

Chemical Database Service (CDS) NEWSLETTER

Issue 17 March 2003



See <http://cds.dl.ac.uk/links/news.html> for this and previous editions of our newsletter

A summary of the main articles

Telnet users are advised to upgrade to Secure Shell. The article on page 2 explains why.

The DETHERM service was terminated at the end of October 2002. The CDS user forum will take place on the 16th of September 2003. See page 3 for more details.

See page 4 for the latest update to CrystalWeb.

More interactive

database demos are now available on our website (page 5).

Three catalogues have been removed from ACD and placed in MDL's Screening Compound Directory (MDL SCD). The new version of ACD now allows you to search and display 3D models. Please see the article on page 6 for more information.

ACD/3D viewer will convert the normally

two-dimensional structures into the three dimensional counterparts. It provides a wide range of features. See page 8/9 for this and other ISIS-add-ins.



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

Inside this issue:

Upgrade from Telnet to secure shell	2
So, what happened to Dethem	3
CDS user forum 2003	3
CrystalWeb Update	4
Online Database Demos	5
Available Chemical Directory (ACD)	6
News Brief	7
ISIS Add-ins	8
ISIS/Draw Tip	9
Databases available from the CDS	10
General Enquiries	11

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.

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

IsoStar: A database of non-bonded interactions.

Special points of interest:

- Upgrade Telnet
- Dethem
- User forum 2003
- ACD
- ISIS Add-ins
- More on-line Demos
- CrystalWeb update

What is Telnet?.....

The term "TELNET" refers to the remote login that is possible on the Internet because of the TELNET Protocol. It gives the user the ability to be on one computer system and do work on another over the Internet. For example, when you "telnet in from your department to CDS", you are using telnet to connect from one computer (your computer) to another computer (CDS's computer) which is in a different location. Once you have established your telnet connection, you then log in to the CDS computer and execute commands remotely on that computer through your telnet interface.

The use of this term as a verb, as in "Telnet to a host" means to establish a connection across the Internet from one host to another. Usually, you must have an account on the remote host to be able to login to it once you've made a connection

Alternative, why upgrade and what you should do.....

Secure Shell (SSH) enables you to connect securely to computers on the Internet that are running SSH. Older protocols such as Telnet, FTP, rsh, rlogin, and rexec transmit everything in plain text over the network for all to see. This means that someone illegally monitoring network traffic can pick up your password. If this happens it is potentially a disaster, since someone with your username and password can gain access to your accounts and all files on your disk space. You need to upgrade to SSH to protect your password. SSH encrypts the information being transmitted, protecting your privacy, passwords, and other sensitive information.

For information on obtaining and installing SSH clients for Windows (TTSSH and PuTTY), Macintosh (Nifty telnet and MacSSH) and Unix (SSH and OpenSSH) see <http://cds.dl.ac.uk/links/news11701.html>.

SSH provides a more secure computing environment than Telnet

So, what happened to Detherm?.....

The DETHERM database is produced by DECHEMA e.V. in cooperation with the FIZ CHEMIE in Berlin and the DDBST GmbH, Oldenburg. The database includes thermophysical property data for about 21,000 pure compounds and 101,000 mixtures. It also contains literature values, together with bibliographical information, descriptors and abstracts.

The full collection of Detherm datasets was made available to all registered CDS users. Initially CDS carried out a preliminary user evaluation trial of the database between September 2001 and March 2002.

As a result of a successful trial and favourable feedback from our Detherm user survey, CDS applied to the EPSRC for long term funding of Detherm and we arranged for continued access by registered CDS users until October 2002, whilst the funding application was being reviewed. The funding application was supported by the comments provided by the users who took part in the Detherm evaluation survey and the research highlights provided by Detherm users.

The funding application was strongly supported by the referees, and went forward to the EPSRC prioritisation panel. Unfortunately it failed at this stage in the face of strong competition for the limited funds available in the funding round. Accordingly the Detherm service was terminated at the end of October 2002, and we are currently re-assessing the situation.

On behalf of the CDS team I would like to thank the users who took part in the survey as well as those who provided research highlights, and we will keep you informed of any developments with regards to future Detherm provision by the CDS. For more information on Detherm see

<http://cds.dl.ac.uk/links/news11702.html>

CDS User Forum 2003

The annual CDS user meeting is scheduled to take place on Wednesday the 16th of September at Daresbury laboratory. Topics for discussion will include

- The future of Detherm
- CDS hardware changes
- Future of ISIS

The CDS user forum will take place on 16th of September

As in previous years 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.

