxalate anions linked to each other via O-H...O hydrogen bonds.

**Formula:** C\(_3\)H\(_7\)N\(_2\)O\(_4\)\(^{+}\).C\(_2\)HO\(_4\)\(^{-}\)
The goal of this project is to provide interactive 3D visualizations of crystal structures and morphologies in order to help educate future materials scientists and engineers worldwide. This website is maintained by Portland State’s Nano-Crystallography Group and utilized for classroom demonstrations in introductory materials science and engineering as well as in introductory nano-science and nano-technology courses. All of our crystallographic data are in open access, i.e. freely available to anybody.

A link to the old frames-based open access crystallography site will be available at this position (on this page) in the future for backward compatibility.

Milestones:

- **February 2013**: 500 small molecule organic CIFs from the free Cambridge Crystallographic Data Centre Teaching Database were added to the local educational subset of the COD. (Acknowledgements of this source are in each individual CIF.) Manual cleaning of data sets.
- **November 2012**: New site interface using Django CMS, an open source Python based content management framework. The old site has been depreciated, but will be available for backward compatibility in the future.
- **June 2012**: Development of new Jmol display menu interface.
- **May 2012**: Updated PyCIFRW to version 3.3 and CIF dictionary to IUCr version 2.1.8. (CIF validation tools).
- **June 2008**: Wikipedia entry 'crystallographic database' written.
- **July-August 2007**: New version of Jmol supports stereo viewing, Wiki Crystallography Database and Crystal Morphology Database created.
- **July-August 2006**: General cleaning up of data, Nano Crystallography Database created.
Several crystallography databases are offered for browsing. You can search the databases, download and display the contained Crystallographic Information Files (CIFs), view 3D models of the encoded crystal structures and morphologies.

We also provide the North American mirror of the Crystallography Open Database (COD). This is the...
about 950 structures: inorganics, organics, a few proteins
**Include these elements:**

Select elements from periodic table. 

*Or enter properly formatted comma separated list ex: Si, O*

**Exclude these elements:**

Shift+Click elements from periodic table

**Strict number of elements:**

**Text (1 or 2 words):** sugar

**Unit Cell (UC) Volume (Å³) min:**

**UC Volume (Å³) max:**

**UC Edge a (Å) min:**

**UC Edge a (Å) max:**

**UC Edge b (Å) min:**

**UC Edge b (Å) max:**

**UC Edge c (Å) min:**

**UC Edge c (Å) max:**
Space group $P2_1$: A screw axis along the $b$ axis means there are 8 more screw axes parallel to [010], including one through the middle of the unit cell.
## Crystal Morphology Database

### Periodic Table

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>Li</td>
<td>Be</td>
<td>B</td>
<td>C</td>
<td>N</td>
<td>O</td>
<td>F</td>
<td>Ne</td>
<td>Na</td>
<td>Mg</td>
<td>Al</td>
<td>Si</td>
<td>P</td>
<td>S</td>
<td>Cl</td>
<td>Ar</td>
<td>K</td>
</tr>
</tbody>
</table>

**Include these elements:**

Select elements from periodic table.

Or enter properly formatted comma-separated list ex: Si, O

**Exclude these elements:**

Shift+Click elements from periodic table
Include these elements: Pt

Select elements from periodic table.

Or enter properly formatted comma separated list ex: Si, O

Exclude these elements:

Shift+Click elements from periodic table

Strict number of elements: 1

Text (1 or 2 words):

Unit Cell (UC) Volume ($\text{Å}^3$) min:

UC Volume ($\text{Å}^3$) max:
There are 4 results.

**Formula:** Pt
**Cell Parameters:** $a = 3.923\text{Å}, b = 3.923\text{Å}, c = 3.923\text{Å}$, $\alpha = 90.0^\circ, \beta = 90.0^\circ$
**Cell Volume:** $60.37\text{Å}^3$

[View CIF]  [View Structure in Jmol V12]  [View Morphology]
[View CIF]  [View Structure in Jmol (large window)]

**Formula:** Pt
**Cell Parameters:** $a = 3.923\text{Å}, b = 3.923\text{Å}, c = 3.923\text{Å}$, $\alpha = 90.0^\circ, \beta = 90.0^\circ$
**Cell Volume:** $60.37\text{Å}^3$

[View CIF]  [View Structure in Jmol V12]  [View Morphology]
[View CIF]  [View Structure in Jmol (large window)]

**Formula:** Pt
**Cell Parameters:** $a = 3.923\text{Å}, b = 3.923\text{Å}, c = 3.923\text{Å}$, $\alpha = 90.0^\circ, \beta = 90.0^\circ$
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[View CIF]  [View Structure in Jmol V12]  [View Morphology]
[View CIF]  [View Structure in Jmol (large window)]

**Formula:** Pt
**Cell Parameters:** $a = 3.923\text{Å}, b = 3.923\text{Å}, c = 3.923\text{Å}$, $\alpha = 90.0^\circ, \beta = 90.0^\circ$
**Cell Volume:** $60.37\text{Å}^3$

[View CIF]  [View Structure in Jmol V12]  [View Morphology]
[View CIF]  [View Structure in Jmol (large window)]
all good open access crystallography resources, e.g. CIFs, space group drawings, history, ...
prices for 3D printing will come down!
**Projet 4500** Multijet™ printer of 3D Systems Corporation, currently the only printer that produces color prints in durable plastics. $69,000 US

ColorJet Printing (CJP) technology platform and new class of durable VisiJet® C4 Spectrum plastics.

