

Chemical Database Service (CDS) NEWSLETTER

Issue 16 Oct 2002

A summary of the main articles

CDS training courses are free of charge to users and potential users. The article on page 2 shows the type of courses we provide and what they entail.

Chirbase as been updated and it is now LitLink enabled. See page 3 for more details.

The CDS website has been revamped after consultation with our user community. Please see the article on page 4 for more information.

CrystalWeb, our web based application for searching crystallographic data has been updated. The new search forms can be seen on page 5.

See page 7 for the latest update to Specs surf.



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

Interactive database demos are now available on our website (page 7).

Two user queries and their solutions are presented on page 8.

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CDS Databases

ISIS: A chemical reaction information management system.

SPEC: SpecInfo is a multi-technique spectroscopic database

ICSD: Inorganic Crystal Structure Data File.

MDF: Metals Data File. It consists of Crystal structure data.

CDIF: Crystal Data Identification File.

ELYS: Electrolyte Solutions Database.

Detherm: Is one of the world's largest

thermophysical property databases.

CSD: The Cambridge Structural Database. Consisting of Crystal class and unit cell data.

IsoStar: A database of non-bonded interactions.

Special points of interest:

- Chirbase now LitLinked
- Website Updated
- Update to CrystalWeb
- Cheminform
- Free CDS training courses
- New on-line Demos

Free CDS training

The CDS provides lectures and one-day training events free of charge to the UK academic community, throughout the year. With students starting post-graduate courses and final year under graduate students thinking about their research projects, organising a CDS presentation day at your institution could prove to be one of the most important decisions of your academic year!

Courses

Service overview (what can CDS do for me): comprises a brief history of the service, the different areas of Chemistry we cover (Crystallography, Spectroscopy, Organic and Physical Chemistry), the main retrieval systems and their datasets, how to access CDS (via website, client/server application or X-windows). Some of the questions CDS can help you answer are listed below:-

Synthetic Organic Chemistry

- Planning a synthesis? Is there a published technique for your proposed chemical transformation?
- What sort of conditions have been tried for a given reaction? What were the yields?
- Should I be taking advantage of specialist datasets such as those covering Protection Group Chemistry, Solid Phase Synthesis, Biocatalysis or Chiral Separation?

Chemical Availability

- Need a compound (ranging from specialist organic and biochemical reagents to bulk inorganic)? Is it (or something similar) available from any chemical supplier worldwide?
- Do you need to pinpoint readily available starting materials and reagents?

Spectroscopy

- Have you recorded an NMR or IR spectrum? What structural features does it imply?
- Do you want to predict the spectrum of the target molecule or intermediate you have planned to make or you think you have made?

Crystallography

- Do you need to continue with this structure? Has it been done before?
- Do you want to explore non-bonded interactions in crystal structures?
- Anything with a cell dimension similar to what you have just measured?
- Will graphics tools help you visualise 3D structures?

Tailored and more Specific courses

Organic Chemistry: consists of our hosted reaction and molecular databases. This course also includes demos and set exercises on the use of each one of these databases.

Crystallography

Information on the Cambridge Structural Database (CSD), which is the only comprehensive collection of small-molecule organic and organometallic crystal structures. A demo of the software (Quest, Conquest, VISTA and Mercury) developed for the search, retrieval, display and analysis of CSD data. A demo of our new web-based crystallographic database tool called CrystalWeb.

Spectroscopy

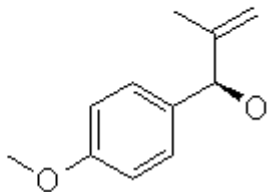
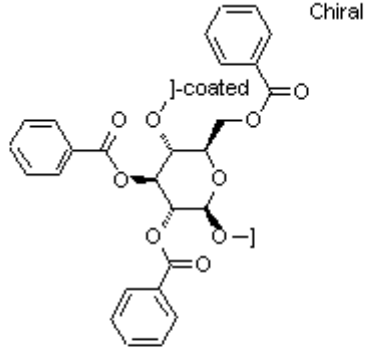
SpecInfo and Specsurf (a web-based version) - a multi-technique spectroscopic database system, covering NMR, MS and IR spectroscopy

CDS group representatives and departmental heads can choose which one would be best suited for their department. We recommend the overview presentation as a starting point. Users already familiar with CDS can choose from the more specialised courses. In order to organise a course we require a minimum of six students and you will need to organise access to local computer training suite facilities.

