

# the Chemical Database Service

## NEWSLETTER Winter 2010

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### Welcome

Welcome to the Winter 2010 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 and what we plan on doing in the near future.

### Latest News

#### Updates to Databases

See the latest news and updates  
*More details on pages 4*

### Database Trials

#### Isestris/DiscoveryGate

An evaluation trial has been available for all of the Symyx databases including Synthesis, Sourcing and Bioactivity databases, either via an Isestris client or via DiscoveryGate.

Please let us know if you found the trial useful and what you think of the databases.

*More details on pages 9 and 10.*

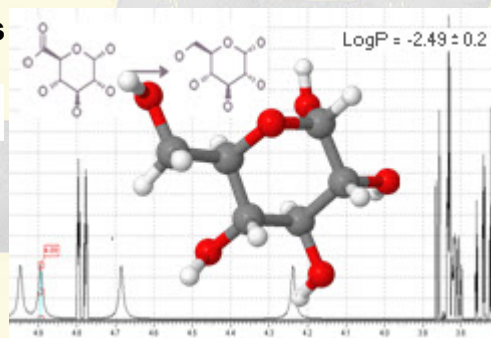
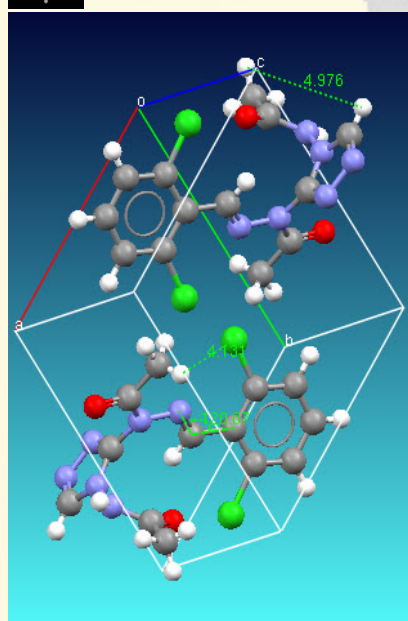
#### ARChem - Retrosynthesis Tool

Design viable synthetic routes for their target molecules

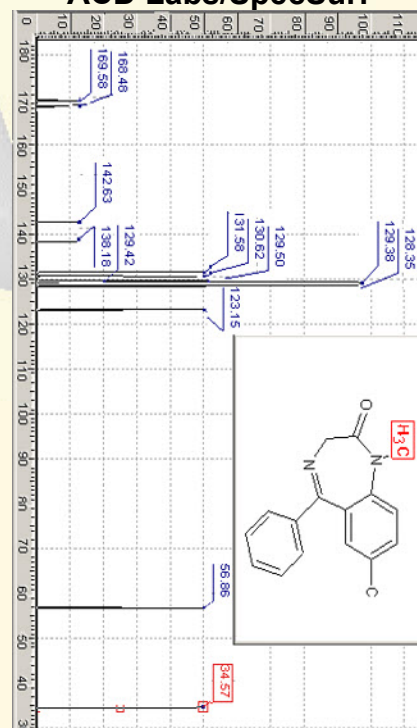
*More details on pages 7 and 8.*



### Crystallography Databases



### Spectroscopy Databases ACD Labs/SpecSurf



### Thermophysical Database

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

#### ACD/I-Lab

##### Boiling Point:

BP (deg C at 760.00 mmHg) =  $431.15 \pm 18.00$

##### Vapor Pressure:

$\log_{10}(p) = -8.516 \pm 2.33$  (p in mmHg)

p (at 25.00 degC) = 0.0000000030 mmHg

##### Enthalpy of Vaporization:

$\Delta_{\text{vap}} H(T_{\text{boiling point}}) = 79.29 \pm 6.0 \text{ kJ/mol}$

# News & Highlights

## Chemical Database Facility

Last year, CDS underwent a Mid-Range Facility Review and **the review panel recognised the importance of such a Facility and thought it to be a priority for EPSRC support.** As a result, CDS were placed in Phase 2 of the tendering exercise for those facilities whose funding did not end until 2010/11.

