

<http://cds.dl.ac.uk/cds/CIG/cig.html>

Future meetings

ONE-DAY TRAINING COURSE ON CHEMICAL INFORMATION

12th October 2004, Burlington House, London
Organised jointly by CSA Trust and RSC-CIG -

Chemical Information for the Non-Chemist

This one day training course will continue the successful meeting last year with a series of presentations which will provide an impartial and critical overview of Chemical Information products. It will be given by specialists from academic information departments, vendor representatives and the pharmaceutical industry.

The theme of the presentations will cover structure searching in relation to chemical reactions, chemical properties and chemicals reported in patents

A booking form is included at the end of the newsletter.

- Why is chemical information different from other types of information?
- How the chemical structure is handled by the chemical information providers (Nomenclature, Registry Numbers, Molecular formulae, Notations, Connection tables)
- Chemical structure drawing packages
- How to search for chemical structures – substructure searching
- Structure databases
- How to search for reactions
- How to search for generic structures

Booking form on last page or see
<http://cds.dl.ac.uk/cds/CIG/CIG-Booking-Form.html>
Any changes to the meeting see
<http://cds.dl.ac.uk/cds/CIG/cig.html#Future>

Past meetings

CHEMICAL INFORMATION FROM Ac to Zr

A full program of eight speakers showed that there is a wealth of chemical information available in other areas beside organic chemistry and patents.

The meeting started with a presentation by **Eva Dimmock** and **Susan Bates** from **INSPEC** on how Inspec can help to solve chemical search problems. The talk first covered the background, content, structure and coverage of the databases then went on to concentrate on chemicals coverage and search, with examples on how to search.

This was followed by **Chris Gibson** from **Manchester University** who spoke about 'Knovel - beyond eBooks' which included slides on how to search the databases and the many benefits. This data is now available to RSC members.

The Merck Index was **Robert Scoffin's (ChembridgeSoft)** subject, which remains an outstanding source of information, especially as it is now also available on-line.

The morning session was concluded by a very entertaining talk from **Patrick Coulter** of **Granta Design Ltd.** concerning the Materials IT Revolution. He involved the audience in suggesting properties for the material for a plane wing and then showed databases where information could be obtained. Samples of materials were also handed around the audience.

Rainer Poerschke (Springer) travelled all the way from Germany to tell us about the Landolt-Bornstein database, a comprehensive top quality data collection on substance and physical properties (also available on-line through SpringerLink and Knovel).

This was followed by **Don Parkin (Chemical Database Service)** who concentrated on the Detherm database, one of the world's largest thermophysical property databases of pure compounds and compound mixtures.

After coffee, **Mark Leach, Salford University** told us about his Chemical Thesaurus which is free for personal use. Apart from information on chemical reactions, it contains a clickable periodic table with lots of physical data, a molecular weight calculator, plus 'gadgets' for Redox chemistry and thermochemistry.

Finally **Fiona MacDonald (Chapman & Hall/CRC Press)** tried to make sense of Inorganic Chemistry using the Dictionary of Inorganic Compounds which contains information on over 4,000 inorganic compounds. Fiona took us through the decisions as to which compounds and data should be included and the various issues, such as name, and finished with how all the data was organised.

Some of the above talks are available to view on the CIG web site.

NEWS

Scientific Publications Inquiry

The House of Commons Science and Technology Select Committee is investigating access to journals within the scientific community, with particular reference to price and availability. The final Report can be found at <http://www.publications.parliament.uk/pa/cm/cmsctech.htm#reports>

CrossRef Search/Google

A group of leading journal publishers are participating in a CrossRef Search Pilot:

<http://www.crossref.org/crossrefsearch.html> .

This Pilot is initially limited to the content of 25 of the more than 600 CrossRef publishers and societies who collaborate to provide scholars with cross-publisher reference linking such as Blackwell Publishing, Oxford University Press and John Wiley & Sons (full list available at above web reference).

Through a special, reciprocal arrangement between Google and CrossRef, a typical Google search is launched but the results are restricted to the scholarly research content from participating publishers, with the intent of reducing the noise produced by general web searches. Search at the website of one of the participating publishers:

RSC journal archives for £50

JISC funds access to the Royal Society of Chemistry Journals Archive

The JISC has licensed the content of the archive in perpetuity on behalf of the HE community. Institutions can now receive content which would have cost them £25,000 - at no charge with the option of hosting the archive locally or paying a service charge for access to the archive via the RSC's interface.