CrystalWeb update

“LitLinked” enabled reference which gives direct access to the primary electronic literature

Unit cell displayed in Chime

4022

Inorg. Chem. 2001, 40, 4022–4029

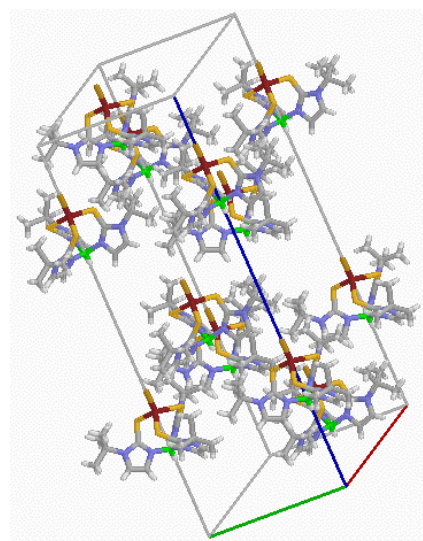
Sulfur-Rich Zinc Chemistry: New Tris(thioimidazolyl)hydroborate Ligands and Their Zinc Complex Chemistry Related to the Structure and Function of Alcohol Dehydrogenase

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The 1-substituted tris(2-thioimidazolyl)hydroborate ligands Ti^R were prepared as the potassium salts from KBH_4 and the corresponding 1-R-2-thioimidazole for $R = t\text{-Bu}$ and $C_6H_4\text{-}p\text{-CH(CH}_3)_2$ (Cum). Their reactions with zinc salts yielded the tetrahedral complexes $Ti^RZn\text{-}X$ with $X = F, Cl, ONO_2$ and $(Ti^{t\text{-Bu}})_2Zn$. With zinc perchlorate the labile perchlorate complexes $Ti^RZn\text{-}OCIO_3$ were obtained. They served as starting materials for the incorporation of substrates which are relevant for the chemistry of horse liver alcohol dehydrogenase: Ethanol led to $[Ti^{t\text{-Bu}}Zn\text{-}EtOH] ClO_4\text{-}EtOH$, *p*-nitrophenol (NitOH) yielded $Ti^{Cum}Zn\text{-}ONit$. Pyridine-2-carbaldehyde and salicylic aldehyde were incorporated as N(pyridine) and O(phenolate) coligands with possible additional O(aldehyde) coordination. Substituted pyridyl methanols ($R\text{-PyCH}_2OH$) yielded the trinuclear complexes $[(Ti^{t\text{-Bu}})_2Zn_3(R\text{-PyCH}_2O)_2] (ClO_4)_2$ with bridging Ti and pyridylmethoxide ligands. Preliminary experiments on the functional modeling of alcohol dehydrogenase have shown that $TiZn$ complexes promote both the dehydrogenation of 2-propanol and the hydrogenation of pentafluorobenzaldehyde.



- Data from the February 2003 Update to the CSD has been added
- Queries from the comprehensive search form can now be saved
- The print references options now outputs unique references
- Download references in EndNote format
- Release 2002-1 of ICSD has now been added.

Available Chemicals Directory (ACD)

Screening Compounds Catalogues Removed

Three catalogues have been removed from ACD and placed in MDL's Screening Compound Directory (MDL SCD). They are SALOR (Sigma-Aldrich Library of Rare Chemicals), MAYBRIDGE and BIONET. This is because most of the chemicals in these catalogues are not 'off the shelf' compounds and are more intended for high throughput screening. This does, however, mean that the remaining compounds in ACD should be readily available compounds. We intend to hold a trial very soon of MDL SCD, which contains over 2 million chemical structures and includes 3D models.

3D Models in ACD

The new version of ACD now allows you to search and display 3D models for over 99% of the structures. You can apply 3D geometric constraints to 3D objects such as points, lines, planes, centroids, and normal vectors. 3D geometric constraints include distances, angles, dihedral angles, exclusion spheres, linearity constraints, and planarity constraints.

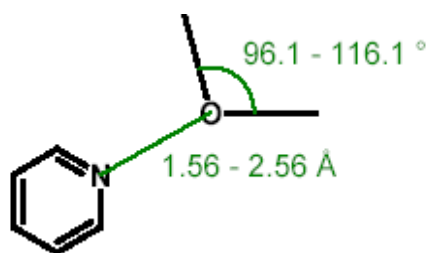
SubStructure Searches (SSS) can be performed on these queries using the MODEL tab in ACD Finder or the 3D Model Query Form on the Web.

Conformationally Flexible Substructure (CFS) searching can also be done from ISIS/Base. It finds 3D structures in the database that contain the query structure embedded within them (SSS) AND those that can be made to fit the query by rotating single bonds in the structure.