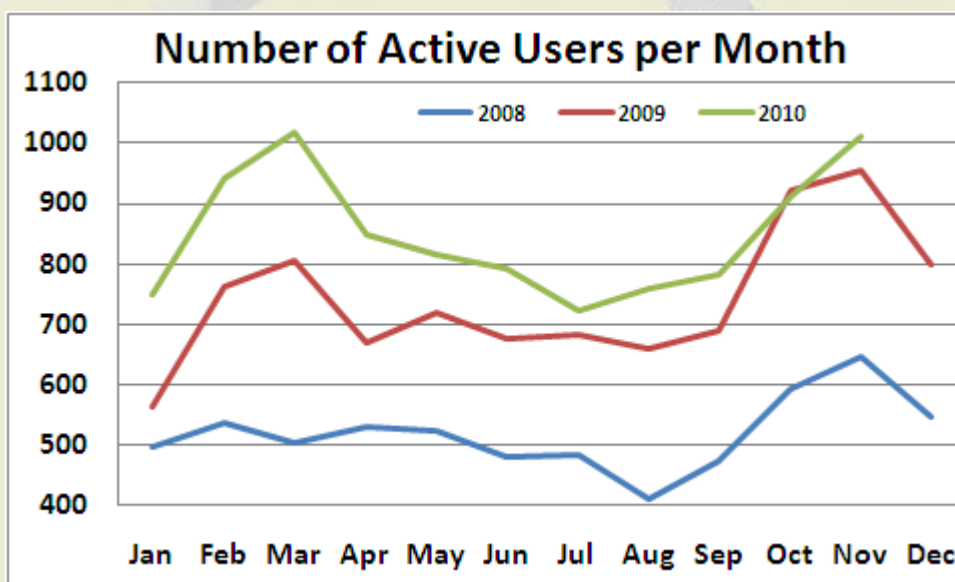
Unfortunately, Phase 1 proceeded slowly (and a new government took office) and, along with the Comprehensive Spending Review in October, it has meant that the tendering exercise was delayed.

However, the renewal process is now underway and hopefully it will be completed before the end of March 2011. **This will mean a Chemical Database Facility being available for the next five years.**

## Usage Highlights

For the academic year 2009/2010, **ALL** usage figures went up from the previous year. CDS now has more registered users than ever before.

- March 2010 **ACCESS** figures were the highest recorded since March 2006.
- The number of **USERS** in March 2010 was the **largest number of recorded users for any month** since the Service started (1,018 Users).
- A record number of **2,946 unique users** accessed the databases over this 12 month period – a rise of 77.5% from the previous year.
- There were, on average, **790 users per month** - the **largest since the Service started.**
- For 2010, **every** month (except October) has shown a higher number of users than the corresponding month in 2009 (averaging **850 users per month** so far for 2010).



# News

## Change to CDS Accord Database Explorer

As a result of the recent Oracle server software upgrade, it was necessary for us to change the configuration of the CDS Accelrys Accord Database server.

**As of September 22nd, 2010**, all CDS users of the Accelrys databases via Accord needed to make a small change to their Oracle client file, located on the Windows PC, in order for it still to operate after this date.

The file that needs changing is the Oracle file "**tnsnames.ora**" to be found in the \network\admin folder e.g. c:\oracle\network\admin\tnsnames.ora but it may be located elsewhere on your system.

The ACCORD3.DL.AC.UK PORT number needs to be changed from 1521 to **1522**

i.e. the entry should read :

```
ACCORD3.DL.AC.UK =  
(DESCRIPTION =  
(ADDRESS_LIST =  
(ADDRESS = (PROTOCOL = TCP)(HOST = cds10.dl.ac.uk)(PORT = 1522))  
)  
(CONNECT_DATA =  
(SERVER = DEDICATED)  
(SERVICE_NAME = ACCORD3.dl.ac.uk)  
)  
)
```

If you do not have write access to the tnsnames.ora file, then you will have to arrange with your system administrator to do it for you after 22nd Sept.

Progress during the changeover was posted on CDS Twitter or RSS feeds.

## ChemSketch Access Problems?

The ChemSketch Client provides a very good access route to the ACD/Labs I-Lab system for spectroscopic and physical properties simulation.

In the past users from a number of sites have experienced problems accessing the CDS ACD/Labs I-Lab server via the ChemSketch Client mechanism. In most cases this was because local Firewalls blocked this access mode. We have received recent evidence that these Firewall problems may have been fixed. If you experienced problems in the past we encourage you to try the system again.

You can download the Client from the CDS via the link:

<http://cds.dl.ac.uk/cds/download/chemsketch.html>

Some of you may have already obtained the ChemSketch Client directly via the ACD/Labs site or have it available via a local installation. In both these cases you need to make slight system modifications. You have to replace a current DLL file (dmillib.dll) with one tailored to access the CDS I-Lab server correctly.

Simply download and replace the existing DLL file. Do this when you have already installed a Client from a source other than the CDS.

Please get back to us if you still encounter problems with the ChemSketch Client.

# News & Updates

## Crystallography

### Cambridge Structural Database System

Version CSD V5.31 (2010 Release)

The latest update (added August 2010) includes 12,212 new entries. The total number of entries is now 525,093 .

The latest data updates are now available via ConQuest, Vista/Mercury and QUEST. and via CrystalWeb.

### Inorganic Crystal Structure Data (ICSD)

This database was updated at the beginning of November. It contains 135,468 crystal structures, including 120,331 fully determined crystal structures with atom coordinates obtained from experimental data and 15,137 crystal structures with atom coordinates derived from the corresponding structure types.

During the update procedure 2,942 new entries were added and 2,308 entries were modified.

## Organic Chemistry

### Available Chemicals

In August, The Suppliers catalogue was updated with new compounds and prices for the following catalogues: Sigma-Aldrich, Fluorochem, Apollo, Key Organics, Life Chemicals and Maybridge Building Blocks.

A new catalogue was also added called Tractus which currently contains 874 compounds.