Staff at institutions can access more than 150 years of essential research at their fingertips as the archive contains all articles published by the Royal Society of Chemistry (RSC) (and its forerunner societies) from 1841 to 1996.

The **RSC Journals Archive** will contain about 210,000 articles and 1,200,000 pages, available as searchable full text. The archive includes top titles such as ChemComm, The Analyst and Dalton Transactions. In addition, the references in the 1990-1996 articles contain 'reference links' to full text and CAS abstracts. A full listing of the journals included in the Archive can be found at

<http://www.rsc.org/pdf/journals/archive/journals.pdf>.

Institutions have two options to Access the RSC journal archives

- **Option A:** they can sign up for three years access via the RSC's secure network. There is an annual access fee, starting from 1st August 2004, which varies, according to the JISC Bands (£462 - £612 Annually)
- **Option B:** they can choose to mount the Royal Society of Chemistry Journals Archive on the institution's local secure network for a one off fee of £50.00 (excluding VAT). However, this requires institution to provide their own searching/indexing/ linking/ authentication services.

http://www.jisc.ac.uk/coll_rsearchive.html

SCOPUS

Scopus, the world's largest abstract and indexing (A&I) database which links to libraries' entitled full text, is in its final phase of development and is being made available for final testing to a select group of librarians.

Launch will follow the successful completion of this testing, and is expected to be in Q4 2004.

With 13,450 peer-reviewed titles, Scopus is designed to be an all science, comprehensive access point for a library, with coverage of 13,000 titles from over 4,000 STM publishers, plus coverage of over 100 open access journals by the summer. Scopus also simultaneously searches the scientific Web using Elsevier's science-only Internet search engine, Scirus. The company aimed to make the Scopus service "as easy to use as Google," with fewer clicks to the full text than any service available. Eilish.McLoughlin@dcu.ie

ChemWeb.com

ChemWeb.com, owned by Elsevier, thought to be closing at the beginning of the year, will soon be transferred to its new owner - **ChemIndustry.com** (<http://www.chemindustry.com>). The new ChemWeb.com will be reshaped into a search resource, in collaboration with users and sponsors.

Resource Guide for Physical Sciences

The Resource Guide for Physical Sciences initiative ended on the 31st of July 2004. The initiative, which was funded by the JISC, has been a great success in raising the awareness of electronic resources with thousands of printed guides distributed, thousands of hits a month to the online website and many talks and presentations given at both national and international conferences across the country.

http://www.jisc.ac.uk/index.cfm?name=rg_phys_main

Platinum Metals Review: E-Journal

Supporting the science and technology of the platinum group metals

Platinum Metals Review is Johnson Matthey's free quarterly journal of scientific research on the platinum group metals (pgms). As from the July 2004 issue, Platinum Metals Review became an E-journal <http://www.platinummetalsreview.com/>

Reed Elsevier

Reed Elsevier, is under fire for the price increases it levies on libraries for access to its publications.

Critics argue that the scientific community should abandon seeking publication in journals of the type that Reed owns in favour of the "open-source" model, in which authors pay to have their research made public.

Elsevier, the scientific publishing division, is proposing a 5.5 per cent price increase — above the rate of inflation. They earned £204 million operating profit in the six months to June 30, down from £219 million a year ago. Profit margins decreased by 1 percentage point to 32 per cent, following what the company said were increased levels of investment.

Last month, MPs on the Commons Science and Technology Committee called on the Government to create a free national archive of all scientific publications, and accused Reed of "not being transparent" about its costs.

News from CAS

CAS Will Extend Access To More Literature From Early Twentieth Century

A significant enhancement to CASM and CPlusSM database coverage, planned for September, is the addition of more information back to 1900! CAS continues to expand its "Scientific Century" project by making thousands of additional early 20th century articles from ACS journals and others available online.

Researchers can now find more than 7,000 additional records back to 1900, including publications even older than the beginning of *Chemical Abstracts*TM (CA). Issues of the *Journal of the American Chemical Society* and the *Journal of Physical Chemistry* provided many of the additional records. Hundreds of other newly added records are for documents published from 1900-1912 in various sources not originally covered in CA but cited in the online files since 1998.

