the Chemical Database Service

NEWSLETTER

Spring/Summer 2009

Contents

Welcome

Welcome to the Spring/ Summer 2009 Newsletter of the Chemical Database Service (CDS)

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

Latest News

Statement of Need

A review by EPSRC of for 'Mid Range' Services means a Statement of Need is required from users for the continued availability of a Service.

More details on page 2

ACD/Labs I-Lab

The EPSRC has agreed further funding of the ACD/Labs I-Labs service provided by the Chemical Database Service. This will ensure continuation of I-Lab on the CDS until at least 31/3/2011

More details on page 5.

SPRESI Database

The CDS has made arrangements to make the SPRESI^{web} system available to its user community until 31/03/2010

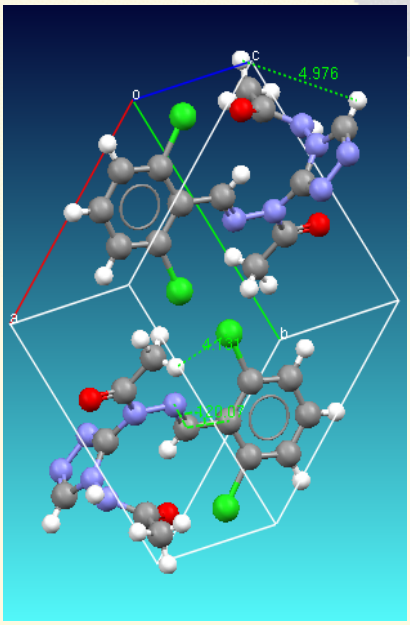
More details on page 7.

Science & Technology Facilities Council

EPSRC

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

Crystallography Databases

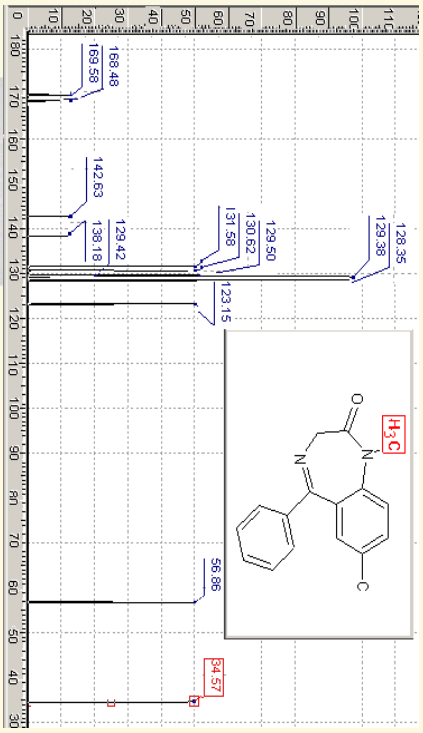


Thermophysical Database

DETHERM ... *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



News

Statement of Need (SoN)

The EPSRC is currently undertaking a review of its support for 'Mid Range' Services. As part of this process it has started a Community Consultation. The Chemical Database Service(CDS) is one of the current Mid Range Facilities and **the community it serves will be directly affected by decisions made by the EPSRC** following its consultation procedure.

As part of the overall review process, the EPSRC has asked all relevant communities to prepare and submit a Statementof Need (SoN). The intention is that these should come from the communities served by Mid Range Facilities rather than the organisations currently providing these services.

A 'petition' has been put in place for the benefit of all community members with an interest in the continued availability of the kind of facilities that are currently provided by the CDS. It gives an opportunity for everyone to lend their support and, if they so wish, to contribute to the framing of the SoN. It can be found at:-

http://www.ipetitions.com/petition/ChemicalDatabaseService/

Please add your name, institution, research area and any other comments you have regarding a central Chemical Database Service (name, institution and research area will be added to the end of the SoN).

If you also feel that any database is needed as "must have" or "desirable" then please indicate this in the comments section. This might include, for instance, data on commercially available compounds, screening compounds and other database systems of potential value to the organic chemistry and more general communities.

EPSRC will use these SoN's to decide on future funding (if any) of this and other facilities. It is, therefore, vital that you make the EPSRC aware of your needs and the importance of the CDS in your research.

