

**Crystal structure visualizations in three dimensions with support from the open access
Nano-Crystallography Database**

P. Moeck^{1*? ♠}, O. Certík^{1,2}, G. Upreti¹, B. Seipel^{1♠}, M. Harvey³, W. Garrick³, and P. Fraundorf⁴

¹ Department of Physics, Portland State University, P.O. Box 751, Portland, OR 97207-0751,
* pmoeck@pdx.edu, phone: 503 725 4227, fax.: 503 725 9525; [?] Advisory Board of the
Crystallography Open Database, <http://crystallography.net>; ♠ Oregon Nanoscience and
Microtechnologies Institute (ONAMI), <http://www.onami.us>,

² Faculty of Mathematics and Physics, Charles University of Prague, Ke Karlovu 3, 121 16
Praha, The Czech Republic

³ Academic & Research Computing for Instruction and Research Services and the Office of
Information Technology, Portland State University, Portland, OR 97201

⁴ Department of Physics and Astronomy and Center for Molecular Electronics, University of
Missouri at St. Louis, MO 63121

ABSTRACT

Crystallographic databases for inorganic materials that are freely accessible over the internet are reviewed. The Nano-Crystallography Database project is described. Instructions are given on how to visualize in three dimensions the atomic arrangements of several thousand entries of the Crystallography Open Database.

Keywords: Open Access, Crystallography, Databases

1. INTRODUCTION

Courses in materials science and engineering, crystal physics, crystal chemistry, and mineralogy typically employ two-dimensional sketches of the atomic arrangement in crystal structures and unit cells. The chapter on ideal crystal structures of the widely used introductory materials science and engineering text by Schaffer et al.¹ contains for example 14 such sketches. Textbooks on mineralogy contain a much larger number of such sketches (e.g. Hibbard's text² features a picture with more than ten ball-and-stick models on the dedication page and approximately one hundred sketches of atomic arrangements in crystal structures and unit cells in the body of the text). Physical three-dimensional models of crystal structures and unit cells are also popular. While academic departments in the developed part of the world may possess some tens of such three-dimensional models and allow their students to explore those hands on, their counterparts in the developing part of the world may consider such models too expensive and fragile for class room usages.

To help remedying this situation we made a survey on crystallographic databases that are freely accessible on the internet and also started our own nano-crystallography database project with on

line three-dimensional (3D) visualizations of ideal and real structures. This paper reports on both the results of the survey and our ongoing project.

2. FREE INTERNET ACCESSIBLE CRYSTALLOGRAPHIC DATABASES

Fifteen years after the development of the World Wide Web, there is already a variety of internet based free-access crystallographic databases. We discuss in this paper the subset of free databases that includes or primarily deals with inorganic crystals.

The free database MINCRYST³ is maintained and hosted by the Russian Academy of Sciences and contains more than 6,000 entries for minerals from which X-ray powder diffractograms can be calculated on the fly. 3D visualization of the entries are provided by means of the java-based freeware program “Jmol”⁴. The Naval Research Laboratory’s Center for Computational Materials Science provides a free on-line database for education and research support under the name “Crystal Lattice Structures”⁵. Currently this database contains 254 entries in 90 space groups. Visualizations of the entries are also provided by Jmol applets. The “Reciprocal Net” is a distributed database of molecular structure information and its main web site is hosted at Indiana University at Bloomington⁶. Information from approximately 400 common molecules (and crystal structures) can be downloaded in the standard Crystallographic Information File (CIF)^{7,8} format (file extension *.CIF). 3D visualizations of these common molecules (and crystal structures) are provided by a range of Java based applets.