New Releases of 2004 Editions of SciFinder[®] and SciFinder Scholar[®] available soon

New releases of the 2004 Editions of SciFinder and SciFinder Scholar will be available this autumn and will include a new SciFinder and SciFinder Scholar toolbar for Microsoft[®] Internet Explorer, improved scrolling, SciFinder Panorama for Microsoft Excel 2003 and reaction display enhancements for SciFinder Scholar. Additional reactions and property information have been added, along with more links to full-text documents.

CAS Records One Million Real-Time Document Requests (RDRs) per Month

With a click of a button, users of CAS electronic services enter a Real-Time Document RequestTM (RDRTM) for the electronic full text of a desired article or patent. Since 2001, CAS Science Spotlight has been tallying RDRs to determine the journal articles and journals that are most sought by scientists in connection with their research. In March, April, and May 2004, the service for the first time reached 1 million RDRs each month and the pace is still accelerating. A comparison of the 2003 Most Requested journal articles vs the 2003 Most Cited has shown no articles in common, indicating that what scientists cite and what they request during the course of their research may be totally different.

Dr Barry Dunne, SII/CAS, bdunne@cas.org

News from STN

Jan Davies, STN Agency UK, daviesj@rsc.org

Version 7.01 of the Analysis Edition of STN Express with Discover

New analysis, data grouping, and visualization functions are now available with Version 7.01 of the Analysis Edition of STN Express with Discover!

Building upon the features of the Analysis Edition (Version 7.0), the new version provides

- New Analyze Plus Wizard for enhanced data grouping, results analysis, and visualization
- Easier access to Discover! wizards and content
- Additional access to the POLYLINK and SEQLINK EXACT commands available via the redesigned CAS Registry Number(R) Wizard
- More experimental and calculated properties in the CAS Registry Number Wizard
- Improved post-processing, with automatic removal of blank cells from displays of patent data in tables and reports

For full details on the web see:-

<http://www.cas.org/ONLINE/STN/discover.html>

STN Adds New CSA Databases

Now available on STN are seven new databases from the renowned database producer Cambridge Scientific Abstracts (CSA). With these new files, STN now offers a total of 26 CSA databases and remains the largest independent online provider of CSA files. Coverage focuses on life sciences, environmental and aquatic sciences, computer sciences, materials sciences, engineering and aerospace. The new files are ANTE, CIVILENG, MECHENG, ENVIROENG, WATER, AQUALINE, and BIOENG.

RSC Journal Prices 2005

The Royal Society of Chemistry journal prices for 2005 can be viewed at

<http://www.rsc.org/is/journals/current/jpricing.htm>

Analytical Chemistry

- The Analyst's popular i-section will publish twice as many articles and will appear in every issue!
- Lab on a Chip will increase to 12 issues
- The scope of Analytical Abstracts will be enhanced to increase coverage of the growing area of proteomics and genomics

Materials Chemistry

- Journal of Materials Chemistry will become the first weekly materials chemistry journal!

Chemical Biology

- New for 2005 - Molecular Biosystems, an interdisciplinary journal for research at the interface of chemistry and biology. Appearing monthly in Chemical Communications from Summer 2005.
- Organic & Biomolecular Chemistry (OBC), will increase the number of communications it publishes.

General Chemistry

- 2005 sees Chemical Communications celebrate 40 years of publication and increases to weekly issues
- Chemical Society Reviews will increase to 12 issues annually
- Chemical Science and Chemical Technology, the two supplements showcasing the latest developments across the chemical sciences, will appear in more RSC journals

CRC Handbook of Chemistry and Physics, 85th Edition

New tables in this edition include:

- Index of Refraction of Inorganic Crystals
- Upper and Lower Azeotropic Data for Binary Mixtures
- Critical Solution Temperatures of Polymer Solutions
- Density of Solvents as a Function of Temperature

By popular request, several tables omitted from recent editions are back, including Coefficients of Friction and Miscibility of Organic Solvents.

Ten other sections have been substantially revised, with some, such as the Table of the Isotopes and Thermal Conductivity of Liquids, significantly expanded.

The Fundamental Physical Constants section has been updated with the latest CODATA/NIST values, and the Mathematical Tables appendix now features several new sections covering topics that include orthogonal polynomials Clebsch-Gordon coefficients, and statistics.