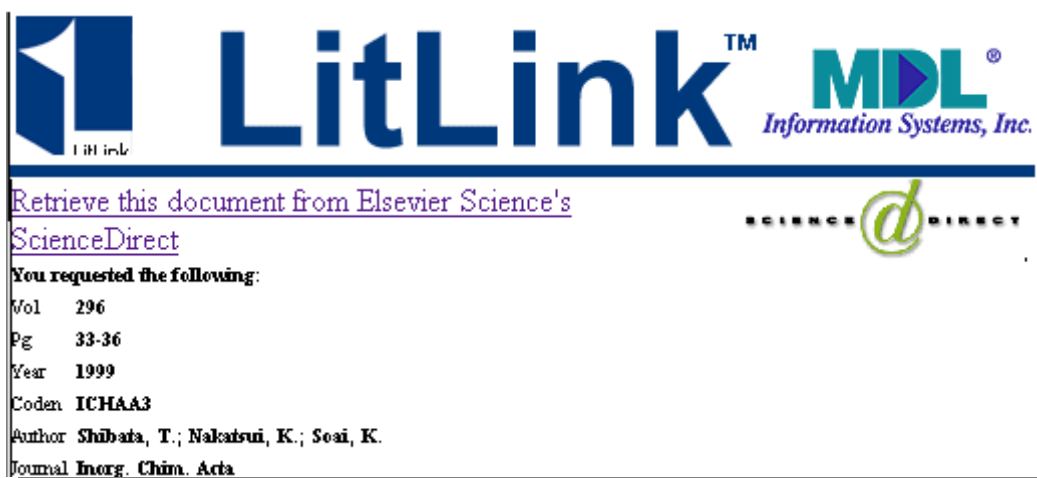
CHIRBASE

Chiral Separations of Enantiomers by Chromatography

[Next](#)
[Previous](#)

Sample				CSP					
									
Rxn No.	Ref. No.	1st	2nd	k1	k2	k2/k1	Res	Rt1	Rt2
45902	1	R	S					21.000000	37.000000
Reference									Ref.No
Shibata, T.; Nakatsui, K.; Soai, K.; Inorg. Chim. Acta, 296, 33-36, 1999.									25838

Chirbase: a powerful information system for chiral separation of enantiomers which is available via the web (<http://cds.dl.ac.uk/chirbase>) and the ISIS/Base client is now LitLink enabled. When the result of a search is retrieved, users can simply view the primary electronic literature by clicking on the highlighted journal reference.



LitLink™ **MDL®**
 Information Systems, Inc.

[Retrieve this document from Elsevier Science's ScienceDirect](#)

You requested the following:
 Vol 296
 Pg 33-36
 Year 1999
 Coden ICHAA3
 Author Shibata, T.; Nakatsui, K.; Soai, K.
 Journal Inorg. Chim. Acta

*“Chirbase is
now LitLink
enabled”*

Clicking on the reference opens a LitLink page containing links to the literature. Users are only able to gain access to the full text of the article free of charge if their institution subscribes to the journal.

New CDS Website

The CDS website has been updated. The site was updated because:

- It was too cluttered
- Users had to scroll to see all the information on a page - especially on low resolution screens
- The horizontal drop-down-menu at the top of the homepage did not work with new versions of browsers (Netscape 6.0)
- No obvious links for accessing web-based databases

