Chemical Database Service (CDS) NEWSLETTER

Issue 21 Apr 2005

See http://cds.dl.ac.uk/cds/newsletters.html for this and previous editions of our newsletter

A summary of the main articles

The CDS Road Show round-up. See the article on page 2 and 3.

Some differences between MDL ISIS and Beilstein are presented on page 3.

See page 4 for training information on the CDS website.

For how to check your details and change your password see Page 6.

See page 7 for news on the CDS website.

Improvements to Crystalweb are presented on page 9.

The CDS is funded by the Engineering and Physical Sciences Research Council

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CDS Road Show 2004/05 Round-up

In order to increase publicity CDS, embarked on a tour of universities.

The road show included a poster display, registration of students/staff for an account and a CDS overview presentation. The overview covered the various chemistry datasets hosted by the service (Physical Chemistry, Organic Chemistry, Crystallography and Spectroscopy) and their access methods (via client software, a Web Based Interface or X-windows). A copy of the presentation slides can be downloaded from http://cds.dl.ac.uk/overview.ppt

Visit	Site	Date
1	Liverpool	29-Oct-2003
2	Manchester	30-Oct-2003
3	Loughborough	26-Nov-2003
4	Sussex	20-Apr-2004
5	Imperial College Chem. Eng.	08-Jun-2004
6	Oxford Chemistry	30-Sep-2004
7	Warwick Chemistry	04-Oct-2004
8	UCL Chemistry	06-Oct-2004
9	Swansea Chemistry	13-Oct-2004
10	Cardiff Chemistry	14-Oct-2004
11	Nottingham Chemistry	15-Oct-2004
12	Leeds Chemistry/Chem Eng	21-Oct-2004
13	Sheffield Chemistry	26-Oct-2004
14	Newcastle Chem Eng	28-Oct-2004
15	Durham Chemistry	29-Oct-2004
16	St. Andrews Chemistry	08-Nov-2004
17	Edinburgh Chemistry	09-Nov-2004
18	Glasgow Chemistry	11-Nov-2004
19	Strathclyde Chemistry	12-Nov-2004
20	Bangor Chemistry	19-Nov-2004
21	Liverpool Chemistry	25-Nov-2004
22	Manchester Chemistry	30-Nov-2004
23	Southampton Biological Sciences	25-Jan-2005
24	Bath Chemical Engineering	09-Feb-2005
25	Bristol Chemistry	10-Feb-2005
26	Loughborough Chemical Engineering	17-Feb-2005
27	Birmingham Chemistry	01-Mar-2005
28	Cambridge Chemistry	08-Mar-2005
29	York Chemistry	15-Mar-2005
30	Belfast Chemistry	22-Mar-2005

CDS Road Show Round-up

CDS Road Show 2004/05 Round-up

We travelled over 7500 miles, registered 344 users and presented to nearly 500 students/staff. If you would like your University to be added to our 2005/06 road show list, the procedure is to contact your group representative (http://cds.dl.ac.uk/cgi-bin/reg/findrep.html) or contact us yourself (if you have no representative). Group representatives or interested/potential users can contact CDS via email: cdsbb@dl.ac.uk or phone: (01925) 603-163. We will require a seminar room with internet connection (in the afternoon) and a poster stand space with internet connection (in the morning).

Many thanks to CDS Reps., librarians, departmental secretaries, users and I.T. staff who made our job easier and helped make the road show a great success.

2005/06 CDS Road show starts in Sept.

MDL ISIS Reaction Databases versus Crossfire Beilstein Database

ISIS (which is hosted by CDS) is a chemical reaction database management system that is designed to store, search, retrieve, and display molecules and reactions along with their associated data. A variety of chemical databases can be searched within ISIS that cover over 50 years of published literature, providing established and current awareness in synthetic organic chemistry, and now contain over 1.3 Million searchable reactions.

The Beilstein database (which is hosted by Manchester Information & Associated Services) is based on Beilstein's Handbuch der organischen Chemie. The Database covers organic chemistry from 1771 to date and contains over 8.2 million structures and 10 million reactions.