An inexpensive monochrome printer from 3D Systems Corporation (less than $1,000 US), on the basis of their Plastic Jet 3D printing technology.

One does not need to own a 3D printer, there are professional over-night print shops, e.g. [http://www.3dsystems.com/quickparts](http://www.3dsystems.com/quickparts)
*cif to *.stl

Open Access Resources for Crystallography Education in Interdisciplinary College Courses: Crystallographic Databases and 3D Printed Models

Peter Moeck1, Jennifer Stone-Sundberg1, Trevor J. Snyder1,2, and Werner Kaminsky3

1 Nano-Crystallography Group, Department of Physics, Portland State University, Portland, OR 97207-0751, U.S.A.; pmoeck@pdx.edu, jbs2@pdx.edu, and jensundberg@comcast.net
2 3D Systems Corporation, Wilsonville, OR, Trevor.J.Snyder@3dsystems.com, and t.snyder@pdx.edu
3 Department of Chemistry, University of Washington at Seattle; kaminsky@chem.washington.edu

ABSTRACT

Complementing a multitude of activities around the International Year of Crystallography, we report here on a few resources that are helpful for integrating basic crystallography into interdisciplinary college education. We concentrate on four resources with which we are directly involved: The Crystallography Open Database (COD) features currently more than 270,000 entries and has over the last decade developed into the world’s premier open-access source for the structures of small molecules and small to medium sized unit cell crystals. Educational offshoots of the COD with approximately a thousand entries combined provide structural information on small molecules, selected macromolecules, crystal structures, grain boundaries, and crystal morphologies in the well documented Crystallographic Information Framework (CIF) file format. This information can be displayed interactively on the websites and freely downloaded. Files that allow for the printing of selected database entries on any 3D printers have recently been added to these databases and can also be downloaded for free. These files were created with the program Cif2VRML and WinXMorph that convert CIF files directly into 3D printing files. Interested college educators are invited to visit our open access crystallography resource portal and suggest other resources that should receive wider exposure over this portal.

Fig. 5 3D printed models of (a) a caffeine molecule, (b) a C60 molecule, (c) a hemoglobin molecule in backbone representation and (d) unit cell representations of the cubic closest packing of equally sized spheres that can be used to demonstrate structural prototypes, e.g. halite and fluorite, which are derived from the copper prototype by fitting additional spheres of smaller sizes into the exposed tetrahedral and octahedral interstices.


Fig. 2a) Cif2VRML (16) screenshot with the sucrose molecule including hydrogen bonds. b) One of our very first printed 3D models with Werner, the creator of the conversion program, in the background (August 2011).

Fig. 3a) WinXMorph (17) screenshot for rendering crystal morphologies, sucrose as example. b) Printed out sucrose 3D morphology models in Jennifer’s hand (March 2014).

W. Kaminsky et al., One-click preparation of 3D print files (*.stl, *.wrl) from *.cif (crystallographic information framework) data using Cif2VRML, Powder Diffraction, accepted
P. Moeck et al., Enlivening 300 level general education classes on nanoscience and nanotechnology with 3D printed crystallographic models, J. Mater. Education, accepted

converted from CIF to STL with Cif2VRML and WinXMorph

designed with a CAD program
sucrose (with hydrogen bonds)

deoxyribonucleic acid
(containing a planar phenoxyazine-derived bi-functional spectroscopic probe)

all printed from CIFs converted to *.wrl (say ‘vormel’) in durable VisiJet® C4 Spectrum plastics with ProJet 4500

chlorophyll
1998

Timothy Herman:
"I was so intrigued with the technology that I left my position at the Medical College of Wisconsin and opened the ... “

in Milwaukee.
http://cbm.msoe.edu/

J. Graber, 3D Printer World, December 9, 2013

RP Rasmol, exports STL and VRML

**Jmol** & **JSmol**
(Robert Hanson & coworkers)


"Models function as thinking tools that stimulate questions and are a key component of the Next Generation Science Standards".
3D Printing Crystal Structure Research Groups

Posted on July 23, 2014 by vfscalfani

 Bookmark the permalink.

Research Groups

Amar Flood (Indiana University Bloomington)
Dean J. Tantillo (University of California, Davis)
Leroy Cronin (University of Glasgow)
Marvin L. Hackert (University of Texas at Austin)
Peter Moeck (Portland State University)
Ronald Zuckerman (Lawrence Berkeley National Laboratory)
Tim Herman (Center for BioMolecular Modeling)
Vincent F. Scalfani (University of Alabama)

Bookmark the permalink.
Welcome to the 3D Printing Crystallography Community Website! The purpose of this website is to provide a collection of resources related to 3D printing crystal structures.

