STRUCTURES

The Structures databases contain a comprehensive collection of organic, organo-metallic and inorganic compounds, metals, alloys and protein **crystal structure data**.

CSD - **C**ambridge **S**tructural **D**atabase.

Crystal structure data for over **615,200 organic and organo-metallic compounds**. New releases of this database are received and mounted quarterly.

*__ConQuest__ is the graphical front end which has 3D search capabilities.

***VISTA** performs numerical, statistical and graphical analyses.

*__Mercury__ provides comprehensive facilities for visualising crystal structures in three dimensions.

*__IsoStar__ A knowledge base of non-bonded interactions derived from the CSD, the Protein Data Bank (PDB) and molecular orbital calculations. Uses a simple web interface.

* **Mogul** A knowledge base of molecular geometries using data derived from the CSD.

WWW interface not yet available.

ICSD - **I**norganic **C**rystal **S**tructure **D**ata File.

Over **150,000 inorganic structures** - the companion file to the Cambridge organic file (though in a different format).

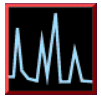
CRYSTMET

Crystal structure data for over **150,000 metals, alloys and intermetallics.**.

CDIF - **C**rystal **D**ata **I**dentification **F**ile.

Crystal class and unit cell data for **237,671 crystal structures**.

CrystalWeb/CrystalWorks - a simple **web interface to ALL of the crystallographic databases** that allows bibliographic and cell data searching along with structure display for **992,552** entries.



SPECTROSCOPY

The Spectroscopy databases are designed to aid the chemist in structure elucidation and spectral interpretation problems.

SPECINFO

SpecInfo is accessed using **SpecSurf,** a **Web graphical user interface** that makes drawing structures, creating peaklists and viewing hit lists easy. Searches can be conducted by inputting then matching a query spectrum (or fragment), a (sub-) structure or bibliographic information such as name, formula or CAS number. The ability to predict an NMR spectra for any trial structure using statistical information taken from the spectra stored in a database can be very useful in identifying a molecule.

ACD/Labs I-Lab

The data can be accessed via **ChemSketch**, a PC based structure drawing package or via the Web using the graphical interface **I-Lab**. In addition to NMR searching and prediction, ACD/Labs I-Lab has compound name generation and property prediction programs.

No.of Records	^{13}C NMR	^{1}H NMR	^{15}N NMR	^{17}O NMR	^{31}P NMR	^{19}F NMR	^{11}B NMR
SPECINFO	359,647	130,025	7661	5184	16,561	25,442	10,238
ACD/Labs	200,100	210,700	9,287	-	27,000	17,000	-

SPECINFO **IR Spectra** = 20,898 **Mass Spectra** = 138,727

ACD/Labs **pKa** = 16,000 **LogP** = 18,400 **Solubility** = 5,000

PHYSICAL CHEMISTRY

DETHERM

One of the world's largest thermophysical property databases of pure compounds and compound mixtures Contains over **7.5 Million data sets** for around **160,500 systems** (around 36,500 pure substances and 124,000 mixtures) covering around **500 property fields**.

Each property orientated package of data is checked and maintained by academic experts. Details are available as a function of temperature, pressure, density etc. Search Wizard and Extended Search options available.

Detherm can be accessed via Client server software or via a Web interface.

ORGANIC CHEMISTRY

SPRESI

Allows you to search Molecules, Reactions, References and associated data. Contains synthesis planning tool. **Direct access over the web** to:

* 8.7 million structures * 4.1 million reactions
* 32 million factual data entries

extracted from: 658,000 references; 164,000 Patents

Specialist Databases – using Accord software:

Protecting Groups

Selected protection, deprotection and transprotection reactions.

Solid Phase Synthesis

Information related to combinatorial synthesis.

BioCatalysis

Biomolecules as catalysts in organic synthesis

Available Chemicals/ Screening Compounds/Building Blocks

Searchable catalogue data from 9 off-the-shelf suppliers, 12 Library Suppliers and 7 Building Block Suppliers. Uses ChemAxon's **JChem** software over the web.

UTILITY PROGRAMS

A variety of utility programs are available, including links to electronic literature, chemical file format conversion and molecule viewers.

CrossRef/DOI

The Digital Object Identifier links citations in databases to the original journal article stored on the relevant electronic literature site. CrystalWeb, ICSD-WWW and ConQuest are all enabled.

Crad

A **c**rystal **rad**ial distribution calculation program.

File Format converters

BEDLAM is a generalised format converter very similar to the widely used converter program, BABEL, but handles crystallographic data better.

BABEL remains the package of choice to handle formats for a whole range of molecular modelling packages.

Help

A variety of help is available for registered users of CDS

- Exercises and Tutorials
- Flash movies showing quick overviews plus more detailed use.
- Online manuals
- Single sheet guides to most of the major packages
- FAQ Database
- Training courses (free of charge)
- 'Overview of CDS' PowerPoint presentation (**http://cds.dl.ac.uk/overview**)

To **register as a user** see the CDS website at:

http://cds.dl.ac.uk/cgi-bin/reg/express_uk

and follow the instructions on that page.

Shibboleth access now supported

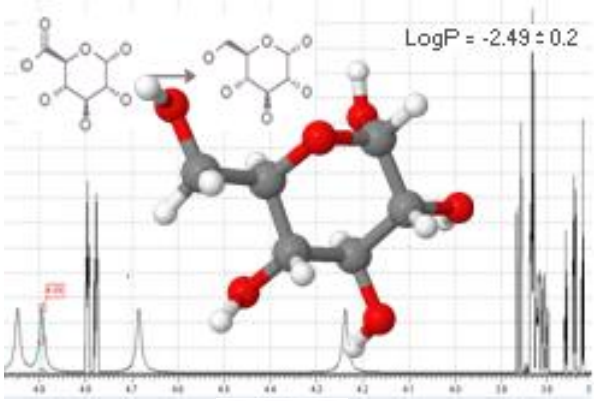
The CDS can be contacted at:

Chemical Database Service
Daresbury Laboratory
Warrington
WA4 4AD
Tel: (01925) 603162
Email: cdsbb@stfc.ac.uk

Funded by the Physical Sciences Programme of the EPSRC

Daresbury Laboratory is part of the Science & Technology Facilities Council

Chemical Database Service



CDS

Daresbury Laboratory

http://cds.dl.ac.uk

The **Chemical Database Service** (**CDS**) is a National service, funded by the Physical Sciences Programme of the EPSRC.

The specific aim of the Service is to ensure that the growing body of information from chemical research is conveniently accessible to UK academics. We provide

FREE OF CHARGE

to all **UK academics** :

- **Networked access to up-to-date, high quality, comprehensive chemical databases.**
- **Help, support, training and advice by postdoctoral chemists.**

The databases available are :