

the Chemical Database Service

NEWSLETTER Winter 2008

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Welcome

Welcome to the Winter 2008 Newsletter of the Chemical Database Service (CDS)

The new Service started in April 2008 following a successful tender bid to supply chemistry databases to the UK academic community for at least the next 3 years.

See inside for details of the current state of the Service and what has changed over the past 6 months.

There is also news of new databases and access methods.. See pages 6/7 and 8.

Latest News

ACD/Labs I-Lab

Version 11 server is now available. Increased database size and improvements to the algorithms mean enhanced prediction capabilities. More details on page 3.

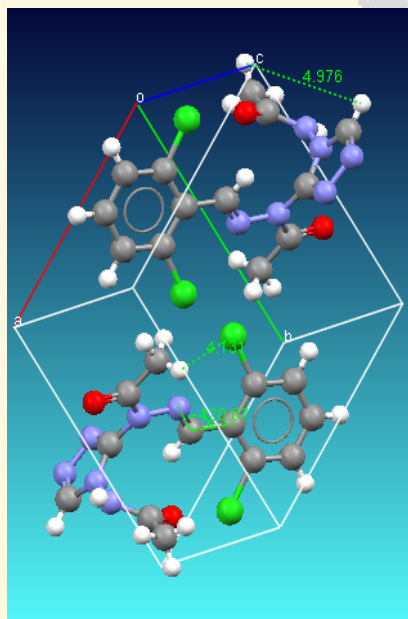
Security

In order to improve our security, we have withdrawn support for normal ftp clients so that plain text passwords are not transmitted over the network. See page 5.



Links used in this Newsletter can be found at:- <http://cds.dl.ac.uk/letterlinks>

Crystallography Databases

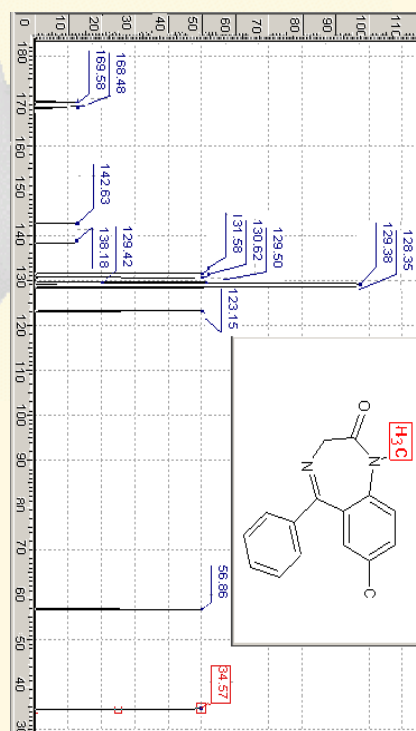


Thermophysical Database

DETERM ... on the WEB
Thermophysical Properties of Pure Substances & Mixtures

No.	T boiling K	vapor pres Pa
1	260.74	0.10
2	265.99	0.20
3	269.16	0.30
4	271.45	0.40
5	273.26	0.50
6	274.75	0.60
7	276.03	0.70
8	277.14	0.80
9	278.13	0.90
10	279.03	1.0

Spectroscopy Databases



New Updates and News

Detherm

Detherm has been updated. Version 2007 now contains nearly 6 Million data sets covering 28,000 pure substances and 106,000 mixtures.

This new data can be accessed by either the Web or by Client software.

Users should also download the latest version of the Detherm client.

For details follow the download link: <http://cds.dl.ac.uk/cds/download/detherm.html>

Versions 2.1 and 2.2 of the client software should still work with the new data, but we advise you to upgrade to the new client when convenient. Versions 2.0 and earlier will not work with the new data and users should upgrade immediately.

Crystallography

The Cambridge Structural Database System has been updated. The August 2008 Update has been made available via ConQuest, QUEST and CrystalWeb This Update adds 20,244 new structures making the total number of entries 456,628 . Cambridge has sent their apologies for the delay between this and the last (January 2008) Update. A new update is also due around December 2008.

CCDC User Survey

The CCDC has recently launched a User Survey to help determine future developments for the Cambridge Structural Database. They would particularly value responses from as many as possible within the CDS user community. The survey is not just relevant to practicing crystallographers. The CCDC wishes to obtain opinions from as many general users as possible, to inform decisions on future data content and delivery. For further details of the survey follow the link: http://www.ccdc.cam.ac.uk/products/csd/user_survey The survey has eleven sections, but there is a prize draw. You are automatically entered into the draw if you complete the survey by the 31th December 2008 closing date!

CrystalWeb

CrystalWeb now contains data from repositories such as Southampton - **before they get into Cambridge Structural Database**. CDS extracts the latest data as meta-data from the Southampton eCrystals archive for Crystal Structures generated by the Southampton Chemical Crystallography Group and the EPSRC UK National Crystallography Service and adds it to CrystalWeb. This could be 3 or 4 months before a new update from CCDC is received.

