Available crystallographic software.

Installation packages and/or licenses are deliver on request.

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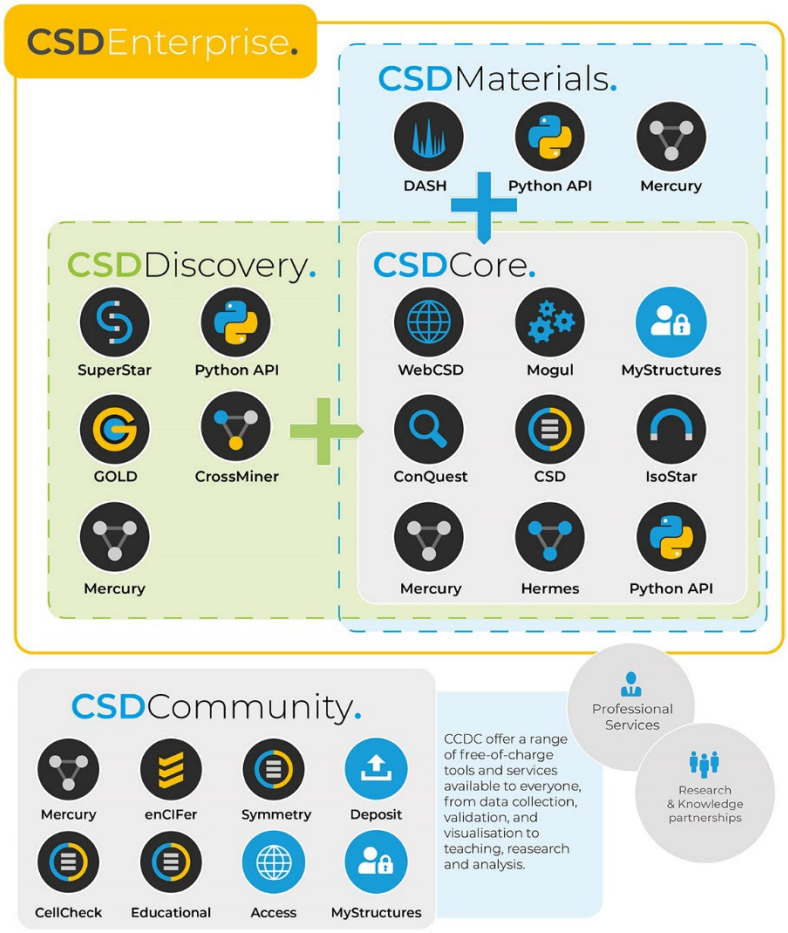
Database: ConQuest, webCSD and Pearson’s Crystal Data.

Visualization: Mercury, Diamond4.

CCDC software

All software from the CSD-Material suite are available. Data sheet



Software link/license on demand

ConQuest :

https://www.ccdc.cam.ac.uk/solutions/csd-core/components/conquest/

ConQuest is the primary program for searching and retrieving information from the Cambridge Structural Database (CSD). Local in-house databases generated using PreQuest can also be searched alongside the CSD using ConQuest.

ConQuest provides an extensive range of flexible search options enabling you to discover the knowledge contained within more than 1 million crystal structures. These include:

- *A full range of text and numeric database search options allowing you to locate structures based on compound name, formula, elemental composition, literature reference and experimental details.*

- *Chemical substructure searching including the ability to define chemical constrains such as charge, hybridization state and cyclicity.*
- *3D geometric searching enabling you to quickly analyse molecular dimensions and determine conformational preferences.*
- *Intermolecular and non-bonded contact searching allowing you to explore interactions of all types and to locate pharmacophoric patterns.*

How to use it

Mercury:

https://www.ccdc.cam.ac.uk/solutions/csd-core/components/mercury/

Mercury offers a comprehensive range of tools for 3D structure visualisation and the exploration of crystal packing. With a long pedigree and over 10,000 downloads, Mercury is firmly established as the visualiser of choice within the crystallographic community.

Mercury is available as a free download with more advanced Mercury features and exploration of the full Cambridge Structural Database (CSD) available with a CSD licence. Advanced features will be greyed out in the absence of such a licence. If your institution has a CSD licence, you may obtain this functionality by registering your copy of Mercury. To check if your institution has a CSD licence or for information on how to obtain a CSD licence, please contact us. More information about these advanced features is available on our CSD-Core Mercury page.

How to use it

webCSD :

http://www.ccdc.cam.ac.uk/structures

WebCSD provides easy and convenient access to the wealth of structural knowledge contained in the Cambridge Structural Database (CSD).