The screenshot shows the old CDS website homepage. On the left is a large, vertical navigation menu with links like Home, Site Navigation, Service Information, Registration, How to Access CDS, Utilities, Help/Documentation, News/Highlights, Downloads, and Links/Other Info. Below this is a search box and a 'Search Site' button. The main content area features a horizontal menu at the top with categories: CRYSTALLOGRAPHY, ORGANIC CHEMISTRY, SPECTROSCOPY, and PHYSICAL CHEMISTRY. The central text reads 'New website' and 'DARESBUY LABORATORY Gateway to CDS WEB Interface'. To the right is a 'TELNET to the CDS Server' button. The main heading is 'CDS ON-LINE THE UK NATIONAL DATABASE SERVICE' and 'Chemical Database Service'. Below this is a 'Welcome to the Chemical Database Service' section with a grid of buttons for services like 'Map of this Site', 'CDS About the Service', 'Becoming a User', 'Packages Available', 'On-line Documentation', 'Access to the Data', 'Help for Users', 'News Archive', 'Downloads', 'Links', 'FAQ Database', and 'Newsletters'. At the bottom, there is a section for 'Latest News' dated October 2001, mentioning 'ChimePro 2.6 SP3' and 'Dethern database'. Logos for EPSRC and CSE are also visible.

Thanks to those of you who took part in our on-line questionnaire.

Conclusion from questionnaire

- Most people use the site to access the databases
- 25% of those who replied thought the home page was too cluttered

- The site should be simple with no "Las Vegas effect"

Advantages of the new website

- Consistent look and feel - Colours, text etc, increased speed of download - No large graphics files, Support all available browsers (version 4 and greater) on all machines, and easily updated (e.g. scripts put in *.js files)

Crystal Web

Crystal Web (<http://cds.dl.ac.uk/cweb>), CDS in-house web-based interface for accessing crystallographic databases available from the Cambridge Structural Database (CSD), Inorganic Crystal Structure Database, CrystMet Database and Crystal Data Identification File has been updated.

- Formula searching is now case insensitive and single letter elements are now

handled correctly

- Cell data and formula search forms are now available
- An element count search option is now available on the formula and comprehensive search forms
- Data from the May, July and September 2002 release of CSD has now been added

- An on-line CrystalWeb demo is now available at http://cds3.dl.ac.uk/cds/help/cweb_demo5_test.htm
- Structure downloads in CIF format are now supported for data from the CSD.
- Options to download references in EndNote format and a simple printable format have been added.



CrystalWeb

Formula search form

Click on individual field names to get help on searching that field.

Search

[Elements](#)

[Element count](#) =

[Compound name](#) contains

Switch to



CrystalWeb

Cell data search form

Click on individual field names to get help on searching that field

Search

Cell lengths	Cell angles
a <input type="text"/>	alpha <input type="text"/>
b <input type="text"/>	beta <input type="text"/>
c <input type="text"/>	gamma <input type="text"/>

*Flash animated
on-line
CrystalWeb
Demo now
available*

News Brief

ChemInform

Cheminform Reaction Library has been updated. The update includes new data from the weekly compendia of ChemInform, 2002, issues 1-26. This adds a total of 36,407 reactions and 50,631 molecules to the ChemInform database. There is a NEW database component file (cirx2003) which has been added with this update. ISIS/Base users MUST update their reaction browser file to take

account of this new component file. Otherwise they will fail to access the data added with the update.

In order to access all the CIRX databases the following list of Hviews should be in the Browser file :-

```
cirx2003+cirx2002+cirx9701+  
cirx9296+reflib+jsm+chc+  
orgsyn+sps+ spg+biocat
```

CDS User forum 2002

CDS's annual user meeting was staged on the 10th of July 2002. Users were introduced to the service's new development and the future direction of the service. To view the powerpoint presentation from the meeting see :-

http://cds.dl.ac.uk/CDS_forum2002/index.htm



LitLink

LitLink, which enables a one click access to primary electronic literature reference has been updated. Links to America Chemical Society (ACS), Chemweb and Wiley, which were previously broken, are now fixed. Please see:-

<http://cds.dl.ac.uk/cds/datasets/orgchem/isis/chemscape/litlink/litlink.html>

for more information on Litlink.

Solid-Phase Synthesis (SPS) Database

Solid Phase Synthesis (SPS) has been updated. Version 2002.1 of SPS contains 20,406 reaction collated from 3,487 published papers. New updates are

Cambridge Structural Database (CSD)

CSD updates are now more regular (every two months). The last update was on the 13th of Sept. 2002, containing over 2215 new entries.

Detherm

Thanks to those of you who took part in our on-line Detherm survey. Due to the very encouraging result and comments

obtained from the survey, a grant application for the long term funding of Detherm has been submitted to EPSRC. The result of this application will be known in November 2002.

