# Chemical Database Service

# NEWSLETTER

**Issue 14** **June 2001**

CDS plans to go ahead with a trial of the **Detherm** thermophysical properties database in September. See page 4 for more details. We will be conducting additional publicity for the trial nearer the time.

We have significantly enhanced the knowledge base associated with our **LitLink** server to include new sites, new journals and a working patent retrieval system. In addition, the **Accelrys** Protecting Groups and Solid Phase Synthesis databases now work with LitLink. LitLink enhancements are described on page 2, whilst Accelrys database changes are described on page 6. These improvements will make it more likely that a retrieved reference from ISIS or Beilstein can be automatically linked to a source of the article in electronic format.

**This year's CDS User Meeting will be held on July 17th at Daresbury. See page 9 for more details.**

The **CDS website** is due for a significant overhaul. We have already sought input from the user community through a survey last month. Details of initial ideas and progress are given on page 9.

David Osa-Edoh joins the CDS team after completing an MSc in Information Systems at Liverpool University. He will be taking over some of the user support functions, assisting in the website redesign and editing the Newsletter.

## Contents



The Chemical Database Service is funded by the Engineering and Physical Sciences Research Council

# LitLink update

LitLink links citations in the ISIS and Beilstein databases to original journal articles stored in electronic format at sites such as Elsevier (ScienceDirect), American Chemical Society, or Royal Society of Chemistry. Articles are delivered to your Web browser as HTML or PDF image files. Articles not available online can be received by email or fax via an appropriate document delivery service.

Recently we have made extensive enhancements to the LitLink system. New sites have been added (e.g. iucr and patent links), as well as a number of new journals e.g. SynLett and Synthesis. In addition we have expanded the links for existing journals to better match the needs of the UK academic community. For example, many more journals now link to the SwetsNet website, which is the access point for NESLI (National Electronic Site Licensing Initiative) agreements. We have also increased the number of links to the Beilstein Abstracts database, a service available free on ChemWeb.

There are over 15,000 patent references in the organic reaction databases. We have made modifications in order that these are picked up by LitLink. Suitable sites, such as the European Patent Office, are selected.

The only database with a significant number of patents which do not work with LitLink is BioCatalysis. We hope that this will be remedied with the next release of this database, later this year.

**Using LitLink**

Both the ISIS Reaction Browser and the Beilstein Commander can be configured to use LitLink. To do this you need to download and install the LitLink client software from the CDS website. Instructions can be found at the following URL

http://cds3.dl.ac.uk/cds/chemscape/cdslitlink.html

The LitLink client software is only available for PCs.

The web based ReactionWeb interface can use LitLink by default. There is no need to download any software and you are not limited to using a PC.

The figure on the next page shows the steps in retrieving a full text article using Beilstein.


In Beilstein, click on LitLink to open a web page with links to sites where the article may be found. (You will need a CDS ID and password).

If your University subscribes to the Journal, then the links should lead to the full article.

**Desktop access to full literature articles from Beilstein and ISIS**

# Trial of the Detherm database

This Autumn CDS plans to run a trial of the Detherm thermophysical properties database. The trial will run from September to December and it is intended to provide unlimited access to the full system and all associated datasets.

We believe that these data may be of interest to many people who are not current CDS users, particularly chemical engineers. We would be grateful if you could pass this information on to any colleagues who might be interested. CDS will be providing additional publicity nearer the time for the trial, and will be targeting chemical engineering departments in particular.

**Database description**

The Detherm database provides thermophysical property data for about 19,200 pure compounds and 92,500 mixtures. Detherm contains literature values, together with bibliographical information, descriptions and abstracts. Currently there are some 3.75 million data sets containing the following properties

- phase equilibrium data
- vapour pressures, critical data
- thermodynamic properties
- transport properties
- surface tensions
- electrolyte data

More information about the database is available on the Dechema website at the following URL:

http://www.dechema.de/f-infsys-e.htm?englisch/dbMain.htm

We also provide a link from the CDS website.

**Technical aspects**

The Detherm database runs under a client/server system, similar to the ISIS software. The data is stored inside an Oracle database running on one of the CDS servers, whilst the client software used to access the data runs on your local PC.

We will be making the client software available free to users. You will be able to download it from the CDS website in a similar fashion to the ISIS client. The Detherm client software only runs under Windows, and this situation is not likely to change.

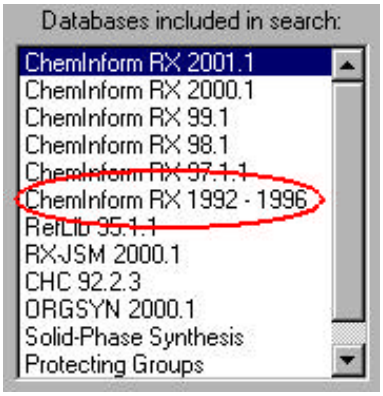
# New CDS staff

The CDS team has expanded with the addition of a new member of staff, David Osa-Edoh, who joined us in February. David gained a B.Sc. in Applied Biochemistry from Liverpool John Moores University (1993-1997) and a M.Sc. in Information Systems from Liverpool University (1999-2000). He also worked for Unilever Research (Port Sunlight) as a Research Associate / Database Administrator from 1998-1999.