Since its adoption in 1990 by the International Union of Crystallography as the standard file format and syntax for communicating crystallographic information between both human beings and computers and between different kinds of software programs and computers, CIF has become a crystallographic entity in its own right of such a significance that a volume of the latest edition of the International Tables for Crystallography⁸ is dedicated to describing it comprehensively. A free on-line check of the syntax of CIFs is provided by the International Union of Crystallography at the URL given in ref.⁹

The free on-line American Mineralogist Crystal Structure Database (AMCSD) was erected in 2003 and contains more than 8,000 critically evaluated entries^{10,11}. Files can be downloaded from this database in CIF and the American Mineralogist Crystal data format (file extension *.amc). A range of PC based freeware programs, for e.g. the visualization of crystal structures (XtalDraw) and for the calculation of powder X-ray and neutron diffractograms (XPow), is available for downloading from the AMCSD site at ref.¹². The database is maintained under the care of both the Mineralogical Society of America and the Mineralogical Association of Canada. Ref.¹⁰ states that approximately 75 % of the submitted manuscripts to the journals “American Mineralogist” and the “Canadian Mineralogist” possess errors of one sort or another. (For comparison, ref.¹³ states that about 40 % of the CIFs received for inclusion into the commercial Cambridge Structural Database contain errors that arise mainly from the manual editing of these files by their authors.) The critical evaluation of data to be included in a crystallographic database is, therefore, a major concern for both commercial and free databases.

Records of approximately 24,000 full crystal structure determinations in the form of CIFs are freely accessible on-line at the Crystallography Open Database (COD)^{14,15}. This database was also started in 2003 and is rapidly growing as more and more crystallographers and scientific institutes/societies/academies donate their collections of CIFs and upload them over the internet so that anybody with access to the World Wide Web can access them for free. The COD also contains all the data sets that are in the AMCSD. An approximately 2,000 entry subset of the COD is named PCOD for Predicted Crystallography Open Database^{14,15} and allows 3D displays

of structural polyhedra and wire frames in the so called Virtual Reality Modeling Language (VRML)¹⁶ format by using common (HTML based) web browsers (if necessary with plug-ins such as COSMO¹⁷ player).

The long term objectives of the COD initiators are summarized on the COD web page¹⁵ as: (i) providing free access to comprehensive crystallographic data (including the atomic coordinates) on all known inorganic, metallic, organometallic and organic crystalline compounds and (ii) complementing the existing commercial databases (which typically specialize on only one or two classes of crystals and contain in addition to crystallographic information a range of physical properties). Another major concern of the COD initiators is supporting crystallographers in emerging countries. By providing the opportunity to check rapidly and early on in an investigation (i.e. already after the cell parameters have been determined) if the structure of the particular crystal under investigation has already been solved, the COD also helps increasing the productivity of structure determinations world wide. To insure a high quality of the data entries, the policy of the COD is that only those CIFs that result from structure refinement software can be uploaded by the general public.

3. THE NANO-CRYSTALLOGRAPHY DATABASE PROJECT AND VISUALIZATION OF CRYSTAL STRUCTURES IN THREE DIMENSIONS

As a complementary project with a similar philosophy to both the COD and the AMCSD, the nanocrystallography group at Portland State University started in 2005 the Nano-Crystallography Database (NCD) project¹⁸. Since structure and morphology of nanocrystals are crucial to their physical properties, the NCD is collecting entries on both the full structure (including atomic coordinates) and the typical morphology (tracht and habit) of inorganic nanocrystals in the form of CIFs. The experimental morphological information that is collected in the "Bestimmungstabellen für Kristalle"¹⁹ will be the first to be included in the NCD. Since we consider the surface of nanocrystals and the possible presence of single or multiple twins as important real structure, the NCD project will collect and later on display such information as well (together with visualizations of other important crystal defects).

As many electron microscopist work on rather simple inorganic structures, we are writing and uploading CIFs to support their work. A good starting point for this are the descriptions of the about 150 full structure determinations in the second edition of Wyckoff's classical reference book "Structure of Crystals"²⁰. To insure a high quality of the data entries, we provide a comprehensive on-line syntax check for CIFs²¹. Only those CIFs that pass both this test and the test that is available at the IUCr web site⁹ will be uploaded to the NCD.