In September, The Suppliers catalogue was further updated with new compounds and prices added for Acros and Maybridge, and in November the SigmaAldrich set of databases were updated, bringing the total to 258,265 entries..

### SPRESI<sup>Web</sup> 2.8

InfoChem recently upgraded the SPRESI<sup>Web</sup> software to version 2.8

This has had some unfortunate effects on web browsers access:

- Internet Explorer (version 6) has a missing search box, seemingly due to access through the CDS site. Version 8 appears to work correctly.
- Safari, Opera and Chrome all have a search button that does not respond.

NB Currently Firefox and IE (V8) are the only recommended browsers to use on Windows, Mac and Linux platforms

# CrystalWorks

## Coming Soon

CrystalWeb has been a key component of the Chemical Database Service, providing a single point of access to search and retrieve data from all the commercial crystallographic databases supported by the Service.

New display features are being developed - called CrystalWorks - which will be added to the basic CrystalWeb system in due course.

An automated system to monitor and download data from the Southampton eCrystals archive is now in place. We anticipate that many additional centres will set up repositories which can also be harvested and displayed within CrystalWorks.

### Top Level Display menu.

It has been designed to allow a rapid scan of summary information for a Hits List of entries. Information is presented on the fly for the item picked out from within the scrollable Hits List box or database Collection Code.

### Top Level Display Menu

Select database entries for display by:

using a collection code menu to the right  
or  
clicking an item in the Hits List below

#### Enter collection code

Database

ICSD

Collection code

36144

Select Entry

#### Browse the databases

Database

Southampton Repos.

Entries subset

soton: 19 - 1231

Collection Code

soton: 277

#### Access your own Hits

Search CrystalWeb

Access Hits

Litref entries

Username logon

#### Hits List

```
icsd - 36144 ~ Bozorth ~ 1923 ~ Fd-3m ~ As4 O6 ~ Tetraarsenic oxide
csd - podsor ~ Castaneda ~ 2008 ~ P-1 ~ C25 H25 O4 P1 ~ Methyl isopropyl 2-(triphenylphosphoranylidene)malonate
icsd - 64639 ~ Murayama ~ 1988 ~ P4/mmm ~ La Ba2 Cu2 Ta O8 ~ Lanthanum dibarium dicopper tantalate
icsd - 26425 ~ Er-Rakho ~ 1981 ~ P4/mmm ~ La3 Ba3 Cu6 O14 ~ Trilanthanum tribarium pentacopper copper(II) oxide
icsd - 41404 ~ Mikhalenko ~ 1980 ~ Pbam ~ Al Yb2 B6 ~ Aluminum ytterbium boride (1/2/6)
crystmet - 511823 ~ Macaluso ~ 2007 ~ Pbam ~ Yb Al B4
crystmet - 511825 ~ Macaluso ~ 2007 ~ Cmmm ~ Yb Al B4
csd - hicwof ~ Bunn ~ 1947 ~ P-1 ~ (C12 H22 N2 O2)n ~ poly(hexamethylene adipamide)
csd - testom ~ Busetta ~ 1972 ~ P21 ~ C19 H28 O2, H2 O1 ~ Testosterone monohydrate
csd - bejvan ~ Cox ~ 1982 ~ P21 ~ C20 H30 O2 ~ 17beta-Hydroxy-7alpha-methyl-androst-4-en-3-one
csd - laddup ~ Hirschmann ~ 1992 ~ P21 ~ C23 H36 O1 ~ 7-(But-3-enyl)-3-oxo-delta-5-androstane
csd - cholme02 ~ Huey-Sheng Shieh ~ 2002 ~ P1 ~ C27 H46 O1, 0.5(C1 H4 O1) ~ Cholesterol methanol solvate
```

#### Selected Entry

**Database Entry:** ICSD - 36144  
**Authors:** R. M. Bozorth  
**Reference:** J. Am. Chem. Soc., 45 (1923), 1621  
**Compound:** Tetraarsenic oxide  
**Formula:** As<sub>4</sub>O<sub>6</sub>  
**Cell:** 11.06, 11.06, 11.06, 90, 90, 90  
**Space Group:** Fd-3m (227)

#### More details for Selected Entry

Literature links & Data aggregators

Coordinates format download options

Jmol structure display options

Output CIF format via Socket

Entry is in current Hits List

Remove from List

### Coordinates format download option Menu

CrystalWorks adds extra format options. It is now possible to scan through the output options very quickly within the browser before choosing one for output to a local workstation file.

It is also possible to output coordinates via IP Sockets to allow close integration with other packages running simultaneously on the user's workstation, e.g. the DLV packages for the visualisation of materials structures and properties.