New Data Spectroscopy



ACD/Labs I-Lab System

**Remember, these set of databases are due for renewal after the end of March 2009.
We need to show EPSRC that they are important so make every effort to use them now.**

ACD/Labs I-Lab Upgrades Predictors and Database Searches to Version 11.0 Capabilities

**¹H NMR database search
(over 193,000 structures)**

New algorithm improvements using a combined approach of:

HOSE code
Neural network
Increments

Improved prediction for stereochemistry

Internal database expansions

Predictions are now based on 1,666,199 ¹H chemical shifts

Prediction of heteronuclear couplings

**¹³C NMR database search
(over 186,000 structures)**

New algorithm improvements using a combined approach of:

HOSE code
Neural network
Increments

Improved prediction for stereochemistry

Internal database expansions

Predictions are now based on 2,430,218 ¹³C chemical shifts

Prediction of heteronuclear couplings

**¹⁵N NMR database search
(over 8,800 structures)**

Internal database expansions

Predictions are now based on 21,435 ¹⁵N chemical shifts

**¹⁹F NMR database search
(over 15,400 structures)**

Internal database expansions

Predictions are now based on 35,014 ¹⁹F chemical shifts

**³¹P NMR database search
(over 26,100 structures)**

Internal database expansions

Predictions are now based on 33,695 ³¹P chemical shifts

**PK_a database search
(over 15,900 structures)**

Version 11 of the pK_a model boasts the addition of >2,000 pharmaceutical lead compounds to the internal database. Analysis of the new subset of compounds along with a portion of the existing dataset generated over 600 new and revised Hammett equations. Improvements to the pK_a model will have a significant effect on our log*D* and solubility modules since pK_a is integral to these modules.

**Log *P* database search
(over 18,400 structures)**

New Model for Log*P* Prediction

A generation model for prediction of log*P* is introduced which combines data for ~12,000 compounds from ACD/Labs' internal training set with new experimental data from >13,000 pharmaceutical lead compounds. All internal fragments and incremental values were recreated using the new combined dataset to provide improved predictions for compounds of pharmaceutical interest, without sacrificing quality of prediction for non-pharmaceuticals. Changes to the log*P* model also impact log*D* and solubility modules due to the inclusion of log*P* in these models.

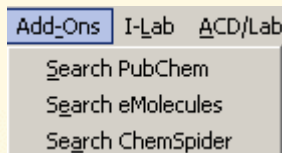
Note: If you use ChemSketch and have problems logging on to CDS, please either download the latest version (Version 11) **from the CDS download area** or, if you are using an earlier version, download the patch (dmillib.dll) and use it to replace the installed version.

Start your download at:- <http://cds.dl.ac.uk/cds/download/chemsketch.html>

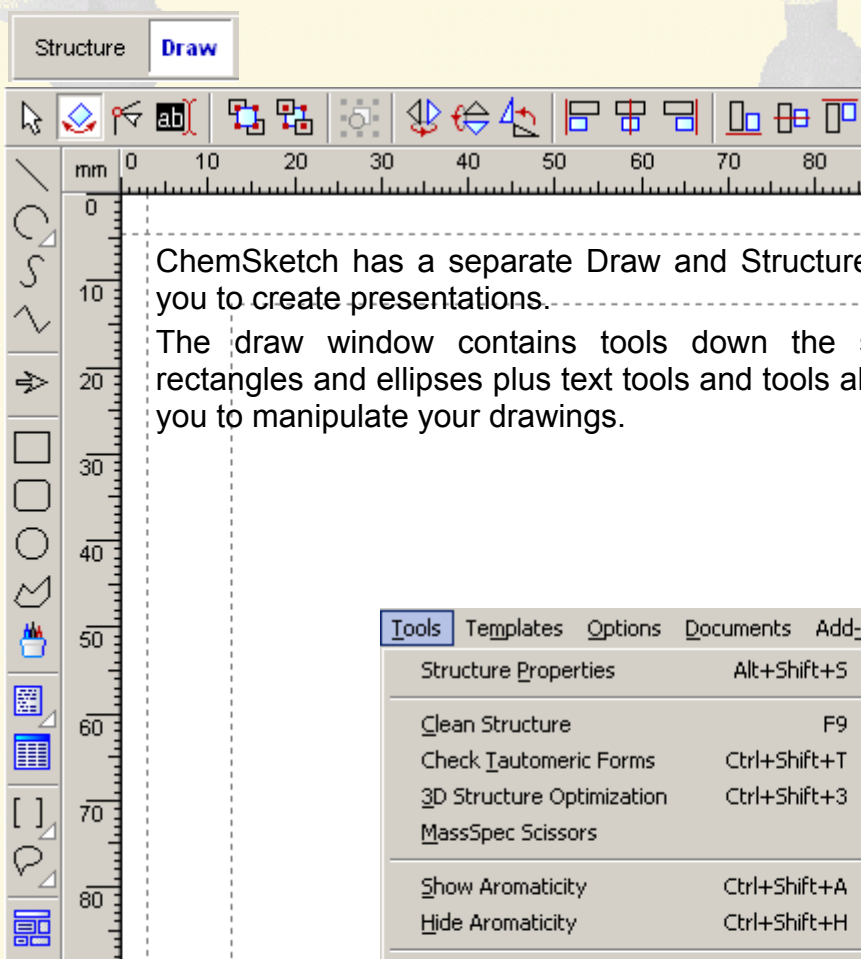
Did You Know

Chemsketch

If you draw a molecule using ChemSketch, you can use it to search PubChem, eMolecules or ChemSpider.