Since the NCD is being developed to support not only materials science education but also image-based nanocrystallography in general (i.e. methods that determine both structure and morphology of nanocrystals from images²²⁻²⁶ taken in transmission electron microscopes), visualizations in 3D of the entries in this database are crucial. For a start, we provide 3D visualizations²¹ by means of Jmol applets for the structural information that is contained in the entries of the COD, Figs. 1 to 5. Next we will work on providing visualizations of the morphological information that will be contained in the entries of the NCD by means of the program "XMorph"²⁷. Fig. 1 shows the opening screen of the website that hosts our local version of the COD. The menu entries are self explanatory and read from top to bottom: *Search the Database, Upload Data, Check syntax errors* and *Insert symmetry equivalent positions*.

Fig. 2 shows the search screen that is accessible from the opening screen, Fig. 1. The elements Au and K were entered into this screen to conduct a search for all the entries that contain these two elements together in one crystal phase. Fig. 3 shows the result screen for the search for the simultaneous presence of Au and K. By clicking on *CIF file* for the second entry in this list, the respective CIF is displayed on the user's computer with the program he or she may select for this purpose. The text editor "Notepad" can be employed to display (and edit) CIFs, but the free program "enCIFer" was specifically designed for the display, editing, and for syntax checks of CIFs. This program can be downloaded for all common platforms at ref.²⁸. Using enCIFer, Fig. 4 shows the CIF for As₂AuK₅.

Fig. 5 finally shows the 3D visualization of the As₂AuK₅ structure in Jmol. Alternatively, the *asymmetric unit* (which is typically just one molecule in molecule crystals) can be displayed. By clicking on *3 x 3 x 3 unit cells*, the content of nine unit cells can be displayed at once. There are options to display only the atoms or the atoms together with a sketch of the unit cell superimposed on the atoms. The unit cell parameters are listed in addition when a structure is displayed with the latter option. As with any Jmol applet, one can zoom into the display of the atomic arrangement by using the Shift key together with the mouse. A range of tools that allow, for example, for the measurement of distances between atoms or the bond angles between three atoms are accessible by a left mouse click directly onto the Jmol structure display. (To display the 3D visualizations with Jmol, the internet browser must support Java 1.4. If not already installed within the browser, the JAVA™ 2 platform is available for free at ref.²⁹.)

The actual visualization of a COD database entry in three dimensions is obtained by turning the displayed atomic arrangement, e.g. Fig. 5, around three mutually perpendicular axes by clicking on *Rot X*, *Rot Y*, and *Rot Z*. Rotations by 45 degrees are default, but arbitrary rotations (with a negative or positive sign) can be realized by either entering the desired rotations in the respective boxes of the rotation menu or by moving the mouse. The option to *Reset to (the) original orientation* also exist.

In the future, we will add to the NCD both interactive 2D fringe fingerprint plots^{25,26} and more crystallographic functionality to the 3D display of structures in order to provide on-line support for image-based nanocrystallography²²⁻²⁶. The NCD shall then become a free internet based research support tool for electron microscopists in addition to providing world wide support for materials science and engineering, crystal physics, crystal chemistry, and mineralogy education.

SUMMARY

Crystallographic databases for inorganic materials that are freely accessible over the internet were reviewed. The objectives, current state of the affair, and future directions of the Nano-Crystallography Database project were described. Instructions were provided on how to visualize the atomic arrangements in three dimensions for several thousand crystals for which entries exist in the Crystallography Open Database.