## Coming Soon

### Literature reference & ChemSpider Menu

Linking to the primary electronic literature has been improved and access to a wider range of chemical information has become possible such as links to [ChemSpider](#), [ChEBI](#) and [NIST WebBook](#)

### Literature links & Data aggregators

[Jmol structure display options](#)
[Coordinates format download options](#)
[Output CIF format via Socket](#)
[Return to Top Level](#)

**Database:** csd **Selected Entry**  
**Entry Code:** testom

**Database Entry:** Cambridge - testom  
**Authors:** B. Busetta, C. Courseille, F. Leroy, M. Hospital  
**Reference:** Acta Crystallographica, Section B - Structural Crystallography and Crystal Chemistry, 28 (1972), 3293  
**Compound:** Testosterone monohydrate  
**Formula:** C<sub>19</sub>H<sub>28</sub>O<sub>2</sub>, H<sub>2</sub>O  
**Cell:** 9.622, 8.099, 11.149, 90, 97.81, 90  
**Space Group:** P21 (4)

**Link Resolver**  
 There is a DOI link to the electronic literature  
 The following is included in the database for this entry  
<http://dx.doi.org/10.1107/S0567740872007861>

ChemSpider provides links to a wide range of articles and data sources together with both spectroscopic, physical property and structural information

**Search the ChemSpider site**

**Search the ChEBI site**

**Search the NIST WebBook**

**Search the NCI/CADD Chemical Structure Lookup Service**

### Jmol structure display options Menu

This has been improved with more options. There is now a full range of display styles from Spacefill through to Ball & Stick to Wireframe.

Displays can easily be switched between say packing diagrams with multiple cell to representations with just the minimal molecule set.

### Jmol structure display options

[Coordinates format download options](#)
[Literature links & Data aggregators](#)
[Output CIF format via Socket](#)
[Return to Top Level](#)

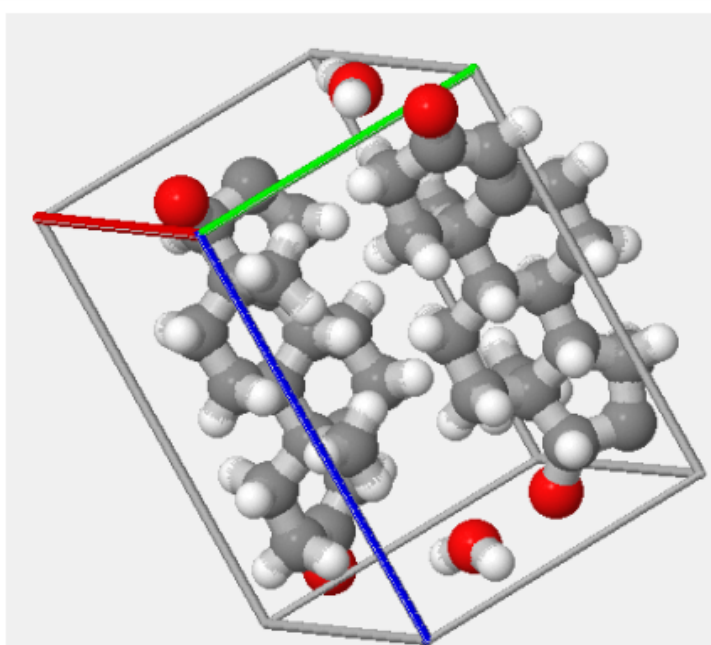
**Database:** csd  
**Entry Code:** testom

Spacefill  Ball and Stick  Sticks  Wireframe  
 Spacefill Size:  Large  Medium  Small

Crystal Cells  Single Cell  Axes  No Axes  
 Full Cell Contents  Unique Molecule Set

No Bond Types  Display Bond Types

Perspective  No Perspective



# Trial Databases

## ARChem - Automating Retrosynthetic Chemistry

**ARChem - Route Designer** from **SynBioSys** is an expert system aimed at helping chemists design viable synthetic routes for their target molecules. The knowledge of the expert system is automatically derived from reaction databases. The system also relies on databases of readily available starting materials for not breaking up the parts that have already been made.

### Features

- Automated extraction of chemical reaction rules from on-line chemical reaction databases (such as Methods in Organic Synthesis [MOS], ChemInform and Beilstein)
- Exhaustive and systematic retrosynthetic search from a target compound to readily available starting materials.
- Capability to identify published synthetic routes for novel drug-like compounds
- Routes sorted according to a merit ranking
- Every step on the route is illustrated with examples from the literature according to the reactions suggested.
- User friendly, web-based front end.

ARChem will be available for a trial period of 3 months from October 2010.

**ARChem** Route Designer  
© SimBioSys, Inc. 2010, <http://www.simbiosys.ca/>

Welcome to the ARChem system

**Select search strategy and upload/draw file**

[A] Upload MOL file for Target Molecule Oriented Search :  Browse... ?

[B] Upload RD file with mapping for Starting Material Oriented Search:  Browse... ?

Draw new Molecule for [A] or new Reaction for [B] Save as (optional) :  ?

**Starting Materials List**

Acros  
 AlfaAesar  
 Aldrich  
 MaybridgeBuildBlocks  
 Gas-Molecules  
 AldrichRareChemicals

**Optional Filter:**  
Max price in USD/mole:

**Reaction Rule Selection**

Name	Minimum number of examples/rule
<input checked="" type="checkbox"/> Beilstein	250
<input checked="" type="checkbox"/> BeilsMixed	4
<input checked="" type="checkbox"/> BeilsMultiStep	60
<input type="checkbox"/> ChemInform	35
<input type="checkbox"/> MOS	All rules (slower search)

[\*] Lower numbers mean use more rules

Synthetic depth: 3  
 Exclude starting materials matching the target molecule.  Send notification email when search is done.