David will be taking over some of the user support functions previously outsourced to the Daresbury Computer Helpdesk. In addition he will play a major part in the website redevelopment and the addition of new training material. He will also be taking over as editor of the newsletter from Dave Fletcher.

# ChemInform Reaction Library 1992 - 1996

Users of the ISIS reaction databases may have noticed that the first five years of the sets comprising the ChemInform Reaction Library (CIRX92 – CIRX96) have now been replaced by a single combined dataset (CIRX9296).




This cumulative database includes corrections to the old individual datasets taken from the weekly compendia of ChemInform, 1991 – 1995 and contains a total of 327,717 reactions and 378,774 molecule entries.

The new set up should achieve faster loading and search times. This change does NOT require users to alter their reaction browser settings.

# Accelrys databases

A number of specialist synthetic organic databases are available from Accelrys (formerly Synopsys). Currently these are Protecting Groups (spg), Solid Phase Synthesis (sps) and BioCatalysis. All of these databases are accessible via the ISIS client / server and ReactionWeb interfaces. Recently we have improved the functionality available for these databases to match more closely that available with the core MDL databases. Specifically we have added the display of specialist data fields in the ReactionWeb interface and we have enabled records retrieved using ISIS to work with LitLink.

## Accelrys databases with ReactionWeb

ReactionWeb is a web based interface to the organic reaction databases. Each hit in a retrieved hitset has a Full Details form (which is displayed by clicking on the 'More details for this record' link). This form now contains fields for displaying all the specialist data from the Accelrys databases. An example display of this data for a record from the Protecting Groups database is shown below.

Synopsys Data

| Substrate | Reaction Condition Keys |
|---|---|
| | Azodicarboxylate Phosphine base |

Protecting Group Data

| Functional Group | Protected Group |
|---|---|
| Alcohol (tetiary)<br>Alcohol* | Isopropyl ether<br>Me2CH- ether<br>i-Pr ether |

Protecting Group Stability

| No. | Stability Conditions | Stability Citations | Stability Keywords |
|---|---|---|---|
| 1 | AlCl3/CH2Cl2/0 C/2 h | J Org Chem, p.5728, 1991 | Al(III), Lewis acid |

Protecting Group Lability

| No. | Lability Conditions | Lability Citations | Lability Keywords |
|---|---|---|---|
| 1 | AlCl3[1 eq.]/CH2Cl2/0 C/2 h | J Org Chem, p. 6726, 1991 | Lewis acid |

Protecting Group Tolerated Groups

| No. | Stable Protecting Group | Derived From |
|---|---|---|
| 1 | Acetonide<br>Me2C- acetal<br>Me2C- ketal<br>Me2C< ketal<br>Isopropylidene acetal<br>Acetonide acetal<br>Me2C< acetal<br>Isopropylidene ketal | 1,2-Diol<br>1,2-Diol*<br>Diol*<br>vic-Diol |

**Full Details record for Protecting Groups data**

## Accelrys databases and LitLink

The main reference for a record retrieved from one of the Accelrys databases is now works with LitLink when using either the ISIS or ReactionWeb interfaces.

However, the author part of the citation is in a different format to that in the MDL database references. As a consequence, although LitLink points to the correct journal provider, once at the site, a list of possible references will probably be displayed instead of just the correct one. However, the required citation should still be present in the list. We anticipate that this complication will be resolved in future releases of the databases.

For example, the following reference is retrieved using ReactionWeb.

References: Citation and Title

| No. | Literature Reference | Title |
|---|---|---|
| 1 | Bull S D, Davies S G, Fenton G, Mulvaney A W, Prasad R S, Smith A D, Chem Commun (Cambridge) (4) p. 337, 2000 | Chemoselective oxidative debenzylation of tertiary N-benzyl amines |

Clicking on the reference and then selecting the ChemWeb site produces 8 hits, whilst the RSC site produces 44 hits. Both contain the required reference.

You searched for records containing [D] in [Authors] and [G] in [Authors] and [G] in [Authors] which were published between 2000 and 2000 in journal 'Chem.Commun.'