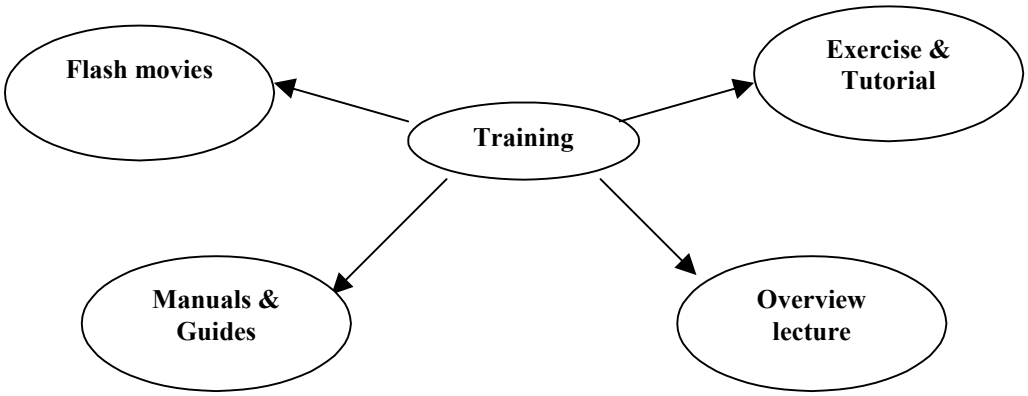
The main difference between ISIS and Beilstein is that Beilstein is a **molecule** database (containing single step reactions using the molecule as reactant or product) where as ISIS is a **reaction** database – the entries being carefully selected because of the transformation.
Another difference is the fact that ISIS contains **overall** reactions. A required transformation may involve two or more single-stage reactions (e.g. A → B → C) so, if your query is A → C, you will not find it in Beilstein but you may find it in ISIS as it contains A → B; B → C **and** A → C.

Beilstein does contain a lot more reactions than ISIS and the overlap in bibliographic data is high. However, the overlap in reaction data is much smaller. This is due partly to the presence of overall reaction data but also because the two databases abstract different journals and also different reactions from the same journals. ISIS contains specialist reaction databases, such as Protecting Groups, and a number of journals not found in Beilstein.

One other fact to remember – ISIS can produce a smaller hit list, useful as a lead, which is easier to look through. Moreover, **clustering** of the hits within ISIS makes looking through these hits even easier.

For a more detailed comparison see:-
Faiz A. Parkar and Don Parkin**.** Comparison of Beilstein CrossFirePlusReactions and the Selective Reaction Databases under ISIS *J. Chem. Inf. Comput. Sci.*; 1999; 39(2) 281 – 288

Training Information on the CDS website



The CDS website has a large number of training and learning information to enable users to learn more about the Service, data/databases we provide and how to use/better use our databases for their research.

Flash Movies

The website has interactive movies covering Spectroscopy, Organic Chemistry, Physical Chemistry and Crystallography database. The movies for each domain of chemistry are made up of specific database searches as well as overviews.

Overview Movies	More Detailed Movies
PHYSICAL CHEMISTRY	
Detherm [Version 1.4] (4:35 mins.) Detherm [Version 2] (5:45 mins)	Direct Search (3:39 mins.) Easy Search (1:15 mins.) Combined Search (1:34 mins.) Results Forms (1:47 mins.) List of Property Fields (V1.4) (0:38 mins.) List of Property Fields (V2.0) (0:26 mins.)

Training Information on the CDS website

Manuals and Guides

Online documentation

Online documentation or manuals are available for the following:

- SpecSurf Guide NEW
- ISIS
- Cambridge Structural Database (CSD)
- CSSR
- Inorganic Crystal Structural Databank (ICSD)
- Metals Data File (MDF)
- Brookhaven Protein Databank (PDB)
- Crystal Data Identification File (CDIF)
- CDS User Guide
- Guide to UNIX on cds
- Guide to display of crystal structures
- Rasmol Molecular Display Program
- Platon Molecular Display Program documentation. There is also a help manual in the application
- Download area. Most manuals can be downloaded for local printing. Many now available in PDF format.

Exercises and Tutorials

Users can download the ISIS exercise and applications such as Conquest have a help menu. There are links to the Conquest user guide and tutorial on the Cambridge Crystallographic Data Centre (CCDC) website.