Note: None of your details apart from your name will appear on the petition's Signatures page and you can even opt to display your name as anonymous.
A donation (to iPetitions) is *not* required. Simply click the Sign petition >> button then close the window.

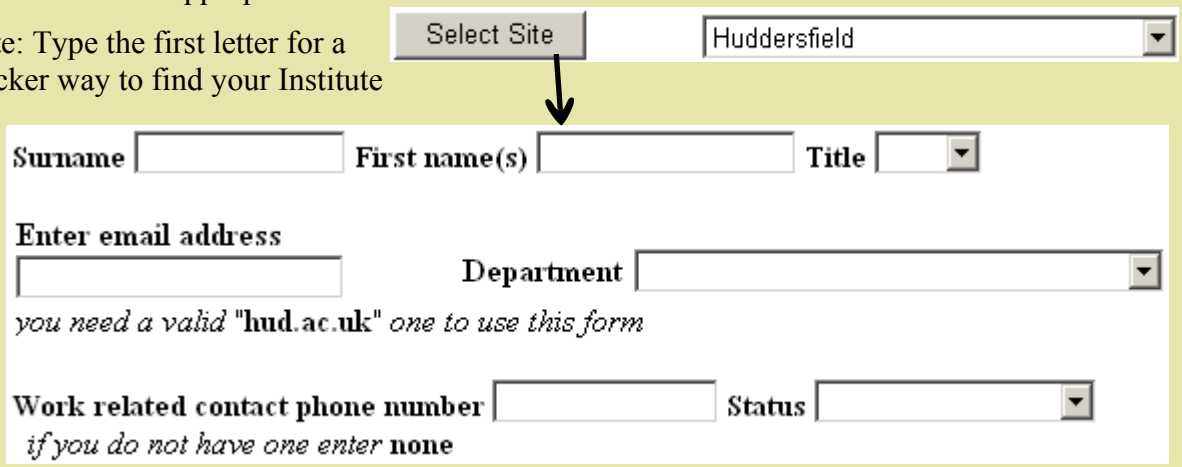
The Statements of Need has to be completed by 12 June 2009 - so please sign this petition now.

Express Login

An *Express* registration procedure is available to members of most academic institutions within the UK

Go to http://cds.dl.ac.uk/cgi-bin/reg/express_uk and select your Institution from the pulldown menu list to access the appropriate Online Form.

Note: Type the first letter for a quicker way to find your Institute



After you submit the registration, your username will be emailed to you **within 10 mins** of completion of the online form

News

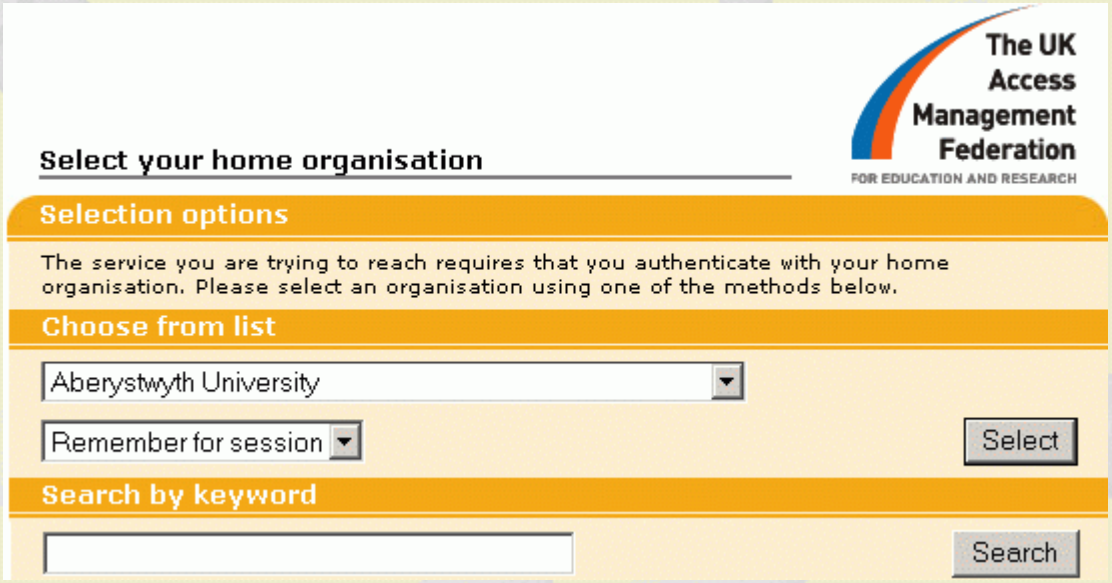
Accessing CDS through Institutional ID's (Shibboleth)

Access to ICSD, CrystalWeb, Available Chemicals and Screening Compounds is now now available **either** by using your CDS ID or by authentication via your Institute ID (Shibboleth ID).