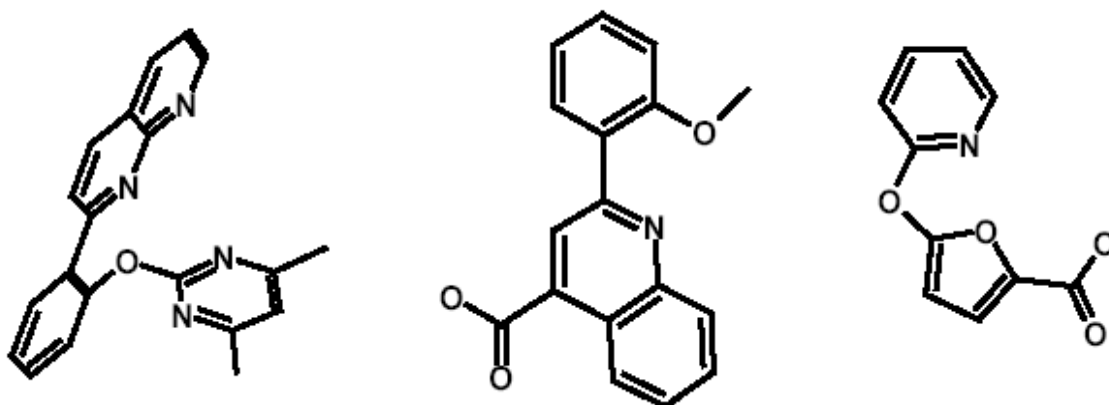
Note: CFS searches can take a long time. Use a SSS search where possible.

Information on 3D queries can be found in the online help in the ACD Finder application on your desktop machine.

For Example, a SSS (or CFS) search using the following Query:-



Should find hits like these:-



News Brief

Annual Research Highlights

CDS is in the process of renewing its EPSRC funding. As part of the grant renewal application we are required to provide highlights of research carried out with the aid of the service. We would like our users to send in research highlights of no more than 600 words (word or pdf document), ideally written for a non-specialist but scientifically literate audience. The format is similar to that of the research summary requested from EPSRC-funded researchers in their final reports. Our current collection of research highlights can be viewed at http://cds.dl.ac.uk/report/res_high.htm. A searchable "LitLinked" (see below) database system of our research highlights collection and their cited references is currently been developed and will be available soon.



Litlink

LitLink allows one click access to primary electronic literature reference and has been recently updated to version 3.0. LitLink Version 3.0 comes with enhanced facilities and an extended journals knowledge base, and we have transferred all the extra Journals we added for our implementation of LitLink 2.2. No reconfiguration is required to use the LitLink facilities available via the CDS version of ConQuest, ICSD-WWW, CrystalWeb, ReactionWeb or the web interface to ChirBase. LitLink currently works with the ISIS Reaction Browser. To "LitLink enable" your Browser, you need to download the LitLink Add-in software, which is available from the CDS website (<http://cds.dl.ac.uk/links/news11705.html>). Some configuration changes are required if you use the LitLink Add-in for ISIS/Base. The relevant configuration parameters are now:

Host Name: cdsLL.dl.ac.uk
Port: 80
Path: LitLink/servlet/LitLink

See <http://cds.dl.ac.uk/links/news11706.html> for further details. If you have a copy of the Cambridge database on your local workstation you can also use the CDS LitLink server but will also need to reconfigure ConQuest to pick up details for version 3.0.

NOTE for ConQuest you may require an additional "/" at the beginning of the path name!