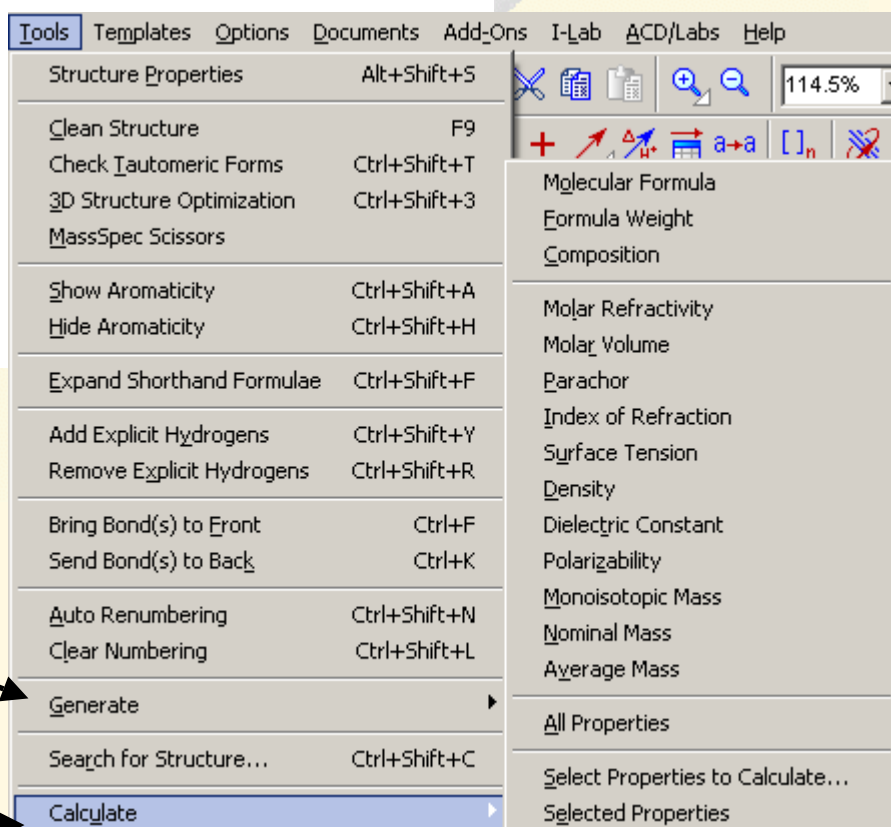


There are icons at the top right hand corner to connect you with these databases or you can use the Add-Ons menu and choose the option there.



ChemSketch has a separate Draw and Structure window that allows you to create presentations.

The draw window contains tools down the side such as arcs, rectangles and ellipses plus text tools and tools along the top that help you to manipulate your drawings.



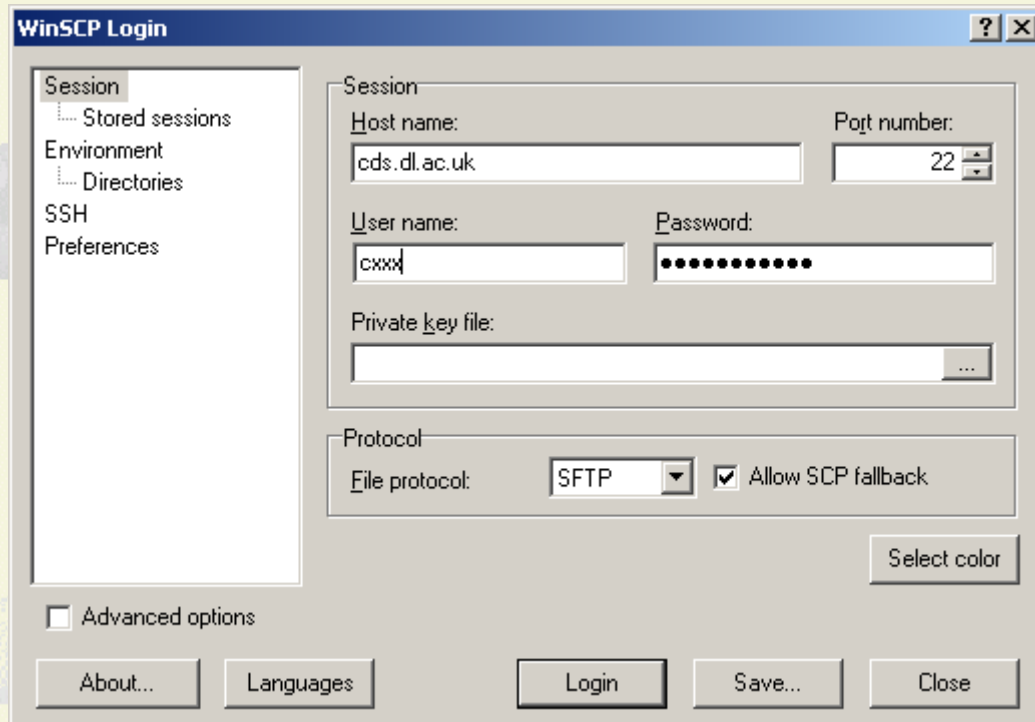
ChemSketch can generate a name, SMILES or InChI from a structure - **and vica-versa**

It can also calculate a number of physical properties - all without connecting to I-Lab.