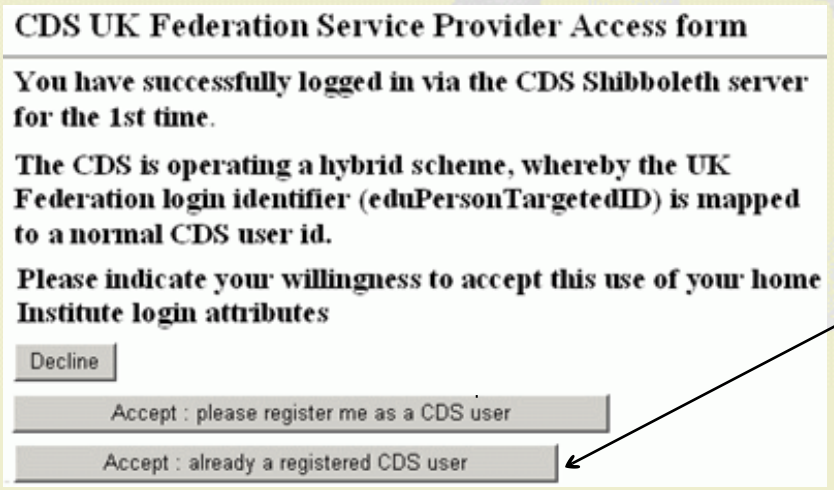
For more details see:- http://cds.dl.ac.uk/cds/help/shibboleth.html

To log in using your Institute ID, first go to the home page and hold your mouse over the **RED** box then choose Institutional Login ("Shibboleth") from the menu.

You should be taken to a login screen. Please choose your Institute from the drop-down list.



Enter your Institutional ID and password when asked. You should then receive notice of a successful login.



If this is the first time you have logged in this way then you can map your Institutional ID to your CDS ID.

Please accept the mapping of ID's

Registered users then need to fill in their existing ID and password.

After successfully logging in, you should be returned to the CDS home page.

Use the **RED** box to access the database of choice.

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

New Updates and News

Crystallography

Cambridge Structural Database System

The latest update (13/02/09) includes 9,005 new entries. The total number of entries is now 472,200

There are also a number of new features in version updates of ConQuest, Mercury, Mogul, IsoStar and PreQuest. For more information see:- http://www.ccdc.cam.ac.uk/support/documentation/csd/rel_install/rel_install.3.3.html

ConQuest 1.11

There is a new **All Text** tabbed view in the View Results window where all textual information for the entry can be viewed. As well as information that is available for all entries such as publication details, chemical formula, unit cell details, supplementary information such as melting points, crystal habit, crystallisation solvent are also provided where available.

Author(s)	F.Marchetti, G.Pampaloni, S.Zacchini
Reference	Chem.Commun. (2008), , 3651
Publication DOI	10.1039/b804432e
Deposition	CCDC [679568]
Formula	$C_4 H_{10} Cl_3 Nb O_3$
Compound	1,2-Dimethoxyethane-oxo-trichloro-niobium(v)
Spacegroup	**Name:** Pbca **Number:** 61
Cell	**a:** 7.327(<1) **b:** 11.974(1) **c:** 23.187(2) **alpha:** 90.00 **beta:** 90.00 **gamma:** 90.00 **Volume:** 2034.294
Reduced Cell	**a:** 7.327 **b:** 11.974 **c:** 23.187 **alpha:** 90.00 **beta:** 90.00 **gamma:** 90.00 **Volume:** 2034.294
Molecular Volume	254.287
Chemical Units	1
Z, Z'	**Z:** 8.0 **Z':** 1.0
R-Factor (%)	2.39
Temperature (K)	100
Density	**CCDC:** 1.994 **Author:** 1.994
Intensity Meas	diffractometer
Average Sigma (C-C)	0.001-0.005Å
Colour	pale yellow
Habit	prism

Mercury 2.2

A number of changes and enhancements have been made to the Materials Module

Mogul 1.1.3

Data libraries are now based on CSD 5.30.