The International Toxicity Estimates for Risk (ITER) Database

NLM has announced the addition of a new database to the TOXNET system - a cluster of databases on toxicology, hazardous chemicals, and related areas. The International Toxicity Estimates for Risk (ITER) Database (<http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?iter>) is a database of human health risk values from major organizations worldwide for over 600 chemicals of environmental concern. It is a product of Toxicology Excellence for Risk Assessment (TERA), a non-profit group whose mission is to protect public health by developing and communicating risk assessment values, improving risk methods through research, and educating the public on risk assessment issues.

1. Collaborative effort wins £0.94m from Aimhigher

The RSC, 12 universities, three pharmaceutical companies and two Sector Skills Councils have come together to win a bid for funding worth £941,446. The money will come from the Hefce Aimhigher National Activity initiative, which aims to help widen participation in UK higher education, particularly among students from non-traditional backgrounds, minority groups and the disabled. Further information is available from Libby Steele in the RSC Education Department (education@rsc.org) and on the Aimhigher website at www.aimhigher.ac.uk/en/home/index.cfm.

2. Campaign for Chemical Sciences reports

The RSC has commissioned three reports as part of its Campaign for Chemical Sciences. The areas covered are: - Supply and Qualifications for Science Teachers - The Right Chemistry: The Choice of Chemistry Courses and Careers - Laboratories, Equipment and Budgets. These reports are available on the RSC website at www.rsc.org/edreports.

3. Manage your membership online

Application forms for transferring between categories of membership, and Chartered Chemist and Chartered Scientist can now be completed and submitted online. You can also use this new online service to pay your annual subscription, pay for ongoing subscriptions to journals, join any of our Interest Groups and update your personal details. You will need your membership number and password (which, unless previously changed, is date of birth in YYYYMMDD format). To access this service, go to www.rsc.org/members.

4. Last chance to register for RSC September 2004 Conferences

There is still time to register for the following conferences: - Faraday Discussion 129: the Dynamics and Structure of the Liquid-Liquid Interface - Frontiers in Chemical Biology: the Chemical Biology of Cancer - CrystEngComm Discussion 2004: New Trends in Crystal Engineering - Materials Discussion 7: From Molecules to Materials - 5th International Symposium on Transition Metals in Organic Synthesis - Non-covalent Interactions in Chemistry and Biology - Molecular Modelling 4 Chemists To see scientific programmes and to register, please visit www.rsc.org/conferences.

5. New from Knovel

Knovel's fully interactive critical tables are searchable by keyword and numeric property value comprising physical data for inorganic and organic compounds and common solvents, with thermodynamic properties. Some have equation plotters to plot thermodynamic properties as a function of temperature. Exploit this membership benefit from the RSC's LIC at www.rsc.org/lic/knovel_library.htm.

LHASA LIMITED ANNOUNCES THE RELEASE OF VITIC 2.0

Based on an original project from the Washington DC-based ILSI Health and Environmental Sciences Institute (HESI), this new version of the database has been substantially extended to include:

- 59,800 Genetic toxicity *in vitro* data records for 2130 chemicals
- 156 Hepatotoxicity data records for 41 chemicals
- 2,700 Skin sensitisation data records for 830 chemicals
- 126 HERG data records for 79 chemicals

Increasing demand for a high-quality, structure-searchable toxicology database led LHASA Limited to initiate a three year research and development project in 2003. The resulting VITIC database is fully structure-searchable, with many potential uses, including data-mining to determine structure-activity relationships.

For further information, please contact:

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Email: info@lhasalimited.org

Web: www.lhasalimited.org

Miner3D

New versions 4.2 of Miner3D ENTERPRISE and Miner3D EXCEL Professional have been released.

New features coming with V4.2 include:

- MovieRecorder - record your animations step by step and save the process of refinement of data model, moves, rotations and also visual querying in Selector. AVI compatible files can be then played in Windows Media Player®, inserted in your multimedia presentations, or emailed.
- HeatMap model improved

For More information and downloads see <http://miner3d.com>

CDS DETHERM Database

The Chemical Database Service has added Detherm to their list of available databases for UK academics. Detherm is one of the world's largest thermophysical property databases of pure compounds and compound mixtures. At present it contains 4.9 Million data sets for around 130,000 systems (over 24,000 pure substances and 106,000 mixtures) covering more than 500 properties fields.



New Odyssey chemistry teaching software for Windows makes chemistry teaching interactive and highly visual.