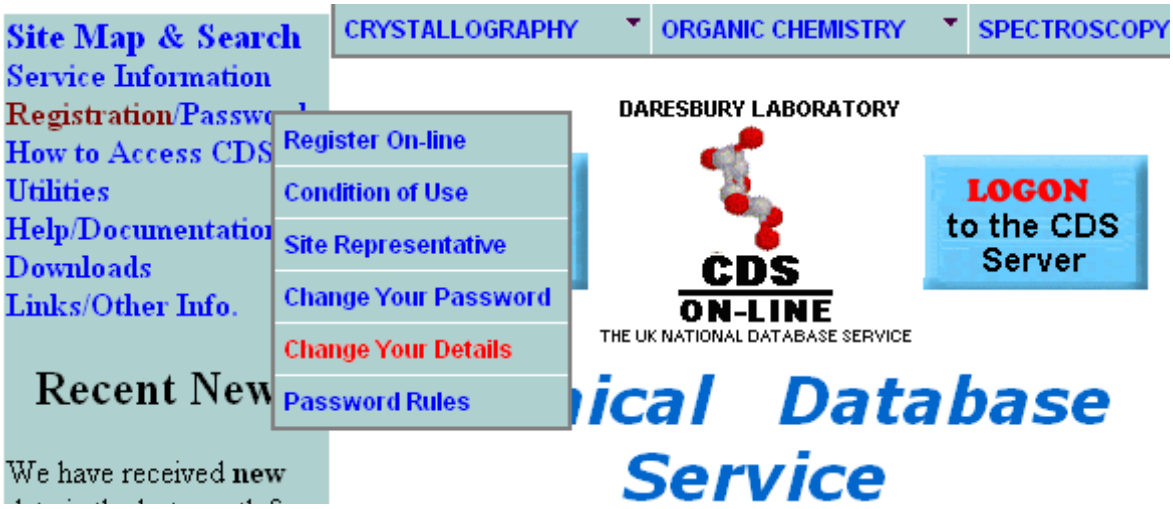
Overview Lecture

Users can also download the CDS overview presentation from http://cds.dl.ac.uk/overview.ppt

CDS Helpdesk: cdsbb@dl.ac.uk or 01925-603-162

Checking your details and changing your password

Users can now check if their details are correct and make changes if required. Move your mouse over "Registration" on the navigation menu and then click on "change your details" on the sub-menu



CDS user details

Use this form to change the details we have stored about your account, including email preferences.
To change your account password click here.

Name

Prof | Lukin | Vierigode

Site

Wolverhampton Applied Sciences
Yeovil Science
York Langwith College
York Physics
leeds electronic and electrical engineering
CCLRC, Daresbury CSE

Electronic mail address l.Vierigode@dl.ac.uk

Telephone number 01925603155

Users can now also change their password via the CDS website.

CDS password change form

ID

Old password

New password

New password (again)

Change password

Passwords must be 6-8 characters long and can consist of letters, numbers and the following non-alphanumeric characters.

_!#$%&()*+,-./:;<=>?@[]^{}|

Each password must contain at least one non-alphanumeric character as well as both upper and lower case characters.

News on the CDS website

News on the CDS website as been updated. News items now have titles rather than file names. News items are listed according to importance and they are dated correctly.

Navigation Menu
Home
Site Navigation
Service Information
How to Access CDS
Registration/Password
Databases
Access via the Web
Utilities
Help/Documentation
News/Highlights
Downloads
Links/Other Info.

CDS News

- Current login message on CDS
- Email message archive
- **BioCatalysis: Biomolecules as catalysts in organic synthesis : Updated 21 Mar 2005**
- **ACD: The Available Chemicals Directory : Updated 21 Mar 2005**
- **DJSM: Derwent Journal of Synthetic Methods : Updated 21 Mar 2005**
- **ICSD: Inorganic Crystal Structure Database : Updated 14 Mar 2005**