IsoStar 2.1

Scatterplot data have been updated and now include 22,161 scatterplots from CSD 5.30, 7,459 scatterplots from the PDB and 1550 potential energy minima.
There are new clients for PC, Mac and Linux workstations

PreQuest

PreQuest is now provided for all platforms including Windows and Mac OS X.

ICSD

There are 4,579 more entries as compared to Version 2008/1. The total number of entries is now 108,258.

CrystalWeb

Data from the recent updates of CSD and ICSD have been made available via CrystalWeb.

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

New Updates and News

Spectroscopy

ACD/Labs I-Lab System

Following a review by the EPSRC, they have agreed to continue funding the ACD/Labs I-Lab set of databases for another two years (up to 31/03/2011)

The server will be updated soon to version 12. This will contain more entries and so increase the search and predictive capabilities of the databases.

ACD/CNMR

- Database contents will increase to 200,100 chemical structures with 2,547,046 13C chemical shifts

ACD/HNMR

- Database contents will increase to 210,700 chemical structures with 1,755,262 1H chemical shifts

ACD/NNMR

- Predictions are now based on 9287 chemical structures with 21,782 15N chemical shifts

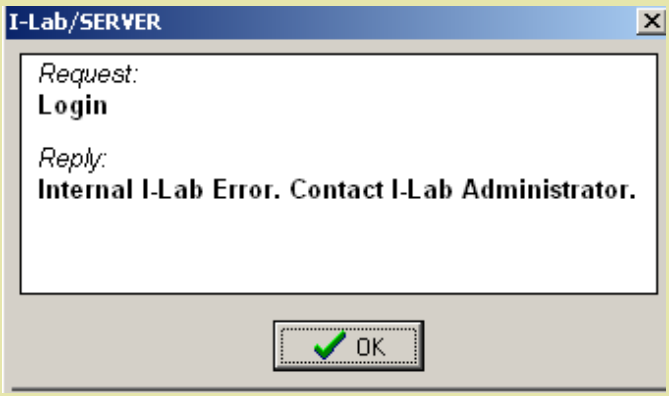
ACD/FNMR

- Predictions are now based on over 17,000 chemical structures with 35,349 19F chemical shifts

ACD/PNMR

- Predictions are now based on 27,578 chemical structures with 34,020 31P chemical shifts

Note: If you use ChemSketch and have problems logging on to CDS, please either:-



i) Download the current version **from the CDS download area** (Version 11) at http://cds.dl.ac.uk/cds/download/chemsketch.html
or,
ii) If you are using an earlier version or obtained a version directly from ACD/Labs (the latest version is Version 12) download the patch (dmillib.dll) and use it to replace the installed version of the dll file.

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

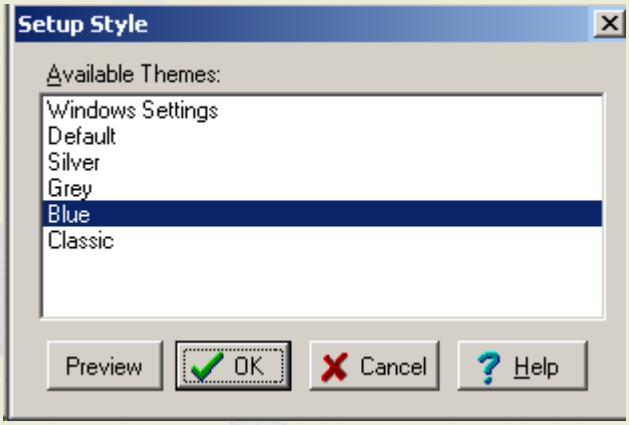
New Updates and News

ChemSketch

ACD/ChemSketch 12 is now available. Key new features are:

- New customizable interface appearance & style
- Improved atom numbering positioning
- Resize and Rotate tools simplification
- Set standard InChI options (updated IUPAC recommendation)