Search

### ARChem Query Screen

# Trial Databases

# Organic Chemistry

## ARChem - Automating Retrosynthetic Chemistry (cont.)

To set up a search you can either:

- Upload a MOL file
- Upload an RD file or
- Draw a molecule or reaction

[If you choose to draw, then ChemAxon's [MarvinSketch](#) will open. ]

There are a number of **starting material catalogues** which you can choose should be used and you results are chosen from **reaction database** such as **Beilstein** and **ChemInform**.

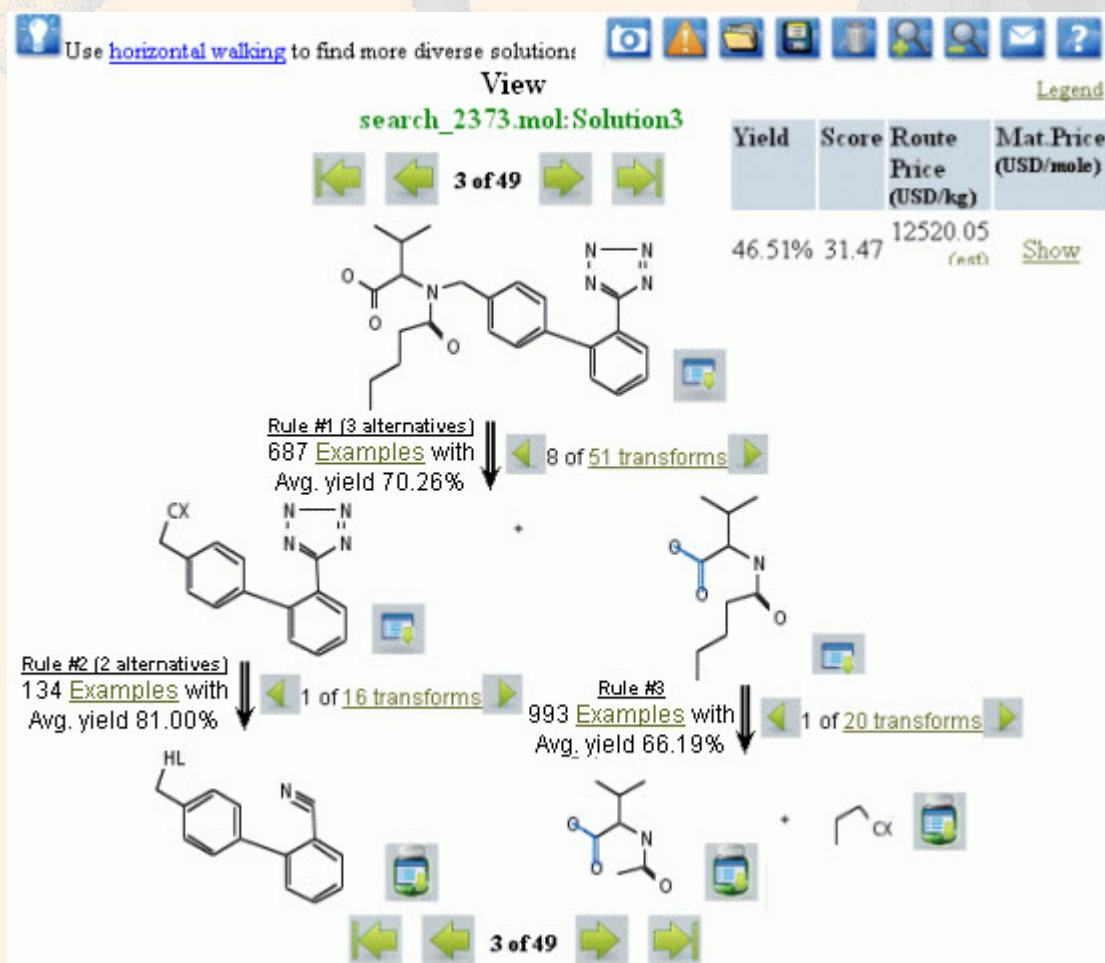
The search may take a while but you can continue to set up other searches. An e-mail will inform you when the search is complete.

## Results

Clicking on View searches will produce a page showing a table which lists all your searches with their parameters, status, and number of solutions.

Click the file name (e.g [search\\_2373.mol](#)) to access the solutions.

Click solution ID (e.g [Solution3](#)) to view full retrosynthetic tree



**Solution to a Product showing number of examples and availability of starting materials.**



# Trial Databases

## Organic Chemistry

### Symyx/Isentris Databases

CDS, in conjunction with JISC, are looking to re-establish the databases that we used to offer in the past using ISIS software, but will now be based on **Isentris** software.

### CDS have been running an evaluation trial

All databases from **Symyx** (now **Accelrys**) have been made available over an extended trial period - which came to an end at the end of November. Access was via an **Isentris client** and via **DiscoveryGate**.

