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CAMBRIDGE STRUCTURAL DATABASE

Access / Logon

Library Access:

Start Menu → Programs → Cambridge Crystallographic Data Centre → X Windows

Password: ccdc@lib At prompt, enter: cq (or: autoseqcq) for ConQuest

To exit: logout

Lab/Office access: <http://ccdc.caltech.edu/docs/index.html>

Database Description

(see: [Acta Cryst. \(2002\). B58, 380-388](#))

The Cambridge Structural Database (CSD) <http://www.ccdc.cam.ac.uk/products/csd/> contains structural information on over 330,000 carbon containing molecules (<1000 atoms) and over 366,000 structures, including organics, see: [Acta Cryst. \(2002\). B58, 407-422](#), compounds of main group elements, organometallics and metal complexes, see: [Acta Cryst. \(2002\). B58, 398-406](#). There is a small overlap between the CSD and the Inorganic Crystal Structure Database, see: [Acta Cryst. \(2002\). B58, 364-369](#), in the area of molecular inorganics.

Life science applications, see: [Acta Cryst. \(2002\), D58, 879-888](#), are exemplified by the crystal structures of the major and minor amino acids and numerous small peptides, and the CSD is a very convenient way to search for structural characterized (non-protein) peptides according to their amino acid sequence. The CSD has recently increased the size limit for polymeric compounds to < 25 residues. Higher oligomers are covered by the [Protein Data Bank](#), see [Acta Cryst. \(2002\). D58, 899-907](#). The CSD covers mono-, di- and tri-nucleotides; higher oligomers are covered by the [Nucleic Acids Database](#), see: [Acta Cryst. \(2002\). D58, 889-898](#).

The CSD reflects the published literature. It is fully retrospective (1923+) and is updated on a current basis. All information is abstracted from primary journals and associated supplementary information in both hard-copy and electronic forms. The CSD is the official depository for crystal structure data for more than 50 journals.

Each CSD entry contains the following information: Author/Journal, Chemical name/properties, Crystal data, Experimental data, Structural diagram, 3D Visualizer.

ConQuest, see: [Acta Cryst. \(2002\). B58, 389-397](#), is a program for searching and retrieving information from the Cambridge Structural Database (CSD). ConQuest, in addition to structure drawing, provides a full range of text/numeric search options (e.g. Author, Journal, Compound name, Formula, Space group, Unit cell, Density, etc).

This latest release of the software incorporates the IsoStar and Mogul programs. IsoStar stores knowledge about intermolecular interactions in the form of scatterplots. Each scatterplot shows the distribution of a contact group (for example, an O-H donor group) around a specific central group (for example, a charged carboxylate group) displayed in a RasMol window. Mogul provides easy access to information on the preferred values of bond lengths, valence angles and acyclic torsion angles, using data derived from the CSD.

CSD - Documentation / Tutorials

Brief tutorials are listed under the 'HELP' on the 'Conquest' menu page

Full Documentation and tutorials are available at:

http://www.ccdc.cam.ac.uk/support/csd_doc/zdocmain.html

User support is available at Caltech's X-ray Facility: <http://www.its.caltech.edu/~bi/bicatalog.html#xray>

WebCite is a database of published research applications of the Cambridge Structural Database and other CCDC products. http://www.ccdc.cam.ac.uk/free_services/webcite/

Literature references for CSD products: http://www.ccdc.cam.ac.uk/support/product_references/

ICSD (Inorganic Crystal Structure Database)

<http://icsdweb.fiz-karlsruhe.de/>

The ICSD is a comprehensive collection of crystal structure data for solid state inorganic compounds, such as simple salts, silicates, oxides, etc. It contains more than 76,000 entries and covers the literature from 1915 to the present. (see: [Acta Cryst. \(2002\). B58, 364-369](#))

Web based searching by empirical formula (elements = **Y Ba₂ Cu₃ O**), ANX formula (**AB₂C₃X₇**), mineral names, crystal data and author names, etc. (see: [Acta Cryst. \(2002\). B58, 370-379](#))

Powder Diffraction File

<http://www.icdd.com/>

SFL CIRCULATION DESK - Laptop #1

PDF-4/Full File 2004 contains over 163,000 entries and includes data originating from ICDD sources and collaborations with FIZ and NIST. The compilation includes metals, minerals, inorganic compounds, and experimental organic compounds. It has been edited to include over 30 searchable diffraction and physical property fields, plus experimental preparation and literature citations.