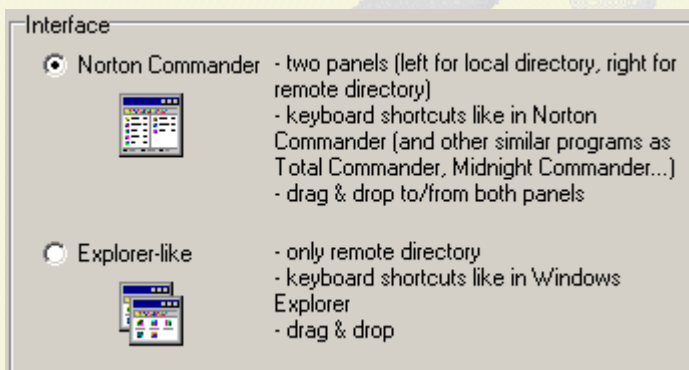
What's New

Security Updates

Secure Shell is a secure replacement for programs that login remotely to other hosts -- programs such as **telnet**, **ftp** and **rlogin**. In order to improve our security, we have withdrawn support for normal ftp clients so that plain text passwords are not transmitted over the network. Please use **SFTP** and **Secure Shell (SSH)** clients such as [WinSCP](#), [PuTTY](#), [Open SSH](#), [MacSSH](#) or [SSH Secure Shell](#) [**CDS recommends PuTTY and WinSCP**]

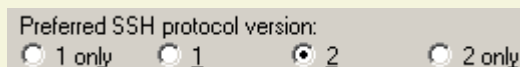


WinSCP is an open source SFTP client for Windows. Its SSH protocol core is based on PuTTY. Its main function is the secure file transfer between a local and a remote computer. Telnet and Rlogin are old protocols offering minimal security and should not be used.



With WinSCP you can even choose the type of interface.

The SSH protocol must be level 2 (not 1) for safer password encryption. Setting up version 2 SSH is easy with WinSCP and PuTTY - just tick the appropriate box

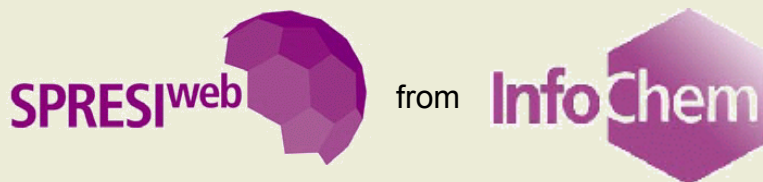


PuTTY can also be used with Exceed to provide X-windows (need to *Enable X11 forwarding*)

See http://cds.dl.ac.uk/cds/interface_and_utilities/secureshell.html for more details.

Coming Soon

(January 2009)



SPRESIweb is a chemical **STRUCTURE** and **REACTION** database that provides direct access to over:

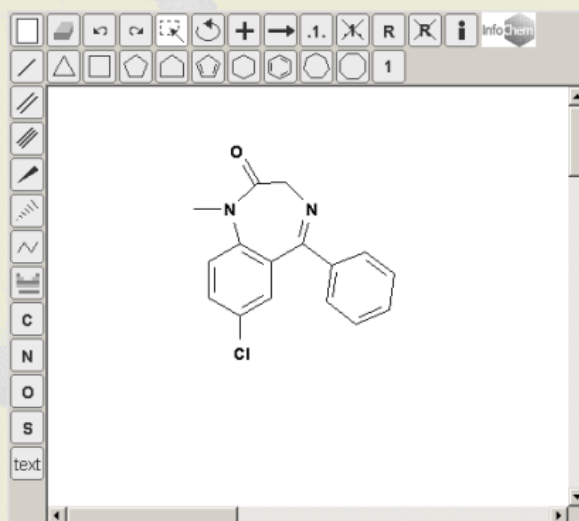
- 6.0 million structures
 - 3.8 million reactions
 - 28 million factual data entries
- extracted from**
- 627,000 references
 - 164,000 patents.

History

In the 1970s the All-Union Institute of Scientific and Technical Information of the Academy of Sciences of the USSR (VINITI) in Moscow and the German Zentrale Informationsverarbeitung Chemie in Berlin (ZIC) began to build a chemistry database. This data collection was designed to include structures, chemical properties, physical properties, keywords, and factual data for the substances. Ever since, VINITI has provided regular updates. Since 2002 the research application SPRESIweb has enabled access to this database.

Structures

- Perform exact and substructure search as well as parent, tautomer and isomer search.
- Retrieve property data (physical properties and keywords) as well as trivial/trade names and synonyms.
- See immediately if the compounds in your hit list are commercially available.
- Download your result lists as SDfiles.
- Choose your favourite structure editor (ISIS/Draw, ChemDraw or InfoChem's Java applet *ICEDIT*) to formulate your query.



Access

SPRESIweb has a user-friendly, highly intuitive web interface. Start your web browser; log in to CDS and follow the links to SPRESI web.

7-Chlor-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-on

Molecule data

Molecular Formula: $C_{16}H_{13}ClN_2O$
Molecular Weight: 284.75
Spresi RegNo: 0012368-300
[» More Names/Synonyms](#)
[» Show details](#)

Calculated Properties

logP: 3.109
Rotatable bonds: 2
H-Acceptors: 2
H-Donors: 0
Calculated with MOE 2004.3
(Chemical Computing Group Inc.)