In the mean-time there will be continued access for users until the end of October this year.

If the grant application is successful there might be a temporary stoppage in the service, while we await the funds to come through.

quarterly and it is estimated that at least 2,000 new reactions will be added annually.

*Detherm currently runs until
the end of October 2002*

Specsurf Upgrades

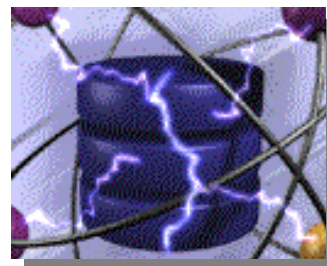
SpecInfo upgrades

In May the SpecInfo server was upgraded to version 4 and the SpecSurf web interface was upgraded to version 2. In addition a new dataset, the Aldrich Collection of H-NMR spectra, was added. This contains 11,678 H-NMR spectra and structures.

The X-Windows client is unchanged, but the SpecSurf web client is much improved. It loads faster and has some new functionality including H-NMR

prediction and stereochemistry recognition. In addition, the speed of some of the search routines has been improved

The SpecSurf web client is now sufficiently mature for us to recommend it as the best way to access the SpecInfo data.



SpecSurf XS is our new, easy-to-use, web browser client for accessing SpecInfo, MS and IR spectroscopy

On-line Demos

SpecSurf

Click on the links below to see movie introductions.

[Quick overview of SpecSurf.](#)

The following are more detailed overviews.

1. [Starting SpecSurf and a look at Menu Options](#)
2. [SpecSurf Structure Editor](#)
3. [SpecSurf Peaklist Editor](#)
4. [SpecSurf - Structure Search Results](#)
5. [SpecSurf - Spectrum Search Results](#)
6. [SpecSurf Spectrum Prediction](#)

On-line interactive demonstration programs of **SpecSurf**,

(<http://cds.dl.ac.uk/help/specsurf.html>)

Reaction Browser

(<http://cds.dl.ac.uk/help/reactionbrowser.html>)

and **CrystalWeb**

(http://cds.dl.ac.uk/cds/help/cweb_demo5_test.htm) are now available.

These on-line demos are intended to act as a learning aid for both novice and seasoned users of the service. In the future these demos will form part of an online training package, consisting of Power-Point presentations (of our training courses) and set exercises. So, if you would like to see some of the functionality as well as the ease of use of our databases, then try-out the online demos. You do not have to be a registered CDS user to view the demos.

ISIS/Base Reaction Browser

Click on the links below to see movie introductions.

[Quick Overview of Reaction Browser.](#)

1. [Starting Reaction Browser](#)
2. [Query Assistant Form](#)
3. [Expert Query Form](#)
4. [Selecting which databases to search](#)
5. [Looking at the Results](#)
6. [Schemes](#)
7. [Clustering your Hits \(and Examples\)](#)
8. [Derivative Reactions](#)

Two CDS user queries and their solutions.

1. CNMR prediction problem

Dear CDS, I am currently experiencing some problems in trying to predict C-13 NMR spectra using the SpecInfo package. These problems seem to have arisen since the recent upgrade. Briefly, when I try to do the prediction I get an error message "404 - file not found". I have not changed anything at this end, and I have previously used this program successfully for quite a long time. I am still using the X-windows interface (I did try the SpecSurf interface but it

caused my PC to lock up - "shortage of virtual memory"). I would be grateful for any suggestions you might have to get this working again as I have found the program very useful in the past.

Solution

With the upgrade of SpecInfo, new versions of all of the databases have been installed in the version 4 server. Due to the nature of the installation, the ordering of the databases is not the same as it was for the old version.

In essence, this means you are probably trying to do a C-13 NMR prediction with the data from a HNMR database. To solve this, you need to click on the Databases menu in the Assignment Editor and choose an appropriate database.

The StandardMixed database contains the bulk of the CNMR data, though there is some in the CNMR_Nat_Prod database. If you want to use all of the CNMR data, then you need to define a set of databases to use. You can do this by selecting Edit Database Sets from the Edit menu in the main window.

2. ISIS Database configuration

Dear CDS, I Cannot access ACD via ISIS/Base. This is the error message I get.