### Databases

#### Bioactivity

- \* Comprehensive Medicinal Chemistry (CMC)
- \* MDL Drug Data Report (MDDR)
- \* Metabolite
- \* National Cancer Institute Databases - The NCI 127K, Plated Compounds, AIDS, and Cancer databases
- \* Toxicity - A compendium of toxicological data.
- \* RTECS (Registry of Toxic Effects of Chemical Substances)

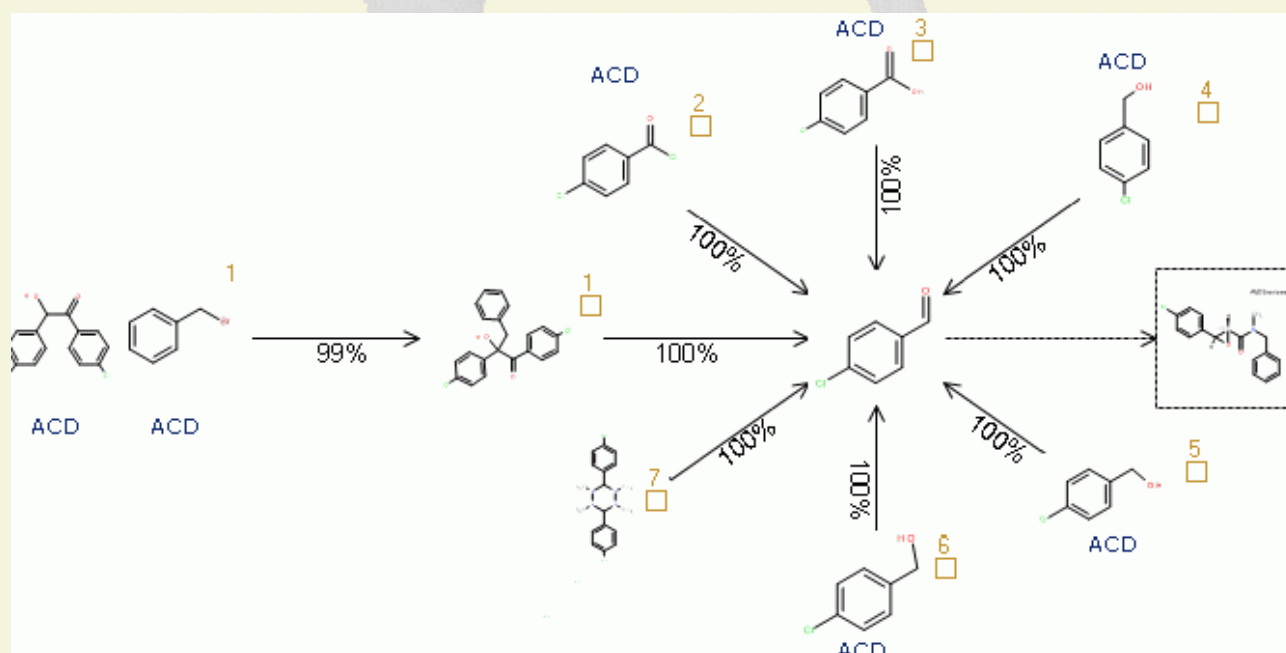
#### Sourcing Databases

- \* Symyx Available Chemicals Directory (ACD)
- \* Symyx Screening Compounds Directory (SCD)

#### Synthesis Databases

- \* ChemInform Reaction Library (CIRX)
- \* Current Synthetic Methodology (CSM)
- \* Derwent Journal of Synthetic Methods (DJSM)
- \* ORGSYN Database
- \* Reference Library of Synthetic Methodology (RefLib)
- \* Solid-Phase Organic Reactions (SPORE)
- \* SPRESI (also available now via CDS)

In addition, Isentris can be used for **Synthesis Planning**, producing reaction schemes that also show if the starting material is commercially available.



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

# Trial Databases

## Symyx/Isentris Databases (cont.)

Initially **users must contact CDS** and they will then be sent login credentials to access the databases via DiscoveryGate. Isentris client software is also available to download and access the data.

DiscoveryGate requires that Java 2 Runtime Environment (JRE) 1.5.0\_12 or later is available on your PC and will install it if not found.

The Java based **Symyx Draw** is also made available on your desktop machine for entering structural queries.

Viewing: Applications/MDL Isentris client/ACD/Details.browse.xml

### *A hit from Available Chemicals Directory using Isentris*

**Symyx ACD contains pricing and supplier information for over 1,160,000 unique chemicals, including 3D models, from 840 suppliers worldwide.**

Getting started information is available at::

<http://cds.dl.ac.uk/cds/datasets/orgchem/symyx/discoverygate.html>

<http://cds.dl.ac.uk/cds/datasets/orgchem/symyx/Isentrisinstal.html>

Funding details of the databases has still to be worked out, but it is likely that the following 'packages' would be offered on an individual, Institutional or UK wide model.