References

[» Journal articles:](#) 269
[» Patents:](#) 50
[» Other references:](#) 26

External Links

[» Use ACD/I-Lab for Predictions](#)
[» Search in MetaXchem](#)
[» **NEW:** NMR prediction \(SpecInfo\)](#)
[» Search in ChemNavigator](#)

Select Supplier ...

Reactions

Discover new individual synthesis pathways with SPRESIweb.

- Define reactant and/or product to perform a reaction substructure search.
- Look for *similar reactions* having the same chemical transformation.
- Search for a particular reaction mechanism using the unique *name reactions* tool *ICNameRXN*
- Retrieve reaction conditions (catalyst, temperature, solvent, etc.).
- See at a glance if the reactants or products of your hit list are commercially available.
- Download your hit list as an RDfile.

References

Journal Articles	
1	Del Pozo Carlos, Macias Alberto, Lopez-Ortiz Fernando, Angel Maestro Miguel, Alonso Eduardo, Gonzalez Javier: Diastereo- and enantioselective synthesis of novel beta-lactam-containing 1,4-benzodiazepines through a ketene-imine cycloaddition reaction (JOURNAL) Eur. J. Org. Chem., (2004) N 3, 535-545
2	Cholbi-Cholbi M. F., Martinez-Pla J. J., Sagrado S., Villanueva-Camanas R. M., Medina-Hernandez M. J.: Determination of anticonvulsant drugs in pharmaceutical preparations by micellar liquid chromatography (JOURNAL) J. Liq. Chromatogr. and Relat. Technol., 27 (2004) N 1, 153-170
3	Ghosh Priyankar, Krishna Reddy M. M., Ramteke V. B., Sashidhar Rao B.: Analysis and quantitation of diazepam in cream biscuits by high-performance thin-layer chromatography and its confirmation by mass spectrometry (JOURNAL) Anal. Chim. Acta, 508 (2004) N 1, 31-35
4	Gunnar Teemu, Mykkaenen Sirpa, Ariniemi Kari, Lillsunde Pirjo: Validated semiquantitative/quantitative screening of 51 drugs in whole blood as silylated derivatives by gas chromatography-selected ion monitoring mass spectrometry and gas chromatography electron capture detection (JOURNAL) Journal of Chromatography B, 806 (2004) N 2, 205-219
5	Sawtschuk S. A., Simonow E. A., Sorokin W. I., Dorogokupech O. B., Wedenin A. N.: Primenenie metoda fiksachii wremen uderzhiwanija pri khromato-mass-spektrometrijskikom i khromatografitskikom opredelenii narkoticheskikh sredstw (JOURNAL) Zh. anal. khimii, 59 (2004) N 10, 1059-1069
6	Salem A. A., Barsoum B. N., Izake E. L.: Potentiometric determination of diazepam, bromazepam and clonazepam using solid contact ion-selective electrodes (JOURNAL) Anal. Chim. Acta, 498 (2003) N 1-2, 79-91
7	Hamerak Zdenko, Gao Dajana, Kova Spomenka, Herold-Brundi Antonija, Vickovi Ivan, unji Vitomir:

Access patent references and scientific literature published by the most relevant chemistry journals back to 1974.

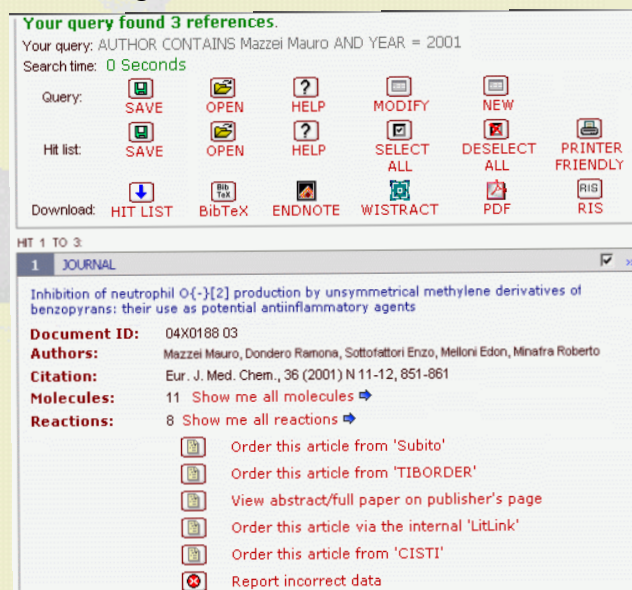
File your literature references by downloading hit lists in BibTex and EndNote format.

Links

Thanks to the web-based architecture, SPRESIweb offers direct links to:

- Catalogue data of several chemicals suppliers

- A full text article or abstract on the publisher's web site
- Document delivery services
- Direct view or purchase of patents
- Cheminformatics services such as ChemNavigator, ACD/Labs Online, Chemie.de.



Your query found 3 references.