Users can also troll through the CDS email message archive

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CDS email message archive

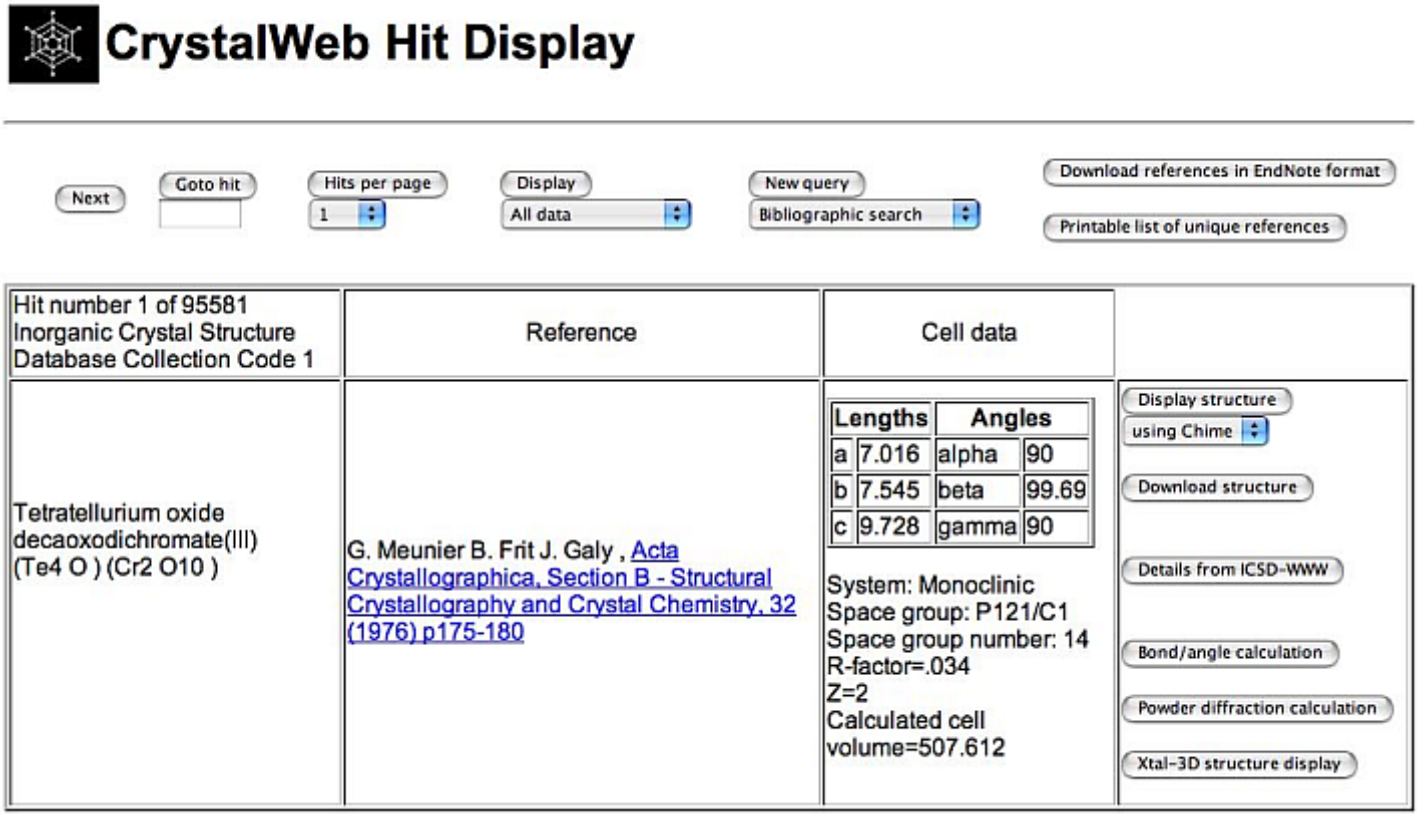
- Database updates for BioCatalysis, DJSM and ACD : Sent 23 Mar 2005
- ICSD Web Interface Upgrades and Error Correction : Sent 16 Mar 2005
- Update to Cambridge and other database systems : Sent 19 Jan 2005
- New Version of the DETHERM Client and withdrawal of ELYS : Sent 3 Nov 2004

Improvements to the Crystallographic Web Interfaces

Web interfaces are becoming an increasingly popular method of accessing the crystallographic databases. CDS currently makes available the CrystalWeb system to search all of the crystallographic databases as well as the dedicated ICSD-WWW system, which only searches the Inorganic Database but has functionality not present in CrystalWeb.

A variety of improvements and fixes have been applied to these web interfaces in recent weeks. ICSD-WWW has had its file output routines tweaked; CIF format now has the correct symmetry operations in all cases and ShelX format has the correct site occupancies (these problems were not present in CrystalWeb). In addition the input to auxiliary functionality, such as powder diffraction calculations and 3D display, has been augmented so that these functions now work for all space groups and settings, without the requirement for manual intervention for "non-standard" space group settings.

CrystalWeb has also been augmented. Behind the scenes work has enabled linking retrieved entries to some of the ICSD-WWW functionality in a "black-box" fashion, i.e. without expert crystallographic knowledge on the part of the user. In particular users can now perform a powder diffraction (including neutron) plot calculation on any entry from the three major databases (CSD, ICSD and CrystMet) with co-ordinate data and derive bond distances and angles between arbitrary atoms in a structure.