Error message when using ISIS/Base to access ACD:-

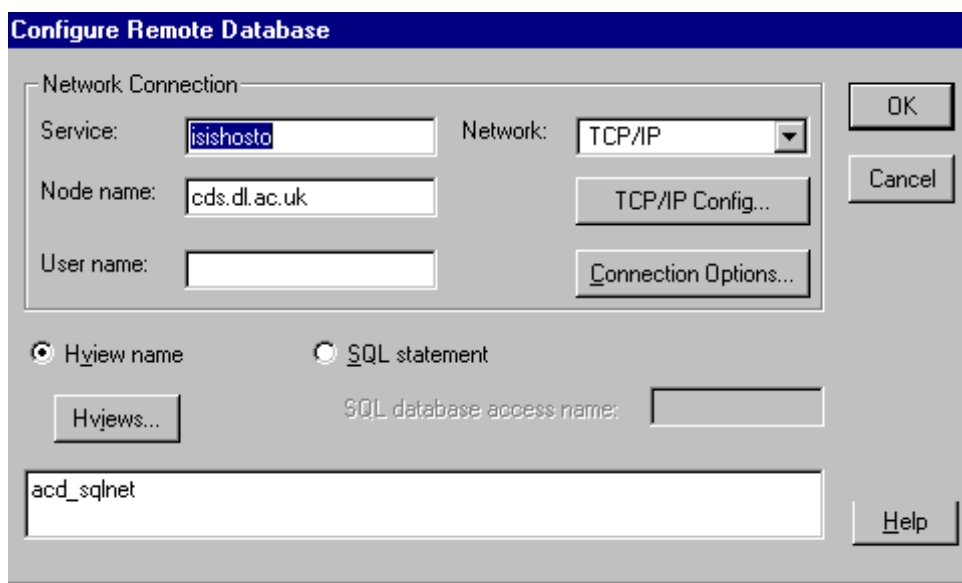
```
"Cant access network service:  
#TCPIP#@193.62.124.48@2055  
@#isishost0#test#password  
Please give an alternate:"
```

Solution

Start ISIS/Base. From the File menu select Configure Database (if you already have the database open, you will need to close it

before you can configure it).

Select the file acdfind.db from the acdfind directory and click on open. Reconfigure acdfind.db by changing servicehost to isishosto and hvview to acd_sqlnet.



Reconfigure database if you cannot access ACD via Isis-Base

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 1,149,537 searchable reactions. Specialist Databases available include Protecting Groups, Solid Phase Synthesis, BioCatalysis and Chiral

CSD: The Cambridge Structural Database. Crystal structure data for over 272,090 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.

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 11,000 entries.

Separations. In addition there is the Available Chemicals Directory (ACD) which contains supplier information on over 380,000 different compounds from over 651 different suppliers and National Cancer Institute Database.

This database is produced using data and structures from the National Cancer Institute (NCI) Developmental Therapeutic Program (DTP).

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.

Detherm: Is one of the world's largest thermophysical property databases of pure compounds and compound mixtures. For instance, in the field of vapour-liquid-equilibrium data, it contained more than 95 % of data published worldwide. It contains:-

3.75 Million data sets for around 120,000 systems (over 21,000 pure substances and 101,500 mixtures) covering more than 200 properties

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 102,459 ¹³C NMR; 999 ¹⁵N NMR; 856 ¹⁷O NMR; 2,183 ³¹P NMR; 1,825 ¹⁹F NMR; 10,600 ¹H NMR; 20,898 infra-red spectra and 128,000 mass spectra.

ICSD: Inorganic Crystal Structure Data File. Contains about 64,848 inorganic structures - the companion file to the Cambridge organic file. ICSD is now accessible via the CDS website.

“Detherm: Is one of the world's largest thermophysical property databases of pure compounds and compound mixtures”

General Enquiries

Chemical Database Service (CDS)
Daresbury Lab
Daresbury
Warrington
WA4 4AD
01925603162
Cdsbb@dl.ac.uk

**CDS website: [http://
cds.dl.ac.uk/cds](http://cds.dl.ac.uk/cds)**

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/cds>
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. Printed manuals can still be ordered from us at the above address.

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
(01925)603163