Your query: AUTHOR CONTAINS Mazzel Mauro AND YEAR = 2001
Search time: 0 Seconds

Query: [SAVE] [OPEN] [HELP] [MODIFY] [NEW]

Hit list: [SAVE] [OPEN] [HELP] [SELECT ALL] [DESELECT ALL] [PRINTER FRIENDLY]

Download: [HIT LIST] [BibTeX] [ENDNOTE] [WISTRACT] [PDF] [RIS]

HIT 1 TO 3: JOURNAL

Inhibition of neutrophil O₂ production by unsymmetrical methylene derivatives of benzopyrans: their use as potential antiinflammatory agents

Document ID: 04X0188 03

Authors: Mazzel Mauro, Dondero Ramona, Sottoraffi Enzo, Melloni Edon, Minafra Roberto

Citation: Eur. J. Med. Chem., 36 (2001) N 11-12, 851-861

Molecules: 11 Show me all molecules

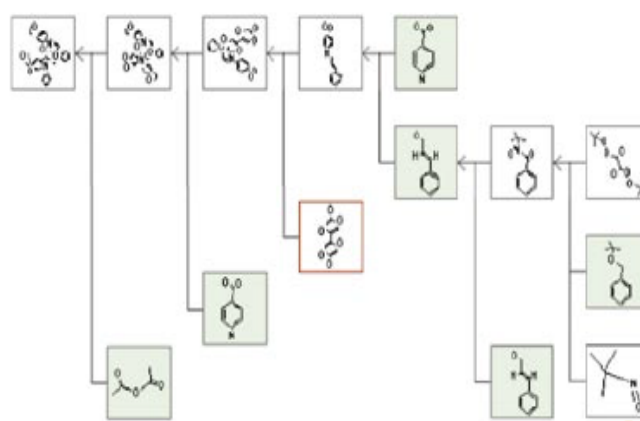
Reactions: 8 Show me all reactions

- Order this article from 'Subito'
- Order this article from 'TIBORDER'
- View abstract/full paper on publisher's page
- Order this article via the internal 'LitLink'
- Order this article from 'CISTI'
- Report incorrect data

STS

Synthesis of given target molecules can be planned interactively with the synthesis-planning tool *Synthesis Tree Search* (STS).

Choose the best synthesis pathway to your target molecule! With this highly interactive synthesis-planning tool you will be able to build an individual synthesis strategy based on millions of published reactions.



Coming Soon?

WebCSD

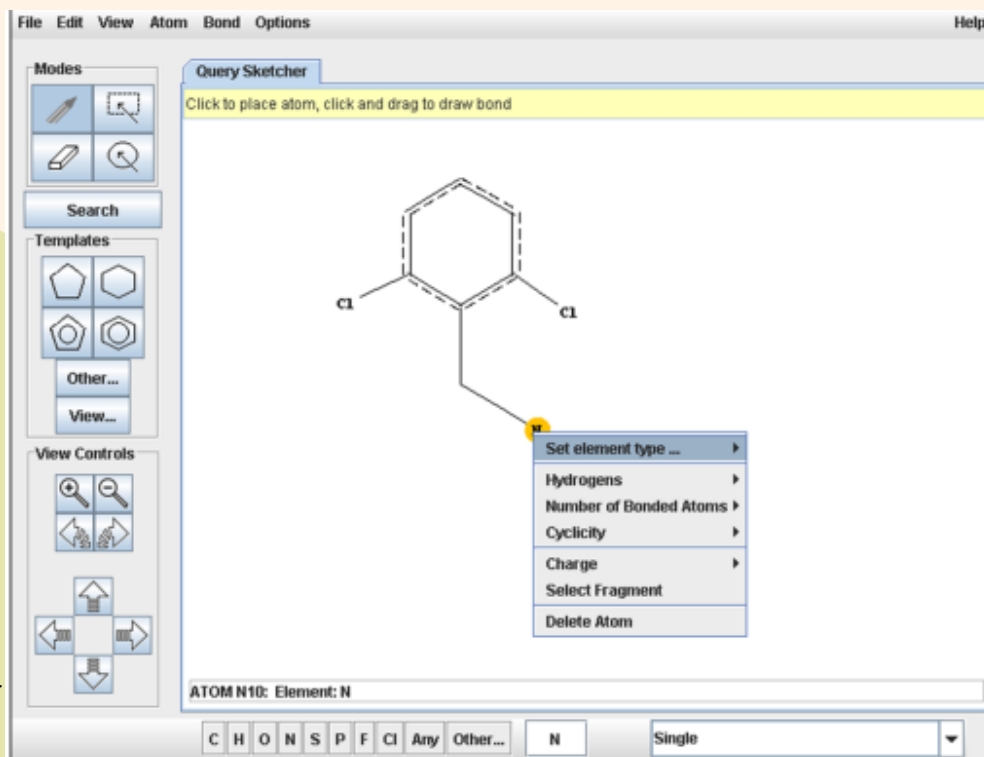
What is WebCSD?

- WebCSD is the new online portal to the [Cambridge Structural Database \(CSD\)](#).
- *Intuitive interface* for easy access to search functionality.

Features

- Substructure searching
- Similarity searching
- Text/numeric searching (Journal reference ; Compound name ; All text)
- Reduced cell searching
- Database browsing
- Customisable 3D display using embedded [AstexViewer™](#) applet - no local software installation required. External viewers also supported.
- Single pane results window
- Easy structure and result export features

WebCSD may be available at the beginning of 2009



Shibboleth

CDS are looking into the possibility of supporting access through Shibboleth authentication by registering as a service provider.

Anyone using resources such as databases or e-journals made available over JANET by data centres or publishers will typically use an **Athens** username and password to gain access. However, JISC has ceased funding it from July 2008, so users will need to subscribe and pay the Athens fee if they want to continue to go through the Athens gateway.

