

# Crystallographic Databases

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# CAMBRIDGE STRUCTURAL DATABASE

<http://library.caltech.edu/collections/engineering/crystal.htm>

The Cambridge Structural Database (CSD) <http://www.ccdc.cam.ac.uk> contains structural information on over 250,000 carbon containing molecules (<1000 atoms), including organics, compounds of main group elements, organometallics and metal complexes. There is a small overlap between the CSD and the Inorganic Crystal Structure Database (ICSD) in the area of molecular inorganics. Information on other metal-containing structures can also be found CRYSTMET.

The CSD has recently increased the size limit for polymeric compounds to no more than 24 residues. Higher oligomers are covered by the Protein Data Bank <http://www.rcsb.org/pdb/>

The CSD contains the crystal structures of the major and minor amino acids and numerous small peptides, and has a very convenient way to search for structural characterized (non-protein) peptides according to their amino acid sequence.

The CSD covers mono-, di- and tri-nucleotides; higher oligomers are covered by the Nucleic Acids Database < <http://ndb-mirror-2.rutgers.edu/> >

The CSD reflects the published literature. It is fully retrospective 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: Bibliographic, textual and numerical information - Chemical diagram - Crystal structure data - Filters (secondary search criteria)

Documentation and tutorials available at:  
[http://www.ccdc.cam.ac.uk/support/csd\\_doc/zdocmain.html](http://www.ccdc.cam.ac.uk/support/csd_doc/zdocmain.html)

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

Password: ccdc@lib

At prompt, enter: cq for ConQuest, or 'isostar' or 'isogen'. (if necessary, click 'next'...)

ConQuest Current Interface for the CSD System

ConQuest is the program for searching and retrieving information from the Cambridge Structural Database (CSD). ConQuest provides a full range of text/numeric database search options, in addition to more complex search functionality, including

Chemical substructure searching

Geometrical searching

Intermolecular non-bonded contact searching

# ICSD (Inorganic Crystal Structure Database)

<http://www.fiz-informationsdienste.de/en/DB/icsd/www-recherche.html>

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 60,000 entries and covers the literature from 1915 to the present.

The ICSD allows for searching in four general categories of Chemistry, Crystal Data, Reduced Cell Symmetry and Reference Data. It includes enhanced features for the characterization of materials based on lattice and chemistry search modules and 3-dimensional visualization and powder pattern simulation of inorganic structures. Internet Search in ICSD:

<http://crystal.fiz-karlsruhe.de/fiz/products/icsd/icsd.htm>

"Normal screen" and "Expert screen" (contains an "expert query" field for crystal commands). You may start your search with a double click on one of the screen options. If you need help just click on a field name/

## CRYSTMET Database

The CRYSTMET database <http://www.tothcanada.com/toth/crystmet/overview.html> is a structure and powder database for metals and intermetallic compounds. CRYSTMET was based on:

A handbook of lattice spacings and structures of metals and alloys, which was continued by Pearson's handbook of crystallographic data for intermetallic phases.

Crystmet is not currently available thru the Caltech Library System).

## METADDEX (Metals Abstracts/Alloy Index)

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

Metadex covers the worldwide literature on metallurgy and materials. The METADDEX database is offered by STN (a PPV system), and currently contains more than 1.3 million records.

## Structure Reports (MIL-8 REF QD 901 S8)

Much 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)

Much 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

Structure data of elements and intermetallic phases - Part 3, v.6

Structure data of organic crystals - Part 3, v.5 & v.10

# Biological Macromolecule Crystallization Database

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

The BMCD contains crystal data and the crystallization conditions, compiled from the literature. The current version of the BMCD includes 3547 crystal entries from 2526 biological macromolecules for which diffraction quality crystals have been obtained. These include proteins, protein:protein complexes, nucleic acid, nucleic acid:nucleic acid complexes, protein:nucleic acid complexes, and viruses. The BMCD also contains the: NASA Protein Crystal Growth Archive which includes crystallization data generated from studies carried out in a microgravity environment supported both by NASA and other international space agencies.

## Crossfire (Beilstein / Gmelin)

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

Library: Start Menu → Programs → Beilstein Commander

Compared with Beilstein and Gmelin, the CSD and ICSD are extremely valuable because Gmelin is not yet up to date with respect to all the literature of the 1990's, and Beilstein has been limited to organic synthesis journals since 1980. Gmelin, however, may have more complete coverage of the older literature.

Beilstein and Gmelin are separate databases, and contain data for over 8.4M organic compounds and 1.5M inorganic/organometallic compounds, respectively. They are searchable by structure, physical property, reaction and bibliographic data

## Combined Chemical Dictionary

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

Compounds in the CCD include:

- Basic fundamental organic and inorganic compounds ...
- Virtually every known natural product, and all currently marketed drugs
- Compounds with an established use (e.g. catalysts, solvents, reagents, etc.)
- Important coordination compounds
- Organometallic compounds representative of all important structural types
- Important biochemical's and minerals
- Miscellaneous compounds of ... active research interest

Literature references to crystal structure determinations are given in the References.