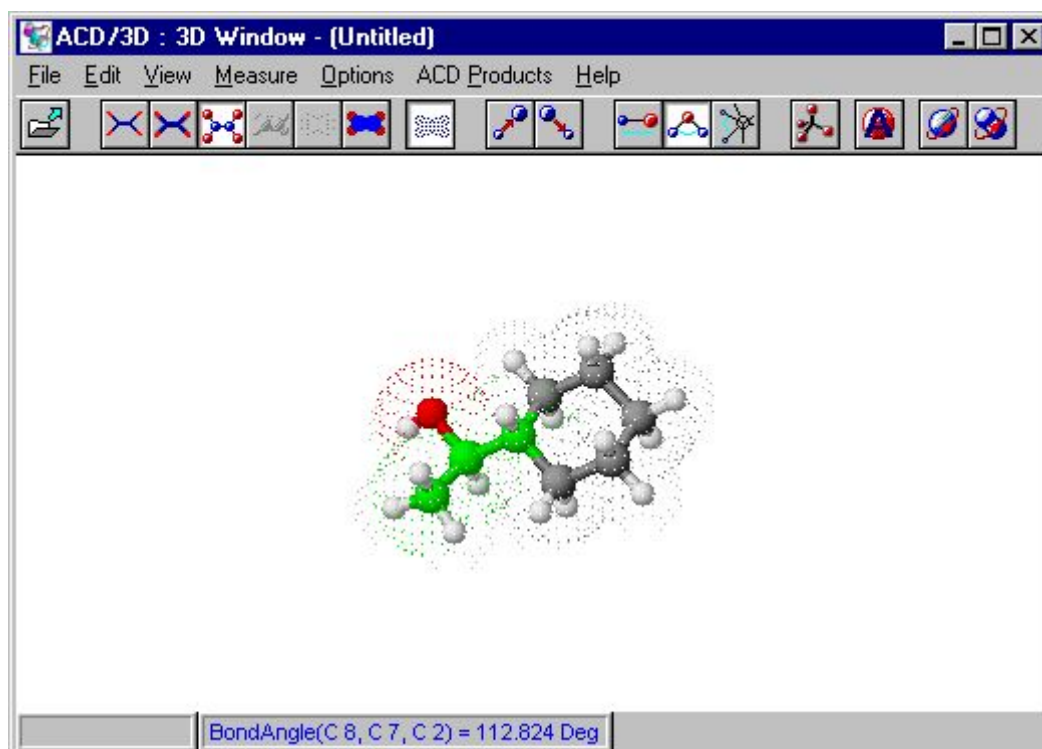
ISIS Add-ins

ACD/3D Viewer

ISIS automatically installs the “View in Rasmol” Add-in but this does not turn 2D molecules into 3D molecules.

ACD/3D will convert the normally two-dimensional structures into the three dimensional counterparts. It provides a wide range of features. You can:

- Specify the representation of the structure displayed: colour and view type of molecules. Structural display options range from using sticks, balls-and-sticks to the more sophisticated opaque space-filling technique or transparent dots-on-a-sphere.
- Copy the contents of the workspace onto the Clipboard using the Copy command (Edit menu). Once the object has been copied, you can paste it into other Microsoft Windows applications, such as word processors or graphics applications.
- Customise fully and individually the atomic radii.
- Perform atom-to-atom measurement, and 3- and 4-vertex (torsion) angle measurement.
- Import structures into a MOL-format file, which is highly compatible with other computational chemistry software.
- Set a structure to auto-rotate, with or without changing the display

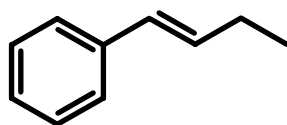


ISIS Add-ins Cont.....

ACD/Name

Version 2.4 of ISIS now includes an Add-in to 'Generate Name with Autonom'. However, ACD/Name is also available which helps you to determine the chemical name according to systematic application of the nomenclature rules agreed upon by the International Union of Pure and Applied Chemistry (**IUPAC**), International Union of Biochemistry and Molecular Biology (**IUBMB**), and the Chemical Abstracts Service (**CAS**).

The freely available version is only for molecules containing no more than 50 atoms, and no more than 3 rings, with atoms from among only H, C, N, P, O, S, F, Cl, Br, I, Li, Na, and K (You can draw over 70% of all known organic compounds and more than 10^{12} of those compounds which have not yet been synthesised!)



ACD/Name:

(1E)-but-1-enylbenzene

AutoNom:

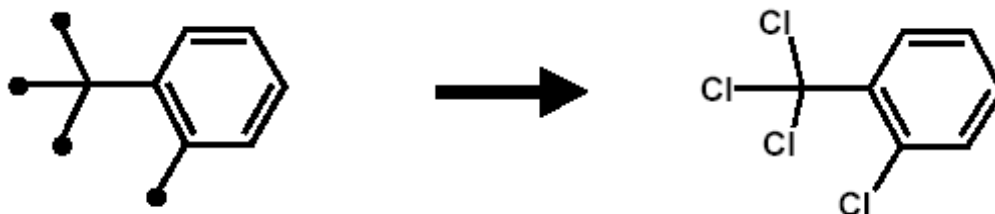
But-1-enyl-benzene

ISIS/Draw Tip

Change Multiple Atoms Quickly and Easily

One way to speed up drawing is to highlight an atom, type in the Symbol then press the Enter key. If you use the **Shift** key you can click on multiple atoms, so you can change more than one atom in a single step.

For example, if you want to draw 1-Chloro-2-trichloromethyl-benzene, draw the structure shown below. Then, holding down the Shift key, click on the 4 atoms where you would like to add chlorine, type "cl" then press the Enter key.



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 almost 1,200,000 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 over 228,246 different compounds from over 650 different suppliers. The National Cancer Institute Database is produced using data and structures from the National Cancer Institute (NCI) Developmental Therapeutic Program (DTP).

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 102,059 ¹³C NMR; 999 ¹⁵N NMR; 856 ¹⁷O NMR; 2,183 ³¹P NMR; 1,825 ¹⁹F NMR; 26,000 ¹H NMR; 20,898 infra-red spectra and 128,000 mass spectra.

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 VISual STATistics 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.

ICSD: Inorganic Crystal Structure Data File. Contains about 67,200 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 11,000 entries.

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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**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:
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