ACKNOWLEDGMENTS

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29. <http://www.java.com/en/download/index.jsp>

About the authors

Peter Moeck is a German-British crystallographer (with more than 20 years of experience in the structural characterization of semiconductors by complementary methods) and currently an Assistant Professor at Portland State University (PSU). In the late 90s he and Phil Fraundorf (a Professor at the University of Missouri at Saint Louis) laid the foundations of image-based nanocrystallography and transmission electron goniometry, i.e. methodologies that can be used with the current generation of high resolution (HR) transmission electron microscopes (HRTEMs), but become much more viable with the wider availability of aberration-corrected TEMs. Peter also volunteers some of this time to services on the international Advisory Board of the Crystallography Open Database. Ondrej Certík is a Czech undergraduate physics student, worked over the summer of 2005 in Peter's research group, and wrote the parser that allows the 3D visualization of CIFs with Jmol. Girish Upreti is a Nepalese graduate physics student in Peter's research group and writes CIFs of simple inorganic structures for uploads to both the COD and the NCD. Bjoern Seipel is a German powder X-ray crystallographer, Adjunct Assistant Professor at PSU, and member of Peter's research group. He writes the software to calculate fringe fingerprint plots from CIFs. Will Garrick heads PSU's Office of Academic & Research Computing for Instruction and Research Services, which kindly provides the infrastructure for this project. Morgan Harvey is an undergraduate student of Computer Science at PSU and works for Will's office. Morgan and Will were instrumental in designing the web pages for this project and provide high level programming support.

Nanocrystallography Visualizations : Crystallography Open Database - Mozilla Firefox

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http://nanocrystallography.research.pdx.edu/cod/

DSPAM v3 Control C... JMOL Ondřej Čertík slovník.cz - Multilingu... JMOL Python Library Refer... CIF file checker

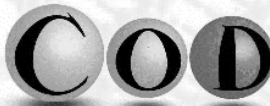
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Fig. 1

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Search

Output limited to 300 entries maximum, see the [hints and tips](#)

Search by physical properties:

Text (1 or 2 words)

With these elements

Without these elements

Minimum and Maximum volume

Strict number of elements

Search by cell parameters:

a (min - max)

b (min - max)

c (min - max)

α (min - max)

β (min - max)

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Fig. 2

Nanocrystallography Visualizations : Open Crystallography Database : Search Results - Mozilla Firefox

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http://nanocrystallography.research.pdx.edu/cod/result.php

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Result : There are 6 entries in the selection Searching elements including Au K

[CIF file](#) Formula : - P 1.00 Au 1.00 K 2.00 -
Comments : Eisenmann, B Klein, J Somer, M Crystal structure of dipotassium catena-phosphidoaurate Zeitschrift fuer Kristallographie (149,1979-) 197 (1991) 277 278
[show](#)
Space group : C m c m
Cell volume: 446.40
Cell parameters: 9.7870 ; 7.3950 ; 6.1680 ; 90.000 ; 90.000 ; 90.000

[CIF file](#) Formula : - As 2.00 Au 1.00 K 5.00 -
Comments : Eisenmann, B Klein, J Somer, M Linear anions (CuAs₂)₅-, (AuP/2)₅- and (AuAs₂)₅- in potassium compounds Journal of Alloys Compd. 178 (1992) 431 439
[show](#)
Space group : P 63/m m c
Cell volume: 546.40
Cell parameters: 5.7300 ; 5.7300 ; 19.2160 ; 90.000 ; 90.000 ; 120.000

[CIF file](#) Formula : - P 2.00 Au 1.00 K 5.00 -
Comments : Eisenmann, B Klein, J Somer, M Linear anions (CuAs₂)₅-, (AuP/2)₅- and (AuAs₂)₅in potassium compounds Journal of Alloys Compd. 178 (1992) 431 439
[show](#)
Space group : P 63/m m c
Cell volume: 514.90
Cell parameters: 5.6360 ; 5.6360 ; 18.7160 ; 90.000 ; 90.000 ; 120.000

[CIF file](#) Formula : - H 4.00 O 2.00 Au 1.00 Br 4.00 K 1.00 -
Comments : Cox, E G Webster, K C The Stereochemistry of Quadricovalent Atoms: Tervalent Gold Journal of the Chemical Society 1936 (1936) 1635 1637
[show](#)
Space group : P 1 21/a 1
Cell volume: 479.90
Cell parameters: 9.5100 ; 11.9300 ; 4.2300 ; 90.000 ; 90.000 ; 90.000