'**Discovery** Package' which includes all the Bioactivity, Sourcing and Synthesis Databases

'**Synthesis** Package' - ACD plus Synthesis Databases

'**Pharmacology** Package' - all the Bioactivity databases.

'**Sourcing** Package' - ACD plus SCD.

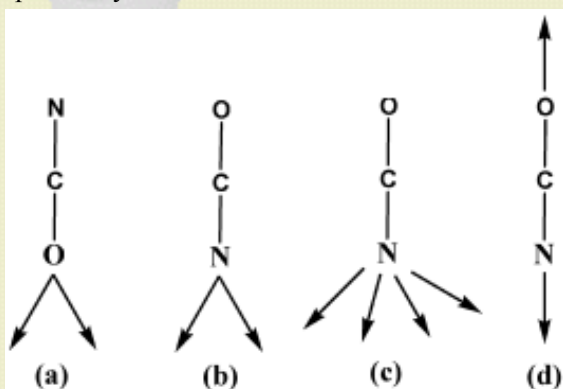
Links used in this Newsletter and others can be found at:- <http://cds.dl.ac.uk/letterlinks>

# Research Highlight

## Na<sup>I</sup>/Cu<sup>I-II</sup> heterometallic cages interconnected by unusual linear 2-coordinate OCN-Cu(I)-NCO links.

Aurkie Ray<sup>a</sup>, Samiran Mitra<sup>a</sup>, Georgina M. Rosair<sup>b</sup>, Ramanan Rajeev<sup>c</sup>, Raghavan B. Sunoj<sup>c</sup>, Eva Rentschler<sup>d</sup>. <sup>a</sup>Jadavpur University Kolkata, India, <sup>b</sup>School of Engineering and Physical Sciences, Heriot Watt University, Edinburgh, UK, <sup>c</sup>Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, India, <sup>d</sup>Johannes Gutenberg – University of Mainz, Institute of Inorganic and Analytical Chemistry, Mainz

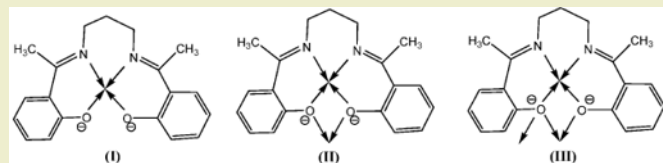
It is well known that the cyanate ion can link a pair of metal centres in *end-on* ( $\mu_{1,1}$ -OCN,  $\mu_{1,1}$ -NCO and unusually  $\mu_{4,1}$ -NCO or *end-to-end* ( $\mu_{1,3}$ -NCO) bonding modes (Scheme 1). In contrast to the *end-on* cyanato-bridged multinuclear metal complexes <sup>1-2</sup> coordination polymers with the *end-to-end* bridging cyanate are comparatively rare.



**Scheme 1** Different types of bridging modes of cyanate (a)  $\mu_{1,1}$ -OCN, (b)  $\mu_{1,1}$ -NCO, (c)  $\mu_{4,1}$ -NCO (d)  $\mu_{1,3}$ -NCO.

Searches of the Cambridge Structural Database using the **Chemical Database Service at Daresbury** found only ten examples of *end-to-end* cyanato bridged copper complexes of which only two complexes showed single  $\mu_{1,3}$ -NCO bridges. A limited number of related linear two-coordinate copper(I) complexes were also found.<sup>3</sup>

Metal salicylaldimines are not only effective complexing agents for p- and d-block elements but also for alkali metal ions. Furthermore, some of the bimetallic systems resulting from alkali metal complexation have particularly important properties concerning electron storage<sup>4-6</sup> and the carrying of polar organometallics.<sup>7</sup> Tetradentate Schiff base ligands with  $N_2O_2$  donor sets can coordinate with 3d/alkali-metal to give rise to heterometallic complexes (Scheme 2) but Na/Cu heterometallic systems derived from a  $N_2O_2$  donor tetradentate Schiff base ligand still remain rare.



**Scheme 2** the  $N_2O_2$  donor Schiff base ligand (H<sub>2</sub>L). **I** and **II** are the usual coordination modes whereas **III** is the most rare and unusual coordination mode of [L]<sub>2</sub>.

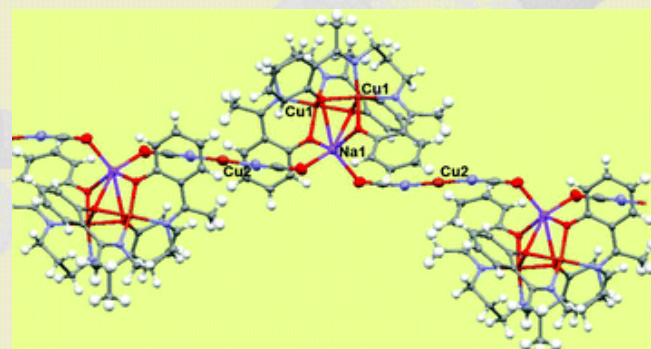
A new Na<sup>I</sup>/Cu<sup>I-II</sup> heterometallic mixed valence coordination complex [Cu<sub>2</sub>L<sub>2</sub>Na(NCO)<sub>2</sub>Cu]<sub>n</sub> (1) with an

unusual architecture was synthesised. To the best of our knowledge this is the first structurally characterised 1D heterometallic coordination polymer propagated by biscyanatocuprate(I) anion. Another key feature is that it is a mixed valence Na<sup>I</sup>/Cu<sup>I</sup>/Cu<sup>II</sup> heterometallic species.