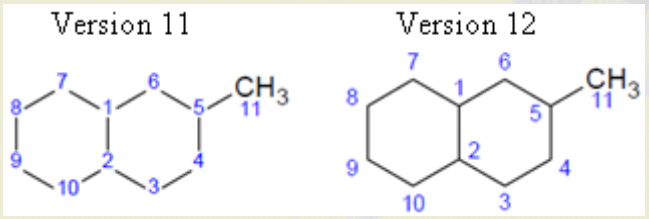
Customizable Interface & Style
*(*under the ACD/Labs menu)
The background color, buttons, and other graphic controls can be made to conform to the Windows setting, the classic ACD/Labs view, or you can create your own theme and preference.



Resize and Rotate tools

The interface has been simplified and behavior made more consistent. Previously, there was a slight discrepancy in **Drawing** versus **Structure** modes when it came to selecting, moving, rotating, and resizing structures and drawings.

The new interface controls for manipulating images and structure objects are made similar to those used by Microsoft Word, ChemDraw, and many other applications. This effectively merges several tools into one, creating a simpler, more user-friendly interface.



Improved atom numbering position

In previous versions, the default position of atom numbers overlapped at the center of the atom node.

In the current version, the numbering is positioned **near** the atom node instead in accordance with current common preferences.

Set standard InChI options (Under Tools> Generate)

New InChI Options proposed by IUPAC have been implemented. The options include:

- Mobile Hydrogen Perception (taking tautomerism into account)
- Excluded bonds to metal
- Absolute stereoconfiguration
- Taking into account narrow ends of stereobonds only

The IUPAC International Chemical Identifier (InChI™) is a non-proprietary identifier enabling unambiguous identification of chemical substances for electronic handling of chemical structural information. These new IUPAC options for InChI reflect the decisions made by the IUPAC InChI project group, and are intended to increase the role of InChI and InChI key as a universal structure identifier.

New Updates and News

Organic Chemistry

SPRESI web from InfoChem

SPRESI web will be available for at least a year (31st March 2010)

Version 2.7 launched in March 2009

New Data

The SPRESI web application now enables you to search over:-

- 7.0 million structures
- 3.9 million reactions
- 31.7 million factual data entries

such as chemical and physical properties, reaction conditions and keywords

extracted from

- 645,000 references
- 164,000 patents.

covering the years 1974 - 2007.

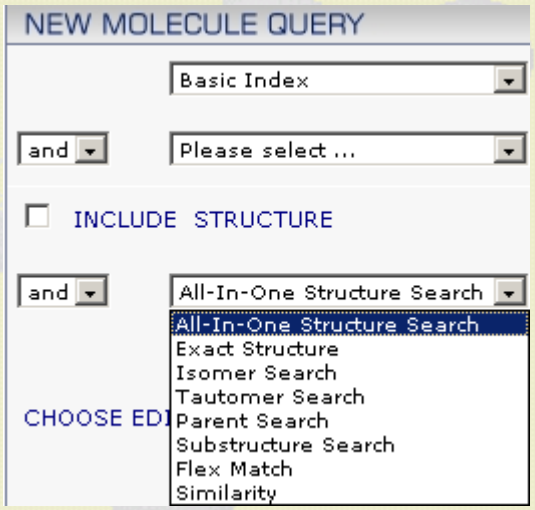
"All-in-one" Structure Search

An 'All-in-One' Structure Search finds molecule records in the database that match your query:-

i) Exactly (see 'Exact Structure', 'Isomer Search', 'Tautomer Search', 'Parent Search' and 'Flex Match')
ii) Contain your query as a substructure wholly within a larger structure (see 'Substructure')
or iii) Similar to your query (see 'Similarity').

The hits are sorted according to this order and the 100 best matches will be shown.

So, instead of specifying multiple queries you get all the results with just one click!



Update of Chemicals Suppliers Catalogues

All the catalogues of the chemicals suppliers included in SPRESI web have been updated. The user can identify which substances contained in his hit lists are commercially available directly during the search and order them right away through the hyperlink to homepage/online catalogue of the particular supplier.