If you have access to the CSD-Core then WebCSD can be accessed by going to:

How to use it

Mogul :

Mogul provides precise information on preferred molecular geometries by enabling access to millions of chemically classified bond lengths, valence angles, acyclic torsion angles, and ring conformations derived from the CSD.

Mogul enables you to rapidly validate the complete geometry of a given query structure and identify any unusual features without the need to construct complex search queries, or carry out detailed data analyses.

Mogul is becoming an essential tool enabling crystallographers to generate ligand restraint dictionaries. Interfaces to Mogul are available in CCP4's Coot, Grade from Global Phasing, and eLBOW from Phenix. Mogul is also used routinely to check the conformations of both computationally and experimentally generated models, and will form an integral part of the PDB's ligand validation pipeline for newly deposited structures. Medicinal Chemists rely on Mogul not only to validate ligand geometries, but also to aid design decisions.

Mogul provides:

- *The ability to load query molecules in a variety of formats (MOL2, CIF, PDB, RES), or sketch a 2D structure.*
- *Easy selection of geometric features of interest and the ability to perform a "one click" validation of all bonds, angles, torsions and ring conformations in the query molecule.*
- *Automatic generation of search substructures. The chemical environment around the feature of interest is encoded ensuring that search results are highly relevant to the query structure. Mogul also has the ability to find structurally related fragments if insufficient hits are found.*
- *Rapid retrieval of geometric data. Results are displayed as a histogram calculated from matching entries in the CSD. Full descriptive statistics and figures of merit are provided allowing easy identification of unusual geometries.*
- *A simple text-based instructions file interface that allows Mogul to be run in batch mode from the command line and enables easy integration with client applications.*

How to use it

Crystal Impact Software

Diamond 4:

https://www.crystalimpact.com/diamond/Default.htm

Diamond is our outstanding molecular and crystal structure visualization software. It integrates a multitude of functions, which overcome the work with crystal structure data - in research and education as well as for publications and presentations.

Diamond does not only draw nice pictures of molecular and crystal structures like most of its competitive programs do. It offers an extensive set of functions that let you easily model any arbitrary portion of a crystal structure from a basic set of structural parameters (cell, space group, atomic positions).

With its high data capacity, its wide range of functions beginning with the generation of molecules reaching up to the construction of rather complicated inorganic structural frameworks, Diamond is a comprehensive tool for both molecular and solid state chemists as well as for surface and material scientists.

Ortep representation in one-step, instruction here

Match!

https://www.crystalimpact.com/match/Default.htm

Match! is an easy-to-use software for phase analysis using powder diffraction data. It compares the diffraction pattern of your sample to a database containing reference patterns in order to identify the phases which are present. Additional knowledge about the sample like known phases, elements or density can be applied easily.

*In addition to this **qualitative analysis**, a **quantitative analysis** (using Rietveld refinement) can be performed as well. You can easily **setup and run Rietveld refinements** from within Match!, with the actual calculations being performed automatically, using the well-known program FullProf (by J. Rodriguez-Carvajal) in the background. Match! provides a **gentle introduction into Rietveld refinement**, from fully automatic operation to the "Expert" mode. The software runs natively on **Windows**, **macOS** and **Linux**.*

*As reference database, you can apply the included **free-of-charge COD database**, 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**.*

Pearson's Crystal Data

Crystal Structure Database for Inorganic Compounds
https://www.crystalimpact.com/pcd/Default.htm

***Pearson's Crystal Data** is a crystallographic database published by ASM International (Materials Park, Ohio, USA), edited by Pierre Villars and Karin Cenzual. It has its roots in the well-known PAULING FILE project and contains crystal structures of a large variety of inorganic materials and compounds. The "PCD" (as it is typically abbreviated) is a collaboration between ASM International and Material Phases Data System, Vitznau, Switzerland (MPDS), aiming to create and maintain the world's largest critically evaluated "Non-organic database".*

The current release 2020/21 contains about 350,000 structural data sets (including atom coordinates and displacement parameters, when determined) for about 195,000 different chemical formulas, roughly 20,500 experimental powder diffraction patterns and about 297,000 calculated patterns (interplanar spacings, intensities, Miller indices). In addition over 53,000 figure descriptions for such as cell parameters as a function of temperature, pressure or concentration are given. To reach this result, scientific editors have critically analyzed and processed over 112,500 original publications.

The database comes with an innovative retrieval software for Windows PCs developed by Crystal Impact. It offers a large variety of new elaborate new features which make retrieval of the desired information extremely easy and comfortable.