Searches can be limited to subfiles (inorganics, minerals, ceramics, metals & alloys, etc.).

Search empirical formulas or elements selected from a periodic table, mineral or zeolite names or classifications, properties/structures (Pearson symbol code, space groups, color, density, MP) or author names ... (see: [Acta Cryst. \(2002\). B58, 325-332](#)) and ([Acta Cryst. \(2002\). B58, 333-337](#))

A history of the PDF is given at: <http://www.icdd.com/products/ICDD.PDF>

American Mineralogist Crystal Structure Database

<http://www.geo.arizona.edu/AMS/amcsd.php>

A crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, and the European Journal of Mineralogy. Data from Physics and Chemistry of Minerals is currently being added. Search with mineral, author or element names, or cell parameters. A description of the database was published in the [Am. Mineral. \(2003\), 88, 247-250](#).

Database of Zeolite Structures

<http://www.iza-structure.org/databases/>

Crystallographic data and drawings for all zeolite framework types, simulated powder patterns for representative materials and relevant references.

Biological Macromolecule Crystallization Database

<http://www.bmcd.nist.gov:8080/bmcd/bmcd.html>

The BMCD (see: [Acta Cryst. \(2002\). D58. \(916-920\)](#)) includes 3547 crystal entries from 2526 biological macromolecules including proteins, protein-protein complexes, nucleic acid, nucleic acid-nucleic acid complexes, protein-nucleic acid complexes, and viruses and the NASA Protein Crystal Growth Archive which includes crystallization data generated from studies carried out in a microgravity environment.

CrossFire (Beilstein / Gmelin)

<http://library.caltech.edu/publications/beilstein/default.htm>

Library: Start Menu → Programs → MDL Crossfire Commander V6

Beilstein and Gmelin are separate databases, and contain data for over 9.4M organic compounds and nearly 2M inorganic/organometallic compounds, respectively. They are searchable by structure, physical property, reaction and bibliographic data. Crystal structure determinations are grouped under Crystal Phase (Beilstein) and Crystal Structure (Gmelin).

SciFinder Scholar

<http://library.caltech.edu/publications/scifinder/>

Library Workstations: Start Menu → Programs → SciFinder Scholar ...

Following a chemical substance search, click 'Get References'. One of the options is to limit retrieval to records that mention 'crystal structure'. This may not be compound specific as retrieval is based on the indexing of the whole article. SciFinder Scholar = Chemical Abstracts ... plus cover-to-cover indexing of 1,350 key chemical journals since Oct. 1994+ ... plus bibliographic information from both 'electronic' articles and from US, EP, WO patents (including machine translated abstracts for JP and DE patents), prior to full CA indexing.

Crystallography Open Database

<http://www.crystallography.net/>

Intended as a light version of the crystal data or powder patterns in the CSD, ICSD, CRYSTMET and ICDD provided at no cost on the Web. Searchable by chemical name, elements, crystal parameters, etc. and returns the CIFs. The guiding principle is that the atomic positions in natural or synthetic crystals are not copyrightable.

Currently contains ~43,000 entries and claims to be more current than the commercial counterparts.

Mineralogy Database

<http://webmineral.com/>

Mineral data for individual species are linked to mineral tables by listings of mineral species, crystallography, crystal structures, X-Ray powder diffraction, chemical composition, physical and optical properties, Dana's New classification, Strunz classification, & mineral specimen images. There also are extensive links to other external sources of mineral data and information.