The following chemicals suppliers (off-the-shelf and screening catalogues) are available:-

ABCR
Acros
Apollo Scientific
ASDI
ChemCollect
ChemiK
ChemPacific
Enamine
Fisher Scientific
Frontier Scientific
Key Organics
Life Chemicals
Maybridge
Oakwood
Otava
PharmaCore
Sigma-Aldrich
Sinova
Synchem Inc.
Synchem OHG
SynQuest
Synthonix
VWR

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

New Updates and News

Organic Chemistry

Suppliers Catalogues

The Suppliers catalogue list is updated whenever a new price list appears. Currently the latest databases were updated on:-
Apollo - March 2009
FluoroChem - February 2009
Sigma-Aldrich - February 2009
Maybridge/Acros - April 2008

Access to these databases is now available via your CDS ID and password **OR** via your Institutional (Shibboleth) ID and password (see page 3)

Symyx Draw 3.1

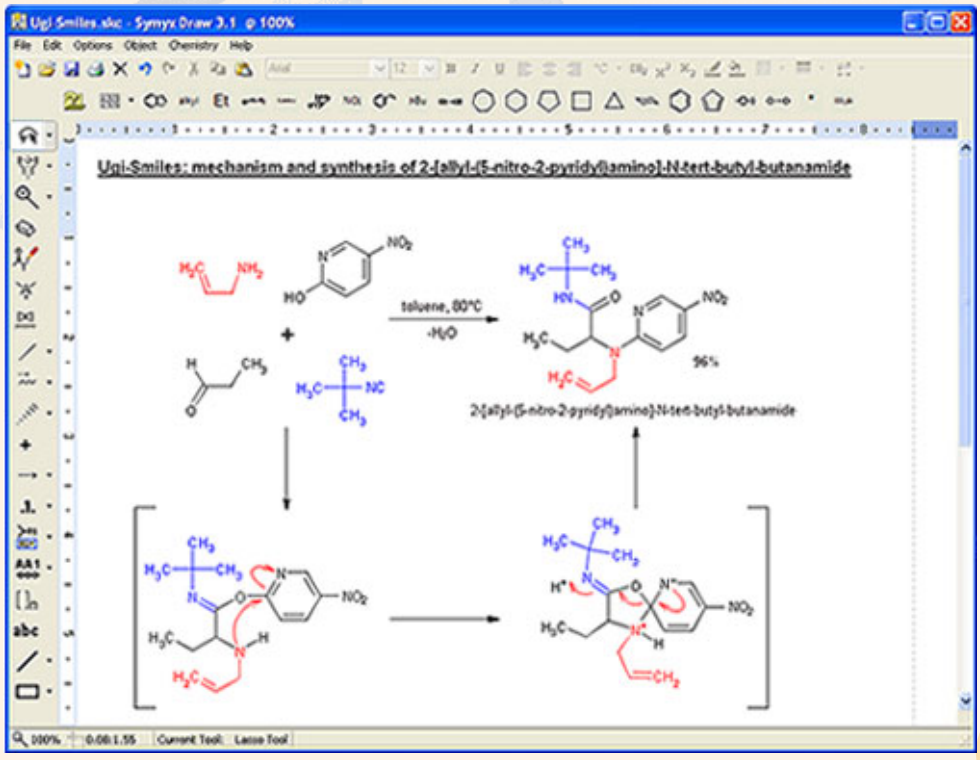
A **No–fee** Symyx Draw chemical structure drawing tool is now available for academic and home use. This is the successor to **ISIS/Draw**. For more information and to download see:-
http://www.symyx.com/products/software/cheminformatics/symyx-draw-no-fee/index.jsp

Symyx Draw benefits

- Built-in structure–to–name and name–to–structure converters for IUPAC, SMILES and InChI using OpenEye's Lexichem™technology
- Improved presentation–quality graphics
- Extensive range of no–charge extensions (add-ins)
- All–purpose drawing tool for rapidly drawing molecules
- Favourite templates for common structures
- Continued use of legacy files and sketches
- Simpler, faster drawing through user interface improvements
- Create and edit polymers, mixtures, and formulations
- Create and edit Markush (Rgroup) queries
- Create and edit 3D queries

Symyx Draw 3.1 is also superior to ISIS/Draw in supporting enhanced stereochemical perception

In addition, the rich presentation- and publication-quality graphics of Symyx Draw 3.1 surpass those of ISIS/Draw.