Cyclic Cu<sub>2</sub>NaO<sub>4</sub> cages constructed by the tetradentate N<sub>2</sub>O<sub>2</sub> donor Schiff base ligand are interconnected to each other by a rare singly *end-to-end* bridged OCN-Cu(I)-NCO link generating 1D chain, with Cu(I) possessing linear 2-coordinate geometry.

The complex has been characterised by elemental, spectral and structural analysis (see Fig.1) The cyclic voltammogram has been compared with the analogous complexes. Density functional theory calculations have been carried out to gain additional insights into the metal and ligand orbitals participating in this unusual structure.

Cryomagnetic susceptibility studies indicate the copper(II) centers in the cyclic Cu<sub>2</sub>NaO<sub>4</sub> cages are antiferromagnetically coupled with  $J = -13.8 \text{ cm}^{-1}$



**Fig. 1** The 1D chain structure propagated by linear 2-coordinate OCN-Cu(I)-NCO linkages.

### References

1. A. K. Boudalis, Y. Sanakis, J. M. Clemente-Juan, B. Donnadieu, V. Nastopoulos, A. Mari, Y. Coppel, J.-P. Tuchagues and S. P. Perlepes, *Chem.-Eur. J.*, 2008, **14**, 2514
2. O. J. Parker, M. P. Wolther and G. L. Breneman, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 1996, **52**, 1089.
3. R. A. Himes, G. Y. Park, A. N. Barry, N. J. Ninian, J. Blackburn and K. D. Karlin, *J. Am. Chem. Soc.*, 2007, **129**, 5352.
4. S. Gambarotta, M. Mazzanti, C. Floriani and M. J. Zehnder, *J. Chem. Soc., Chem. Commun.*, 1984, 1116
5. E. Gallo, E. Solari, N. Re, C. Floriani, A. Chiesi-Villa and C. Rizzoli, *J. Am. Chem. Soc.*, 1997, **119**, 5144.
6. G. Fachinetti, C. Floriani, P. F. Zanazzi and A. R. Zanzari, *Inorg. Chem.*, 1979, **18**, 3469.
7. E. Gallo, E. Solari, C. Floriani, A. Chiesi-Villa and C. Rizzoli, *Inorg. Chem.*, 1997, **36**, 2178.

# 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 **525,000 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 **135,000 inorganic compounds**

*WWW interface available for ICSD.*

## CRYSTMET

Crystal structure data for over **126,400 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.

## 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.

## 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 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	16,561	25,442	10,238
ACD/Labs	200,100	210,700	9,287	-	27,500	17,000	-

**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.

## ORGANIC CHEMISTRY

### SPRESI

Allows you to search Molecules, Reactions, References and associated data. Contains synthesis planning tool.

**Direct access over the web to:-**

- 8 million structures
- 4 million reactions
- 32 million factual data entries

extracted from:- 653,000 references  
164,000 Patents

### Accelrys Accord Databases

#### Protecting Groups

Selected protection, deprotection and transprotection reactions

#### Solid Phase Synthesis

Information related to combinatorial synthesis.

#### BioCatalysis

Biomolecules as catalysts in organic synthesis

#### Sourcing Databases

#### CDS Available Chemicals

Up-to-date catalogue data including prices.

#### CDS Screening Compounds

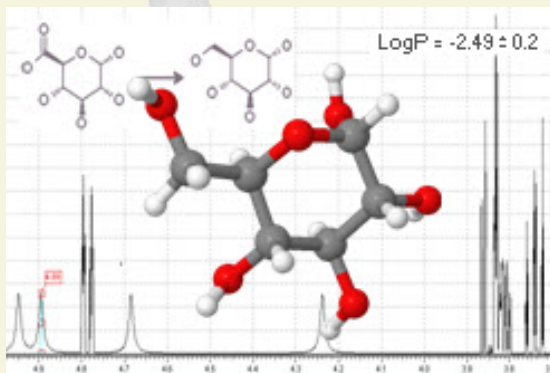
Over 3.5 Million entries from 12 Suppliers

# 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.**

## 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](mailto:donald.parkin@stfc.ac.uk)

Phone: 01925 603 162

Links used in this Newsletter can be found at:

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

## Main Service Machine

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

**CDS Helpdesk:**  
[cdsbb@stfc.ac.uk](mailto:cdsbb@stfc.ac.uk)

or phone  
**01925 603 162**

## 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**

**Cheshire**

**WA4 4AD**

**Tel: 01925 603 162**

**Fax: 01925 603 031**

**Email: [cdsbb@stfc.ac.uk](mailto:cdsbb@stfc.ac.uk)**