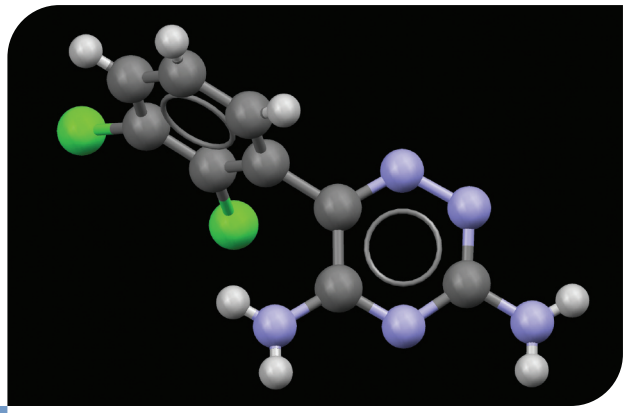
www.ccdc.cam.ac.uk



The Cambridge Structural Database System

Research and Education

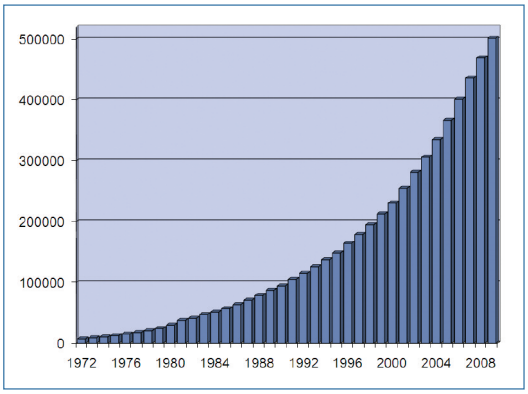
A powerful and highly flexible suite of software, the Cambridge Structural Database System enables you to unlock the knowledge contained within more than 500,000 crystal structures.

Cambridge Crystallographic Data Centre

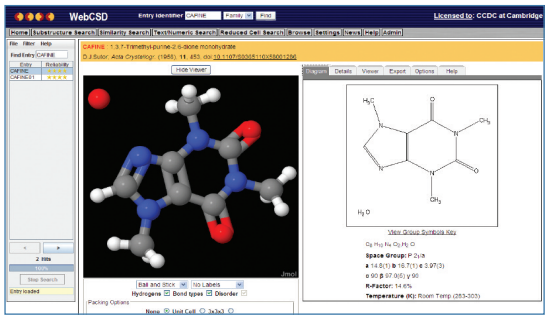
The Cambridge Structural Database (CSD)

Comprehensive and fully curated the CSD is the world's repository of experimentally determined small molecule structures.

- **World's repository:** Established in 1965, the CSD [1] is the world's repository for small-molecule organic and metal-organic crystal structures. Containing the results of over half-a-million x-ray and neutron diffraction analyses this unique database of accurate 3D structures has become an essential resource to scientists around the world.
- **Comprehensive coverage:** With comprehensive and fully retrospective coverage of the published literature you can have full confidence that your CSD searches are returning *all* crystal structure matches. The CSD also contains directly deposited data that are not available anywhere else.
- **Fully curated:** Each crystal structure undergoes extensive validation and cross-checking by expert chemists and crystallographers to ensure that the CSD is maintained to the highest possible standards. Also, each database entry is enriched with bibliographic, chemical and physical property information, adding further value to the raw structural data. These editorial processes are vital for enabling scientists to interpret structures in a chemically meaningful way.
- **Continually updated:** The CSD is continually updated with new structures (>40,000 new structures each year) and with improvements to existing entries. With regular web-updates and early online access to newly published structures you can keep fully up-to-date of the latest research.
- **Build local databases:** In addition to searching published crystal structures, institutions can build their own local structure repositories that are then searchable either independently of, or in conjunction with, the CSD.



The CCDC archived the 500,000th crystal structure to the CSD on December 10th 2009. The half-millionth entry was the anti-convulsant drug Lamotrigine (refcode EFEMUX01). The histogram shows the growth of the CSD from 1970 to present.