Shibboleth has emerged as the front-runner for the most widely adopted standards-based approach and looks like taking over from Athens.

The goal is to allow users to access resources seamlessly and securely using a single, institutionally controlled identity. This will reduce substantially current problems in which users are required to maintain multiple passwords for multiple resources in multiple domains.

Shibboleth does not carry out authentication itself. Instead, Shibboleth defines a set of protocols for the secure passing of identity information between institutions and service providers. For more information see:-

http://www.jisc.ac.uk/publications/publications/pub_shibboleth.aspx

Links used on this page and others can be found at:- <http://cds.dl.ac.uk/letterlinks>

Research Highlights

Investigating Crystal Structure with Solid-State NMR and First-Principles Calculation

Jonathan R. Yates¹ and Chris J. Pickard²

1- Department of Materials, University of Oxford

2- School of Physics and Astronomy, University of St. Andrews

Almost all of the crystal structures deposited in the crystal structure databases held by the CDS have come from diffraction based techniques. However, other experimental techniques can provide information on atomic-level structure. One of the most powerful is solid-state NMR. In recent years there have been significant advances in solid-state NMR driven by the availability of high field magnets and the adoption from liquid-state NMR of sophisticated pulse sequences. The interpretation of NMR spectra can be problematic: while for single crystal diffraction one can use Bragg's Law to go from a diffraction pattern to crystal structure, for NMR there is no such simple relation. The NMR signal is determined by the response of the electrons to the applied magnetic field, as such it is inherently quantum mechanical in nature. In recent years we have been involved in efforts to develop a predictive theory for NMR parameters in solid-state systems[1]. The approach is based on density functional theory using the well known planewave/ pseudopotential formalism. It is now possible to compute the full range of NMR properties: NMR chemical shifts, electric field gradients (for quadru-polar nuclei), and spin-spin (J) couplings. For a given arrangement of atoms one can thus simulate the corresponding NMR spectra

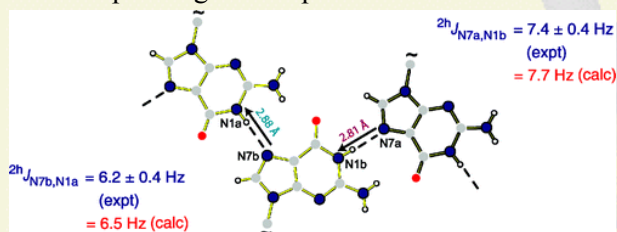


Fig 1. Calculated and measured J-coupling across a hydrogen bond in a molecular crystal[2].

and assign the experimental resonances to individual atomic sites. It is important to note that it is not trivial to invert this procedure and directly determine the crystal structure from an observed NMR spectrum - this is similar to the situation of power X-ray diffraction.

A typical investigation would involve using a crystal structure from a CDS database (ICSD or CSD) as input to the calculations. At a simple level this procedure gives an independent confirmation of the crystal structure, but the information NMR provides is richer than this: spectra are highly sensitive to the precise details of electronic structure, for example distinguishing between differing oxidation states, coordination and bonding.

It is also possible to perform various “computer experiments” to further probe the influence of structure on NMR observables; in a series of studies we have looked at the change in chemical shifts between a molecule first in vacuum and then in its full crystal.

From this it is apparent that intermolecular C-H...O interactions (so called weak hydrogen bonds) have a significant effect on ¹H chemical shifts. Such experiments have also made direct use of the CDS: having established that calculations could be used to assign the ¹⁷O NMR spectrum of one form of glutamic acid, we computed ¹⁷O NMR parameters for several polymorphic forms of glutamic acid, with crystal structures taken from the CDS. This

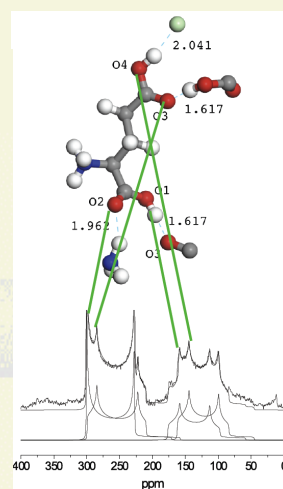


Fig2. Experimental ¹⁷O NMR spectrum of an amino acid and its atomic level assignment provided by first-principles calculation[3].

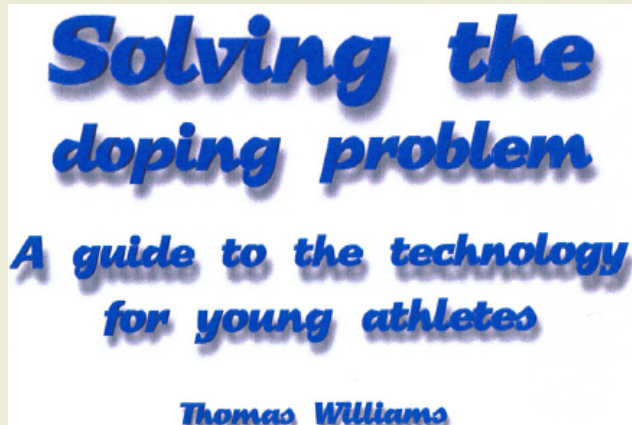
enabled us to find clear correlations between ¹⁷O NMR parameters and hydrogen bonding geometries [3]. Clearly the procedure we have described is dependent on the fidelity of the input crystal structure. An obvious problem occurs with molecular crystal structures determined by X-ray diffraction, as the location of the H atoms is quite imprecise. Using such a database structure directly in calculations leads to gross errors in the predicted NMR spectrum. We therefore ‘improve’ the crystal structures by first optimising the positions of the hydrogen atoms such that their quantum mechanical forces are minimised. When a complete crystal structure is not available the problem is more challenging. One promising route is to include information from NMR experiments and first-principles calculations as constraints for power-XRD[4]. It is also becoming possible to generate candidate structures *ex nihilo*, or from nothing but a knowledge of the stoichiometry of the system[5].