Found 8 matching records, showing results 1 - 8

- Chemoselective oxidative debenzylation of tertiary N-benzyl amines Publication date 2000 *Beilstein Abstracts* [Full Record]

**A part of the ChemWeb site page, showing the retrieved reference**


**A part of the RSC site page, showing retrieved references**

# Password changing

When a CDS account is setup, the password is pre-expired. This means that the system requires users to change their password when they first directly logon. However, many methods of access to CDS, such as via the web or the ISIS client, do not directly logon to the system in the conventional unix sense. In these cases users are not forced to change their passwords and indeed there is no obvious way to do so.

We strongly recommend that users change their passwords, whether they normally directly logon to the service or not, especially if they have been advised of their password by email.

To change your password you need to directly login to the main CDS server, cds.dl.ac.uk, using telnet or a similar program. Upon logging in successfully you will see a screen similar to the following:

```
*****************************************************************************
* 01/05/01  The Solid Phase Synthesis (SPS) database has been updated. The    *
*           latest release (2001.1) contains 16,146 reactions, abstracted     *
*           from 2,842 citations. Go to the CDS website for further details.  *
*                                                                             *
* 15/05/01  The MDPI database of available chemicals has been updated. The    *
*           addition of 229 compounds now brings the total to 9,229 compounds *
*                                                                             *
* 22/05/01  This year's user meeting will be held on Tuesday July 17th at     *
*           Daresbury. All users are invited to attend. Type "forum_news" for *
*           more details.                                                     *
*****************************************************************************

            For help or details of packages available type "help". For
            a list of older login banner items type "omotd".

            There is also a link to a News Archive which includes recent
            and other relevant items on the CDS Web (http://cds.dl.ac.uk/cds).

UX:login: ERROR: Your password has expired.
UX:login: TO FIX: Choose a new one
Old password:
```

In the above case this is the first login and the system is prompting for a password change. If the system, for whatever reason, does not prompt you to change your password, you can do so by typing “passwd” at the cds% prompt. In both cases you will need to supply both your old and new passwords. Note that if you login using Secure Shell (SSH) the system will not prompt you for a new password, this is a bug and you will need to use the passwd command to change your password.

In order to improve password security there are a number of rules which must be followed for a password to be valid.

- Passwords must be at least 6 characters long.
- Passwords must contain at least two alphabetic characters.
- Passwords must contain at least one numeric or special character.

Passwords which do not conform to these rules will be rejected by the system.

# User meeting

This year's Chemical Database Service user meeting is planned to take place on Tuesday July 17th at Daresbury laboratory.

Topics for discussion this year include:

- The forthcoming trial of the Detherm physical property database
- Website redevelopment
- Enhancements to web interfaces to the data
- Future training strategy
- New CDS staff

The user meeting is an ideal opportunity to meet the CDS team, learn about future plans and to discuss any aspects of the Service. User representatives are particularly encouraged to attend, though all users are welcome.

As in previous years, we will be able to cover the travelling expenses of attendees. If you are interested in attending please contact us at cdsbb@dl.ac.uk.