# SciFinder Scholar

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

Library: Start Menu → Programs → Beilstein Commander

Following a chemical substance search (Registry File) click 'Get References'. One of the options is to limit retrieval to papers, in CAplus that mention 'crystal structure'. This is not compound specific as retrieval is based on the indexing of the whole article.

**CAplus** <http://www.cas.org/casdb.html>

Chemical Abstracts 1907+ -- 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 CAS indexing. Records from 1907-1961 do NOT include CA Index Terms or CAS Registry Numbers.

**Registry File** <http://www.cas.org/casdb.html>

A chemical structure and dictionary (CA Index Name, synonyms, CAS RN or MF) database - 1957+. Currently lists over 20M organic and inorganic compounds and over 24M biosequences. Provides links to 'Commercial Availability' and 'Regulated Chemicals Listing'. ACD calculated property data is provided for nearly 12.7M organic compounds along with basic (mp, bp, refractive index, ORD & density) experimental property data for over 800K compounds. 'Dictionary' searching is often faster than structure searching and avoids problems with structure searches that contain multi-component substances because of SFS' philosophy of 'maximizing retrieval'. SFS 2001 and 2002 offer an Additional Options dialog box to exclude: mixtures, isotopes, polymers ...

## Powder Diffraction File

[http://skinbark.caltech.edu/cdroms/Powder\\_Diffraction\\_File\\_2001/campus\\_access/](http://skinbark.caltech.edu/cdroms/Powder_Diffraction_File_2001/campus_access/)

Library: Not Available from library workstations

A collection of 55,000 single phase X-ray diffraction patterns used for identification of crystalline compounds. Retrieval is via chemical name, mineral name, PDF number and three strongest lines of the compound.

## Crystal Lattice Structures

<http://cst-www.nrl.navy.mil/lattice/index.html>

Indexed by: Strukturbericht Designation; Pearson Symbol; Space Group; Prototype and Structures of Intermetallic Alloy Phases.

## Structural Classification of Proteins

<http://scop.mrc-lmb.cam.ac.uk/scop/index.html>

Provides structural and evolutionary relationships between proteins with known structures.

# Crystallography References

The small molecule [X-ray facility in the Beckman Institute](#).

## Ch 122A - MIL-8 Reserve Books

Crystal structure analysis : a primer	Glusker, Jenny
The crystalline state, v.3:	Bragg, William L.
Crystals, X-rays, and proteins	Sherwood, Dennis
Elementary crystallography; an introduction ...	Buerger, Martin
Elements of X-ray crystallography	Azaroff, Leonid
Fundamentals of crystallography	Giacovazzo, Carmelo
International tables for crystallography	Int. Union of Crystallography
v. A - Brief Teaching Edition, 2002	
Introduction to crystallography	Sands, Donald
Mathematical techniques in crystallography ...	Prince, Edward
Methods in x-ray crystallography	Jeffery, James
Space groups for solid state scientists	Burns, Gerald
Structural inorganic chemistry	Wells, A. F.
Structure determination by X-ray crystallography	Ladd, M. F. C.
Symmetry of crystals	Fedorov, E. S.
Vector space, and its application in crystal-structure ...	Buerger, Martin
Vectors and tensors in crystallography	Sands, Donald
X-ray analysis and the structure of organic molecules	Dunitz, Jack D
X-ray crystallography; an introduction to the inv	Buerger, Martin
X-ray structure determination : a practical guide	Stout, George H.

## Additional References:

Crystal Structures, 2nd ed., v.1-4, 1963-71	Wyckoff, F.
International tables for crystallography	Int. Union of Crystallography
v. A - Space Group Symmetry, 2002	MIL-8 Reference
v. B - Reciprocal Space, 2001	MIL-8 Reference
v. C - Math., phys., and chem. tables, 1999	MIL-8 Reference
v. E - Subperiodic Groups, 2002	on order
v. F - Crystallography of biol. Macromol., 2001	MIL-8 Reference

## Caltech Chemistry Library Web Page

### CHEMICALS - STRUCTURE INFORMATION

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

Miscellaneous web sites, e.g. Database of Zeolite Structures, Quasicrystals, etc.

Help Files Examples:

## 8.2 Using the Compound Name Dialogue Box

Type the required compound name, or partial compound name. The search will find structures even if the specified name is interrupted by numbers, commas, hyphens, etc., 'thiazolyl' would find: Azobenzene-N-(4,5-bis(methoxycarbonyl)thiazol-2-yl)imide. To search for more than one name or partial name, use the New Box button. If two separate words are typed into the same box, e.g. benzoic acid, the whole text string, including the space, is matched.

### 10.2.1 Specifying a Chemical Formula

1. Type directly into the input box. The formula may be exact, e.g. C12 O4 H18, or inexact, e.g. C6-8 O > 2 (which means 6, 7 or 8 carbon atoms, and more than 2 oxygen atoms). Element Group Symbols may be used, but must be enclosed in square brackets, e.g. C6 [7A]2 (7A means any halogen atom)

2. Hit Select from Table and set the formula up from the Periodic Table. Click on an element or any of the Element Group Symbols. Then select the required mathematical operator (see Section 2.4.4) and type in the number(s) of atoms that must be present.