Research Highlight

Understanding the Structure and Properties of Amorphous Biomaterials

Dave Pickup and Bob Newport
School of Physical Sciences, University of Kent, Canterbury, CT2 7NH

Amorphous biomaterials have sparked much interest since the discovery by Larry Hench in the late 60s that high CaO- and Na_2O-content silicate glass can promote the regeneration of bone tissue [1]. This led to the development of commercially available Bioglass® (46 mol% SiO_2, 27 mol% CaO, 3 mol% P_2O_5 and 24 mol% Na_2O), which has found widespread use in the clinic. Now much research is focussed on the so-called 'Third Generation' biomaterials which are designed to trigger a response that causes the body to heal itself. As well as silicate-based glasses, phosphate-based glasses have recently become important in this field [2]. Phosphate glasses containing CaO and Na_2O are bioresorbable, and when prepared with high CaO content can actively promote cell proliferation. Furthermore, such phosphate glasses can be used for the delivery of antibacterial ions such as Ag^+ or Ga^{3+} and can readily be prepared as fibres to aid the repair of highly anisotropic tissue such as muscle.

Our research is focussed on understanding the structure of amorphous biomaterials, so that we can gain an insight into why they exhibit the properties they do. Moreover, we have a particular interest in amorphous biomaterials prepared by low-temperature sol-gel synthesis: sol-gel chemistry offers exciting possibilities in this regard, such as the inclusion of drugs in the synthesis which are later released when the material dissolves into physiological fluids at a controlled rate after being implanted, or combining the sol-gel with a biopolymer for improved mechanical properties for bone-replacement applications.

Determining uniquely the structure of an amorphous material is impossible due to the disordered nature of the structure. However, techniques such as X-ray absorption spectroscopy (EXAFS and XANES), MAS-NMR, high-energy X-ray diffraction (HEXRD) and neutron diffraction (ND) can reveal information on the average short and medium range order present. The result of processing the data from EXAFS, HEXRD and ND experiments is normally a radial distribution function that contains peaks that correspond to the atomic distances within the structure. Figure 1 shows examples of such functions obtained by HEXRD for both melt-quenched and sol-gel antibacterial Ga-doped phosphate-based glasses.

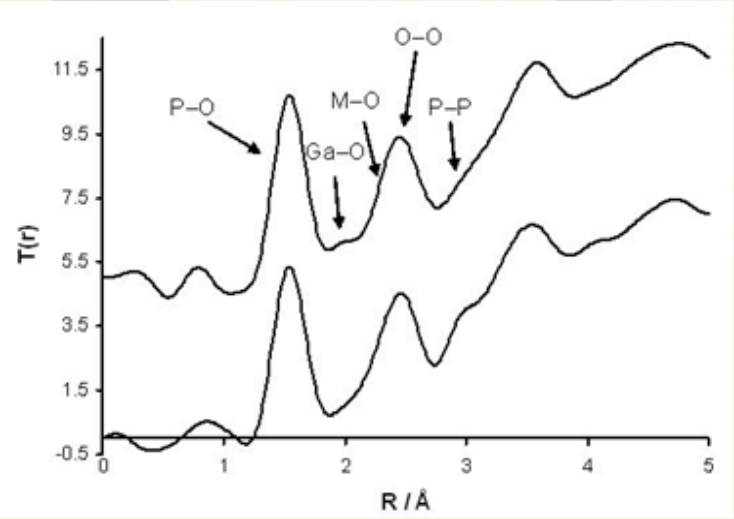


Figure 1: HEXRD pair distribution functions from Ga_2O_3-Na_2O-CaO-P_2O_5 glasses: melt quenched (bottom curve) and sol-gel (top curve)

Understanding the Structure and Properties of Amorphous Biomaterials

Continued

The key to obtaining useful structural information from radial distribution functions is to be able to identify the various atomic correlations present: in multicomponent systems, these correlations usually overlap with one another beyond the nearest-neighbour distances. It is at this point in the data analysis process that the **CDS** becomes invaluable. Using **ICSD**, we can check the analogous bond distances found in crystals containing the same atoms as our amorphous materials and use this information to assign the various correlations in our radial distribution functions. We can also use the information to identify correlations between bond distances and coordination numbers. For example, in the case of gallium phosphates, the CDS data reveal that tetrahedral Ga^{3+} ions have Ga–O distances that fall in the range 1.82-1.84 Å, those for five coordinate gallium are in the range 1.88-1.92 Å and those for octahedral gallium fall within 1.94-1.99 Å. This further corroborates peak assignment.