3D Printing Crystal Structure Listserv

We have an active listserv [3DP-XTAL] hosted by The University of Alabama for discussion related to the 3D printing of crystal structures. If you would like to be added to this listserv, send an email to:

3DP-XTAL-request@LISTSERV.UA.EDU

3D Printing Crystal Structure Related Wiki Pages

Publications
Repositories
Research Groups
Software
NIH 3D Print Exchange

3D model repository for biomedical related 3D print files. Files include custom labware, proteins, macromolecules, cells, and organisms.

NIH 3D Print Exchange

RSC Crystal Data Repository (coming soon)

3D model repository for small molecules and solids. There are currently ~30,000 STL and WRL files that are searchable by name, formula, structure, SMILES, and InChl code.

Bookmark the permalink.
Biennial Conference on Chemical Education (BCCE), August 4, 2014, Allendale, Michigan
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
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.”


CeO$_2$ $\Sigma = 5$ $(310)/[001]$ $36.9^\circ$ tilt boundary, viewed down [001], black white (two color) layer group $p21’$ $am’$

diamond, $\Sigma = 5$ $(310)/[001]$ $36.9^\circ$ tilt boundary, viewed down [001], black white (two color) layer group $p21’$ $am’$

two color layer group $c2’$ $mc’$ – a genuine back-white group, polar physical properties can exist

two color layer group $c2’$ $mm’$ – a genuine back-white group, polar physical properties can exist


CeO$_2$ $\Sigma = 5$ $(310)/[001]$ $36.9^\circ$ tilt boundary, viewed down [001], black white (two color) layer group $p21’$ $am’$

diamond, $\Sigma = 5$ $(310)/[001]$ $36.9^\circ$ tilt boundary, viewed down [001], black white (two color) layer group $p21’$ $am’$

two color layer group $c2’$ $mc’$ – a genuine back-white group, polar physical properties can exist

two color layer group $c2’$ $mm’$ – a genuine back-white group, polar physical properties can exist


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

Aberration-corrected translation-symmetry averaged STEM Z-contrast imaging …

only pure O columns are located at interface

only pure O columns are located at interface

SrTiO$_3$ $\Sigma = 13a$, (510)/[001], 22.6° tilt boundary in [001] projection, sectioned at 1/4
[510], large disks Sr columns, medium disks pure O columns, small disks mixed O and Ti columns
some 350,000 – 400,000 CIFs in open access crystallographic databases

COD in its 12th year, more than 293,000 CIFs

EDU-COD in its 11th year, CMD in its 7th year, approx. 1,000 CIFs total

programs for conversion of CIF (molecule structures, crystal morphologies, grain boundaries, … ) to STL and VRML by Werner Kaminsky http://cad4.cpac.washington.edu/, (color printing only from VRML files)

programs are free for individuals, license from UW for all commercial purposes

3D printing will come down in price significantly, good for hands-on models in class

plans for Bicrystallography Open Database

open access crystallography resource portal, nanocrystallography.net

simply google for “open-access crystallography”
related presentations

Chemical information presentation in the Crystallography Open Database, Andrius Merkys, … and Saulius Gražulis
poster A566, 8/07/2014, 18:30-20:30  CC.P25.A566 (C1710)

Launching the Theoretical Crystallography Open Database, Saulius Gražulis …

COD at the Software Fayre (Fair), Saulius Gražulis and Andrius Merkys, … 8/8/2014, 11:00 – 11:45, room 519b

3D printing of crystallographic models from open access databases, Werner Kaminsky, … and Peter Moeck
poster B422, 8/11/2014, 18:30-20:30  MS84.P08.B422 (C1278)
Leroy Cronin:

“I don’t want chemistry reduced to plastic trinkets, I want new science to occur as a result of use of ubiquitous 3-D printing and molecular design.”

Merci beaucoup pour votre attention!

Thank you very much indeed for your attention!
our first two 3D print files in open access (April 2014)
access statistics: nanocrystallography.research.pdx.edu, June 1, 2012 to July 31, 2014
Caffeine right/large and in Werner’s hand: printed with the so called Z-corp (MIT) technique, dried colored gypsum water mixture dipped into superglue (now ZPrinter series of 3D Systems Corporation, approximately $0.25 US per printed cubic centimeter, but models tend to be a bit fragile).

left/small printed with a ProJet 4500, the utilized proprietary plastic is much more durable

W. Kaminsky et al., One-click crystallographic information framework) data using Cif2VRML preparation of 3D print files (*.stl, *.wrl) from *.cif, Powder Diffraction, accepted
a few 3D printers read *.wrl files (VRML format, say ‘vormel’)

*Herapathite*, the molecule behind the early fortune of the Kodak company