New link to ICSD-WWW functionality from CrystalWeb

Databases available from the Chemical Database Service

A brief description of all the databases currently available from the CDS at Daresbury.

ISIS: A chemical reaction information management system allowing search, retrieval and display of molecules, reactions and their associated data. Currently contains over 1,300,000 searchable reactions. Specialist Databases available include Protecting Groups, Solid Phase Synthesis, BioCatalysis, Chiral Separations and National Cancer Institute Database. This database is produced using data and structures from the National Cancer Institute (NCI) Developmental Therapeutic Program (DTP).

In addition there is the Available Chemicals Directory (**ACD**), which contains supplier information on over 432,000 different compounds from over 660 different suppliers.

Screening Compounds Catalogues

Made up of over 3 million compounds available from around 20 suppliers. Such as **SALOR** (Sigma-Aldrich Library of Rare Chemicals), **MAYBRIDGE** and **BIONET**.

SPEC: SpecInfo is a multi-technique spectroscopic database package intended to cover NMR, IR and mass spectra. The package is designed to aid the chemist in spectral interpretation and structure elucidation problems.
The database currently contains 102,500 ^{13}C NMR; 999 ^{15}N NMR; 856 ^{17}O NMR; 2,183 ^{31}P NMR; 1,825 ^{19}F NMR; 60,700 ^{1}H NMR; 20,898 infra-red spectra and 130,000 mass spectra.

CSD: The Cambridge Structural Database. Crystal structure data for over 338,000 organic and organometallic compounds. Currently available under Cambridge's Quest and ConQuest retrieval software and our in-house software (CSSR). VISTA is a **VI**sual **STA**tistics package which reads the tables files which are when derived geometric parameters are requested with a CSD search. Mercury offers comprehensive facilities for visualising crystal structures in three dimensions. Both VISTA and Mercury can also be called from within ConQuest.

IsoStar: A database of non-bonded interactions taken from the CSD, PDB and theoretical calculations.

Mogul: A knowledge Base of molecular Geometry using data derived from the CSD

ICSD: Inorganic Crystal Structure Data File. Contains about 83,000 inorganic structures - the companion file to the Cambridge organic file. ICSD is now accessible via CrystalWeb on the CDS website.

MDF: (**CRYSTMET**) Metals Data File. Crystal structure data for nearly 82,000 metals, alloys and intermetallics.

CDIF: Crystal Data Identification File. Crystal class and unit cell data for over 237,000 crystal structures.

DETHERM: Is one of the world's largest thermophysical property databases of pure compounds and compound mixtures.

Acknowledging the Service

The results of research using the Chemical Database Service may be published through the normal academic channels provided the following acknowledgement is quoted:

"We wish to acknowledge the use of the EPSRC's Chemical Database Service at Daresbury."

The following publication should also be cited:
The United Kingdom Chemical Database Service, Fletcher, D.A., McMeeking, R.F., Parkin, D., J. Chem. Inf. Comput. Sci. (1996), **36**, 746-749.

General Enquiries

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Cdsbb@dl.ac.uk

CDS website:
http://cds.dl.ac.uk

CDS
ON-LINE

The Chemical Database Service (CDS) provides on-line access to a variety of quality databases in the field of Chemistry, plus support, training and advice.

Access:
The service is available **free of charge** to UK academic research groups for non-commercial work. Each individual user will be issued with a unique ID. It is not our policy to allow shared IDs.

Remit: To provide Chemical Database Service and support to UK academic community as well as helping to maintain/ improve the service according to the service level agreement with the EPSRC

Information

For ISIS specific problems:

Dr. D. Parkin
Email: D.Parkin@dl.ac.uk
(01925) 603162

For SpecInfo specific problems:

Dr. D.A. Fletcher
Email:D.A.Fletcher@dl.ac.uk
(01925) 603492

For crystallography specific problems:

Dr. R. F. McMeeking
Email:R.F.McMeeking@dl.ac.uk
(01925) 603669

World Wide Web Site

Information about CDS, including online help and documentation is available over the World Wide Web at the CDS website, URL: http://cds.dl.ac.uk Web based interfaces to selected databases are also available from this site.

Documentation:

Most documentation is available online and some can be downloaded from the CDS web site.

cds (main service machine):

Internet number: 193.62.124.36
Internet name: cds.dl.ac.uk

Comments:

All comments, questions and suggestions about this newsletter should be sent to:
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