# Website redesign

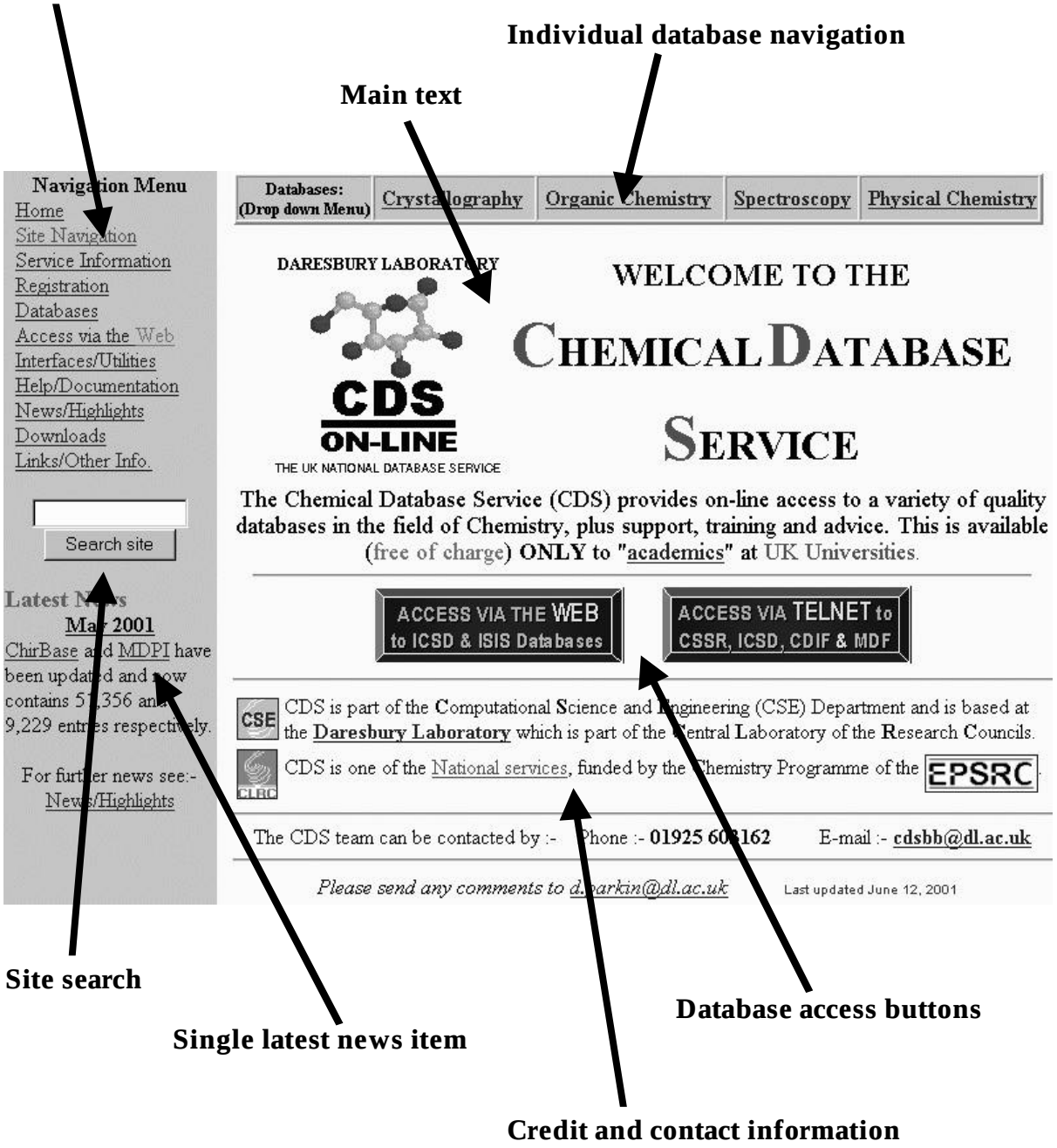
The CDS website has not had a serious overhaul for some years now. During this time the relative importance of a number of features has changed and the website has not adjusted to reflect this. It has merely got bigger and more complex.

We have therefore started a project to redesign the website and produce something that is simpler and laid out more logically. As a first step in this process, last month we ran a web-based survey about the current website. In all there were 130 replies to the survey and we would like to thank all the people who took the time to respond.

The general consensus from the survey responses was that the home page was too cluttered with a number of redundant elements. In addition some links were insufficiently prominent, such as a link to the ICSD and other web interfaces. The major use identified for the site was database access, followed by the downloading of client software.

Based on this information we are now in the process of redesigning the home page and rethinking the logical structure of the whole site. We anticipate the new site will be operational by the end of the summer.

**Possible new CDS website home page**




A prospective design for the site home page, taking the survey results into account, is shown above, with the main features labelled. We would appreciate any comments or suggestions about this design. Please send any such comments to us at cdsbb@dl.ac.uk

# Summary of 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 1,041,000 searchable reactions. Specialist databases available include Protecting Groups, Solid Phase Synthesis, BioCatalysis and Chiral Separations.

In addition there is the Available Chemicals Directory (ACD) which contains supplier information on 315,000 different compounds from over 630 different suppliers.

**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 99,059 $^{13}$C NMR; 999 $^{15}$N NMR; 856 $^{17}$O NMR; 2,183 $^{31}$P NMR; 1,825 $^{19}$F NMR; 5,000 $^{1}$H NMR; 20,898 infra-red spectra and 128,000 mass spectra.

**CSD** The Cambridge Structural Database. Crystal structure data for over 233,000 organic and organometallic compounds. Currently available under Cambridge's Quest and ConQuest retrieval software and our in-house software (CSSR).

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

**ICSD** Inorganic Crystal Structure Data File. About 59,500 inorganic structures - the companion file to the Cambridge organic file. ICSD is now accessible via the CDS website.

**MDF** Metals Data File. Crystal structure data for nearly 61,000 metals, alloys and intermetallics.

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

**ELYS** Electrolyte Solutions Database. Thermodynamic and transport property data such as density, viscosity and diffusion coefficients. Currently contains about 10,000 entries.

# Information

**General queries:**

Chemical Database Service (CDS)
Daresbury Laboratory
Daresbury, Warrington
WA4 4AD
(01925) 603162
Email cdsbb@dl.ac.uk

**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/cds

Web based interfaces to selected databases are also available from this site.

**Registration of new accounts:**

You can now register online for a CDS account from the CDS website.

**Documentation:**

Most documentation is available online and some can be downloaded from the CDS web site. Printed manuals can still be ordered from us at the above address.

**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.

**cds (main service machine):**

Internet number: 193.62.124.35
Internet name: cds.dl.ac.uk

**Comments:**

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

David Osa-Edoh
Email D.Osa-Edoh@dl.ac.uk