NIST Surface Structure Database (not at Caltech)

<http://www.nist.gov/srd/nist42.htm>

The Surface Structure Database (SSD) is a critical compilation of crystallographic information on surfaces and interfaces for over 1250 experimentally-determined atomic-scale structural analyses. For example, the SSD contains: Adatom structures on compound semiconductors, atomic coordinates at the CoSi₂/Si interface, variation of C-C bond lengths in adsorbed hydrocarbons and studies of the Al/GaAs (110) system studied with LEED?

Either search for specific items (e.g. Si substrate, (111) crystal face, Al adsorbate), or for classes of materials or structures (e.g. metallic substrates, molecular adsorbates, reconstructions). Data retrieved includes: full reference and brief summary of the surface structure, details of sample preparation, experimental technique, dataset and theoretical analysis, complete description of the bulk and surface unit cell(s), a scrollable list of coordinates, with error bars, for surface or interface atoms, and a scrollable list of important bond lengths and angles.

3D color graphics that allow visual inspection of all surface structures including:

- * rotation, magnification and choice of perspective
- * display of atoms as circles, disks, shaded spheres, etc.
- * color or gray-scale publication-quality PostScript output
- * full-color or red/blue stereo modes
- * storage and comparison of related structures
- * choice of colors for atoms, bonds and background
- * interatomic distances, bond angles, number and distance of neighbors ...

RCSB PDB (Protein Data Bank)

<http://www.rcsb.org/pdb/home/home.do>

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The online PDB archive is a repository for the coordinates and related information for more than 38,000 structures, including proteins, nucleic acids and large macromolecular complexes that have been determined using X-ray crystallography, NMR and electron microscopy techniques.

For background information:

The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data
Helen Berman; Kim Henrick; Haruki Nakamura; John L. Markley
Nucleic Acids Research 2006; doi: 10.1093/nar/gkl971
<http://nar.oxfordjournals.org/cgi/content/full/gkl971>

Nucleic Acid Database (NDB)

<http://ndb-mirror-2.rutgers.edu/>

The Nucleic Acid Database (NDB) is a repository of nucleic acid crystal structure data. The NDB currently contains ~3,300 structures. A Structure Finder Tutorial is provided:

<http://ndb-mirror-2.rutgers.edu/NDB/structure-finder/tutorials/index.html>

For background information:

The Nucleic Acid Database
H. M. Berman, et.al.
Acta Cryst. (2002). D58, 889-898
<http://journals.iucr.org/d/issues/2002/06/01/an0593/index.html>

METADDEX: Metals Abstracts/Alloy Index (STN)

<http://info.cas.org/ONLINE/DBSS/metadexss.html>

Metadex covers the worldwide literature on metallurgy and materials. The METADDEX database is searchable by librarians on STN, and currently contains more than 1.3 million records.

CRYSTMET Database (not available at CIT)

CRYSTMET <http://www.tothcanada.com/> is a database of critically evaluated crystallographic data for metals (including alloys, intermetallics and minerals) with associated bibliographic, chemical and physical information, including simulated powder diffraction patterns for all of the 70,000 entries, which covers the literature from 1922 to the present. [Acta Cryst. \(2002\). B58, 343-348; 358-363](#)

Combined Chemical Dictionary

<http://www.chemnetbase.com/scripts/ccdweb.exe> (Firefox/Netscape preferred)

The Combined Chemical Dictionary includes all the compounds contained in:

- Dictionary of Organic Compounds (255,000)
- Dictionary of Inorganic/Organometallic Compounds (101,000)
- Dictionary of Natural Products (170,000)
- Dictionary of Drugs (40,000)
- Dictionary of Analytical Reagents (14,000)

CCD's focus is on fundamental organic, organometallic and inorganic compounds; important biochemicals and minerals; compounds of active research interest and virtually every known natural product, and all currently marketed drugs in the US and UK. Literature references to crystal structure determinations (struct) are given in the References.