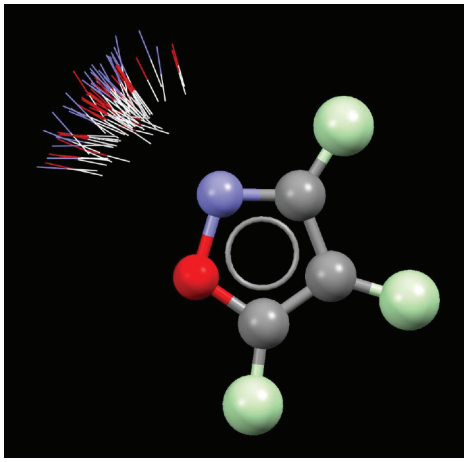


WebCSD interface showing structural information for caffeine (refcode CAFINE). The WebCSD online interface allows you to search, display and manipulate 3D structures all from within a standard web browser.

Educate

A unique teaching resource, the CSDS is the ideal platform for furthering students' understanding of 3D structural chemistry.

- **3D visualisation:** 2D chemical diagrams and idealised computational models cannot convey the levels of comprehension, even wonder, that are opened up to students by the visualisation and interactive manipulation of real 3D molecular structures. Visualisation of crystal structures from the CSD offers instructors unprecedented opportunities to enhance student's learning experiences, spatial abilities and conceptual understanding.
- **Experimentally measured data:** The use of experimentally measured data is of great pedagogical value and is known to enhance student learning. By mining the CSD, students can move beyond their textbook structures and analyse data and trends from real molecular structures. In addition, exposure to real measured data, complete with experimental error and statistical variation, provides opportunities to deal with the uncertainties of chemistry and prepares students for the realities of research.
- **Limitless possibilities:** The educational value of the CSDS is widely recognised and has been extensively demonstrated across the entire span of the chemistry curriculum, e.g. [2]. Now, with rapid online searching via WebCSD, it is easier than ever for faculty and students to fully utilise this major chemistry resource in a classroom environment [3].



IsoStar scatterplot showing O-H and N-H H-bonds to N- and O-acceptors in isoxazole rings as part of an extensive study of H-bond competition effects.

Research

The CSD System incorporates a suite of flexible search and analysis tools allowing chemical knowledge to be extracted from the raw crystallographic data.

- **Widely applicable:** Information derived from the CSD is vital to structural chemistry research in its broadest sense, and in particular to pharmaceutical drug discovery, materials design, drug development and formulation. More than 2,000 papers and reviews [e.g. 4-6] have been published worldwide that describe research applications using the accumulated data in the CSD. Literature references and short synopses are freely searchable at **www.ccdc.cam.ac.uk/free_services/webcite**
- **An essential resource:** The CSD has been crucial in deriving systematic information about molecular conformations for use in drug discovery [7], crystal structure prediction [8] and powder diffraction analyses. It has also been the central information source underpinning the rapid development of crystal engineering. CSD analyses are indispensable in our understanding and control of intermolecular interactions of all types, particularly weaker interactions such as C-H•••X [9], X-H•••π [10] and dipole-dipole interactions, as well as in studies of intermolecular synthons [11] and the systematics of crystal packing [12]. CSD analyses are also vital in structure correlation studies [13], including the mapping of reaction pathways from crystal structure data and correlations of crystal structure geometry with *ab initio* calculations [14].
- **Driving research:** There are clear indications that CSD knowledge will be vital in the development of future materials, such as gas-storage systems, and will play a key role in the development of nano- and green-technologies. As the CSD grows both in size and in the complexity of structures it contains, the database not only helps us to answer our questions about molecular structure and interactions, but helps to formulate what those questions should be.

Case Studies and Educational Resources

Case studies illustrating how the CSD System can be applied to a diverse range of research problems are available from the CCDC website.

Structural chemistry teaching resources including an interactive 500-structure teaching subset [15] and discovery-based learning exercises [16] are freely available from **www.ccdc.cam.ac.uk/free_services/teaching/**

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The Cambridge Structural Database System

The CSDS is an integrated suite of tools comprising the following software components:

The Cambridge Structural Database

comprehensive of the published literature and fully curated

PreQuest

build searchable databases of proprietary structures

ConQuest

search and retrieve information from the CSD

WebCSD*

access newly published structures online

Mercury

visualise and explore extended molecular networks

Materials Module of Mercury**

investigate and analyse solid forms

Vista

interactively analyse numerical data retrieved from the CSD

Mogul

instantly validate molecular geometries

IsoStar

rapidly assess intermolecular interactions

* Available to unlimited licence holders ** Add-on component of the CSD System

Evaluations

To request an evaluation of the Cambridge Structural Database System, please contact **admin@ccdc.cam.ac.uk**

Supported platforms

The Cambridge Structural Database System is supported on Windows, Mac and Linux platforms. For a full list of supported operating systems visit the CCDC website.

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