No CIF Formula : - Au 5.00 K 3.00 Pb 1.00 -
Comments : Zachwieja U; Wlodarski J - K3Au5Pb: Layers of (2)(infinity)[AuAu3/2] gold tetrahedra and (1)(infinity)[Pb-2/2] lead chains - ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE 624 (1998) 1569-1572
Space group : Imma

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Fig. 3

1008878.cif - enCIFer

File Edit Search Tools Help

Blocks: 1

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1 |data_1008878
2 |_chemical_name_systematic      'Pentapotassium diarsenidoaurate'
3 |_chemical_formula_structural   'K5 (Au As2)'
4 |_chemical_formula_sum         'As2 Au K5'
5 |_publ_section_title
6 |
7 |Linear anions (CuAs2)5-, (AuP7)5- and (AuAs2)5- in potassium compounds
8 |
9 |loop_
10|_publ_author_name
11| 'Eisenmann, B'
12| 'Klein, J'
13| 'Somer, M'
14|_journal_name_full             'Journal of Alloys Compd.'
15|_journal_codens_ASTM          JALCEU
16|_journal_volume               178
17|_journal_year                 1992
18|_journal_page_first           431
19|_journal_page_last            439
20|_cell_length_a                5.730(2)
21|_cell_length_b                5.730(2)
22|_cell_length_c                19.21599(400)
23|_cell_angle_alpha             90
24|_cell_angle_beta              90
25|_cell_angle_gamma             120
26|_cell_volume                  546.4
27|_cell_formula_units_Z         2

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Editor Visualiser

Errors - none
Warnings - none
Remarks - none

Loaded dictionary: /home/ondra/encifer/encifer_1.1/dict/cif_rho.dic
Starting new file "untitled1.cif"
Reading CIF "1008878.cif"
Read 80 lines.
No errors, warnings or remarks.

Line 1, Column 1

USA 1008878.cif - enCIFer Sun Aug 28, 14:26

Fig. 4

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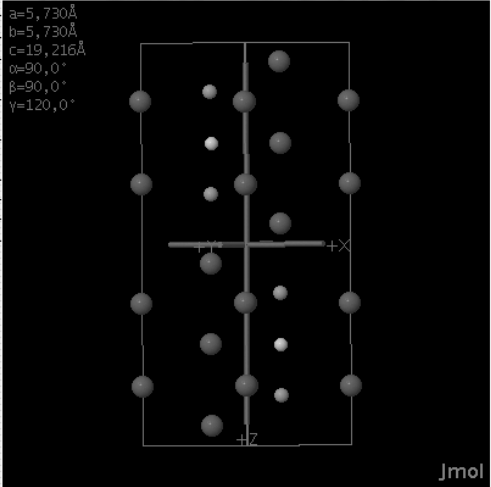
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Showing file '1008878.cif' in a Jmol applet.

$a=5,730\text{\AA}$
 $b=5,730\text{\AA}$
 $c=19,216\text{\AA}$
 $\alpha=90,0^\circ$
 $\beta=90,0^\circ$
 $\gamma=120,0^\circ$



45 45 45 show unit cell

Rot X Rot Y Rot Z

Reset to original orientation mode 1 - asymmetric unit mode 2 - primitive cell mode 3 - conventional cell

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Fig. 5

Fig. 1: Screenshot of the opening screen of the website that hosts our local version of the COD.

Fig. 2: Screenshot of the search screen with entries for the elements Au and K.

Fig. 3: Screenshot of the results of the search for the simultaneous presence of the two elements Au and K.

Fig. 4: Screenshot of the CIF of the second entry in the result list of Fig. 3 displayed by the LINUX version of the free program “enCIFer”²⁸.

Fig. 5: Screenshot of the visualization screen for one unit cell of As_2AuK_5 displayed by Jmol.