In summary the crystallography databases provided by the CDS have proved invaluable in developing a predictive theory of solid-state NMR spectroscopy. In the future we expect to see the databases contain structure determined by both solid-state NMR and computational techniques as well as by diffraction methods. Perhaps the most useful studies will involve a combination of all three approaches.

- 1- see www.gipaw.net for references and details
- 2- *J. Am. Chem. Soc.*, 130, 12663 (2008)
- 3- *J. Phys. Chem. A*, 108 6032 (2004)
- 4- *Magn. Reson. Chem.* 44 325 (2006)
- 5- *Nature Physics*, 3, 453 (2007)

RSC Award winner works for CDS!

Thomas Williams of St Gregory's Catholic High School, Warrington was the Secondary Schools winner of the RSC Bill Bryson Prize for 2008, which had the theme 'The Science of Sport'.



Thomas spent a week working in the CDS office as part of his work experience organised by his school and Daresbury Laboratory. His article entitled "Solving the doping problem" explores the science behind the techniques employed by chemists all over the world to catch the athletes using drugs such as anabolic steroids and stimulants, as well as taking a look at the problematic shortfalls in the technology.

More information can be found at:- <http://www.drugsinsport.tk/>

Or you can download the article at:-

http://www.rsc.org/images/Thomas%20Williams_tcm18-132915.pdf

Training

The CDS web site contains online training material for all of the databases and interfaces that are available. This includes "getting started" and tutorial information as well as structured problem sets, appropriate Flash Movie clips, etc. This will be augmented and updated in line with system developments.

The service offers "hands-on" training courses at University sites on demand. These require the site to have a suitably equipped training room as well as sufficient demand (minimum of 6 people) for a course. Individual sites will **not** be charged for these services.

Where Are We?

We are part of the support and service programme of the Computational Science and Engineering Department (CSED) based at Daresbury Laboratory, Warrington which is in turn now part of the Science and Technology Facilities Council (STFC).



Daresbury Laboratory

Links used on this page and others can be found at:- <http://cds.dl.ac.uk/letterlinks>

Databases Available From The Chemical Database Service

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

STRUCTURES

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

CSD - Cambridge Structural Database.

Crystal structure data for over **456,000 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.

ICSD - Inorganic Crystal Structure Data File.

Crystal structure data for Over **103,000 inorganic compounds**

WWW interface available.

CRYSTMET

Crystal structure data for over **115,000 metals, alloys and intermetallics..**

CDIF - Crystal Data Identification File.

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

CrystalWeb

A simple **web interface to all of the crystallographic databases** that allows bibliographic and cell data searching along with structure display.

UTILITY PROGRAMS

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

CRAD - A crystal radial distribution calculation program.

BABEL and **BEDLAM** - file format converters

SPECTROSCOPY

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

SPECINFO

SpecInfo is a multi-technique spectroscopic database system which covers NMR, IR and mass spectra. A variety of features are available within the program to help with spectrum prediction and searching. It is accessed via the Web interface **SpecSurf**.

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.

The databases currently contains:-

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	7,661	5,184	16,561	25,442	10,238
ACD/Labs	186,000	193,000	8,800	-	26,100	15,400	-

SPECINFO

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

ACD/Labs Physicochemical data:

pKa = 16,000 LogP = 18,400 Solubility = 5,000

Physical property predictions includes pKa, LogP, LogD, aqueous solubility, boiling point/vapour pressure/enthalpy of vaporization, adsorption coefficient/bioconcentration.

PHYSICAL CHEMISTRY

DETERM

One of the world's largest thermophysical property databases of pure compounds and compound mixtures. Contains nearly **6 Million data sets** for around **134,000 systems** (around 28,000 pure substances and 106,000 mixtures) covering around **500 property fields**.

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

General Information

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

The Service is available **free of charge at point of access** 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 ID's.**

Main Service Machine

cds.dl.ac.uk

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

Web Site

Information about CDS, including online help, documentation and up-to-date news items is available over the World Wide Web at the CDS website.

<http://cds.dl.ac.uk>

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

Comments:

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

Dr. D. Parkin

Email: donald.parkin@stfc.ac.uk

Phone: 01925 603 162

Links used in this Newsletter can be found at:

<http://cds.dl.ac.uk/letterlinks>

Documentation:

Most documentation is available online or within the client packages. User Guides, training exercises and tutorials can all be downloaded from the CDS web site.

CHEMICAL DATABASE SERVICE

Daresbury Laboratory

Warrington

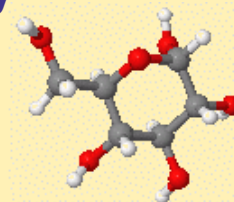
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CDS
ON-LINE