Once we have identified the various atomic correlations in the radial distribution functions, we can obtain bond distances, coordination numbers and disorder parameters by modelling the data numerically. This information allows us to build up a structural picture of the material we are studying. A typical example is Figure 2 which shows part of a model of Bioglass® generated using Reverse Monte Carlo procedures.

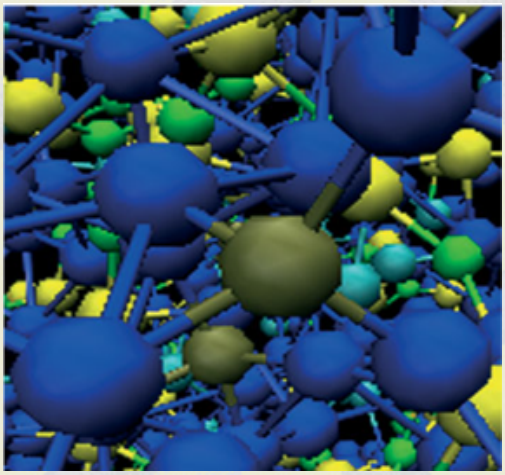


Figure 2: RMC model of Bioglass® showing an orthophosphate group (P = brown, Si = yellow, bridging O = green and non-bridging O = blue). Taken from ref. [3]

Using models obtained by the methods described above, we can begin to understand the properties of amorphous biomaterials. For example, in the case of the Ga-doped phosphate glasses, we discovered that the presence of GaO_6 octahedra in the structure blocks the migration of the sodium ions, which in turn reduces the solubility of the glass and the release of antibacterial Ga^{3+} ions. This explained why there is an optimal gallium content for antibacterial activity [4]. Ultimately, such understanding leads to the design of better biomaterials for the future.

1. Hench, L.L. and J.M. Polak, *Third-generation biomedical materials.* Science, 2002. **295**(5557): 1014.
2. Abou Neel, E.A., et al., *Bioactive functional materials: a perspective on phosphate-based glasses.* J. Mater. Chem., 2009. **19**(6): 690.
3. FitzGerald, V., et al., *A Neutron and X-Ray Diffraction Study of Bioglass® with Reverse Monte Carlo Modelling*. Adv. Fucnt. Mater., 2007. **17**(18): 3746.
4. Pickup D. M., et al., *Structural Characterisation by X-ray Methods of Novel Antimicrobial Gallium-Doped Phosphate-Based Glasses. J. Chem. Phys.*, 2009. **130**(6): 064708.

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 **472,200 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 108,258 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.

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 accesses 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 contain:-

No.of Records	13C NMR	1H NMR	15N NMR	17O NMR	31P NMR	19F NMR	11B NMR
SPECINFO	359,647	130,025	7,661	5,184	16,56	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 Physiochemical 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

DETHERM

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.

ORGANIC CHEMISTRY

SPRESI

Allows you to search Molecules, Reactions, References and associated data. Contains synthesis planning tool.
Direct access over the web to:-

- 7.0 million structures
- 3.9 million reactions
- 31.7 million factual data entries

extracted from:- 645,000 references
164,000 Patents

Available Chemicals

Up-to-date catalogue data including prices for:-

* Sigma-Aldrich
* Acros/Maybridge
* FluoroChem
* Apollo.

using ChemAxon's JChem software over the web.

Screening Compounds

Libraries from 11 Suppliers are available for searching using ChemAxon's JChem software over the web.

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.

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.

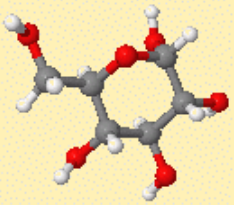
Comments:

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

CHEMICAL DATABASE SERVICE
Daresbury Laboratory
Warrington
Cheshire
WA4 4AD
Tel: 01925 603 162
Fax: 01925 603 031
Email: cdsbb@dl.ac.uk



CDS
ON-LINE