Structure Reports (MIL-8 REF QD 901 S8)

Some of the older data in the CSD, ICSD and CRYSTMET is also available in:

- Structure Reports v.1-29, 1913-1964
 - Section A: Metals and Inorganic Compounds v.30A-57A, 1965-1990
 - Subject / Formula Index 1913-1990
- Section B: Organic and Organometallic Compounds v.30B-49B, 1965-1982
- General Index: 1913-1973

Landolt-Bornstein (MIL-8 REF QD 61 L332)

Some of the older data in the CSD, ICSD and CRYSTMET is also available in:

- Crystal structure data of inorganic compounds - Part 3, v.7, sect. a-h (index 7h)
- Structure data of elements and intermetallic phases - Part 3, v.6
- Structure data of organic crystals - Part 3, v.5 & v.10
 - Organic Substance Index (HTML)
 - <http://lb.chemie.uni-hamburg.de/static/>
 - Inorganic Substance Index (HTML)
 - <http://lb.chemie.uni-hamburg.de/inorg/>

Crystal Data; Determinative Tables (Mil-8 REF QD 908 D666)

Single crystal data is arranged according to the six crystal systems, and sub-arranged by the a/b ratio

v.1(organic) and v.2(inorganic) cover the literature thru 1966, v.3(organic) and v.4(inorganic) cover the literature from 1967-74 and 1967-69 respectively.

Each volume has a formula index.

Crystallography References

Ch 122A - MIL-8 Reserve Books

Crystal structure analysis : a primer, 2nd ed., 1985	Glusker
The crystalline state, v.3: Detn of crystal structures	Lipson
Crystallography made crystal clear, 3d ed., 2006	Rhodes
Crystals, X-rays, and proteins, 1976	Sherwood
Elementary crystallography; an introduction, 1963 ...	Buerger
Elements of X-ray crystallography, 1968	Azaroff
Fundamentals of crystallography, 2nd ed., 2002	Giacovazzo
International tables for crystallography	IUC
v. A - Space Group Symmetry, 5th ed., 1992	
v. A - Brief Teaching Edition, 5th ed., 2002	
Introduction to crystallography, 1969	Sands
Mathematical techniques in crystallography, 3d ed., 2004 ...	Prince
Methods in x-ray crystallography, 1971	Jeffery
Space groups for solid state scientists, 2nd ed., 1990	Burns
Structural inorganic chemistry, 5th ed., 1984	Wells
Structure determination by X-ray crystallography, 4th ed., 2003	Ladd
Symmetry of crystals, 1971	Fedorov
Vector space, and its application in crystal-structure, 1959 ...	Buerger
Vectors and tensors in crystallography, 2002	Sands
X-ray analysis and the structure of organic molecules, 1995	Dunitz
X-ray crystallography; an introduction ..., 1942	Buerger
X-ray structure determination : a practical guide, 2nd ed., 1989	Stout
Conquest 2.0 Tutorials	CCDC
Conquest 2.0 User Guide	CCDC

Additional References:

International tables for crystallography (IUC)	MIL-8 REF QD908 I56
v. A - Space Group Symmetry, 2002 (Ch122 Reserve)	
v. B - Reciprocal Space, 2001	
v. C - Math., Phys., and Chem. Tables, 1999	
v. D - Physical Properties of Crystals, 2003	
v. E - Subperiodic Groups, 2002	
v. F - Crystallography of Biological Macromolecules, 2001	
v. G - Definition and Exchange of Crystallographic Data, 2005	

Crystal structures, 2nd ed., v.1-6, 1963-71

Wyckoff, F.

Caltech Chemistry Library Web Page

Chemicals - Crystal Structure Information

<http://library.caltech.edu/collections/chemistry.htm#CRYSTAL>

A list of additional web sites (e.g., Quasicrystals, Crystal Lattice Structures, Crystals Primer, X-ray Crystallography Research Guide, etc.)