ODYSSEY is a new suite of instructional software for the initial chemistry classes in Universities, colleges, and secondary schools. Featuring molecular simulation technology, *ODYSSEY* provides a highly interactive environment for learning and exploration. Rich content is included to accompany students and instructors throughout the introductory curriculum. Classroom demonstrations as well as student assignments are supported with ready-to-use materials.

Molecular Simulation Approach. *ODYSSEY* addresses more than 70 core chemistry topics. The software allows for stunning molecular simulations that are carried out in real time by a fully-integrated computational engine. With on-the-fly user control of system parameters (temperature, volume, and system composition), compelling classroom demonstrations and innovative student assignments are within reach of every lecturer and teacher.

Discovery-Based Learning. In addition to more than 200 pages of chemistry content, *ODYSSEY* includes a collection of student assignable worksheets and an extensive, annotated library of molecular models (inorganic and organic molecules, gases, liquids, solids, solutions, biomolecules and more).

Visualisation. *ODYSSEY* offers a window onto the molecular world, providing opportunities to interact with molecules and matter like never before. Students carry away an intuitive understanding of chemical structure and molecular motion.

Advanced Interface. *ODYSSEY* operates in a, web-like HTML environment that combines molecular simulations and text content. By introducing students to molecular modelling, *ODYSSEY* provides early exposure to computer-based tools that are a standard part of many teaching laboratories.

Download the demo at:

http://www.wavefun.com/software/odyssey_demo_request.html

MDL CrossFire Commander 7.0

The software to search the CrossFire Databases has been redesigned with numerous new features:

- All actions in Commander are in one Window, instead of two Windows as it was with earlier Versions.
- MDL Look&Feel : MDL CrossFire Commander 7.0 has the same look & feel as any other MDL Software.
- Results can be organized by sorting or grouping. This is especially helpful since the results from a search in Beilstein get bigger while we increase the content
- Alerts: An automatic search retrieves all new data about a research topic from a database update.
- Reaction Classification Codes: All Reaction Databases of MDL are equipped with InfoChem's Reaction Classification Codes, enabling a user to find similar reactions in other databases with this identifier.

All the new features and the redesign are a step into the direction of integrating all content and all clients of MDL under DiscoveryGate.

IUPAC-NIST Chemical Identifier (INChI)

The objective of the IUPAC Chemical Identifier Project is to establish a unique label, the IUPAC Chemical Identifier, which would be a non-proprietary identifier for chemical substances that could be used in printed and electronic data sources thus enabling easier linking of diverse data compilations.

A new test version was made available in July 2004

The test program accepts input in the form of MOLfiles (or SDfiles) and CML files. A single INChI is generated for a single input structure, which can contain multiple components. Identifiers can be created for organic compounds with Z/E and sp³ stereochemistry, tautomers, and isotopes as well as salts, organometallic compounds and protonated forms of a compound.

The 2004 Tony Kent Strix Award

The Strix Award is presented in memory of Dr. Tony Kent, a past Fellow of the Institute of Information Scientists and former Director of Information Services at the RSC, who died in 1997. Tony Kent made a major contribution to the development of information science and information services both in the UK and internationally, particularly in the field of chemistry. The name Strix was chosen both to reflect Tony's interest in ornithology, and the name of one of the last and most successful information retrieval packages which he created. The Award is given in recognition of an outstanding contribution to the field of information retrieval.

The 2004 award has been given to Prof. C.J. (Keith) van Rijsbergen. Professor van Rijsbergen has been at the forefront of research in information retrieval for more than 30 years. He has been particularly effective in introducing a range of theoretical ideas into the field, notably in the areas of clustering, probabilistic models, and non-classical logics including probabilistic logics and inference models. A recent contribution is entitled *The Geometry of Information Retrieval*, and uses a framework from the field of quantum mechanics.

He has also contributed to evaluation questions; an effectiveness measure which he proposed has become widely used, and is the standard measure in text categorisation studies.

He has published extensively, including a substantial number of research papers, but also material aimed at non-specialists or students. His textbook called *Information Retrieval*, first published in 1975, has been very extensively used and cited. The second edition of this book (1979) was the first textbook to give coverage to the emerging probabilistic theory in IR.

His career has taken him to academic positions in Cambridge; Melbourne; a short spell in Berkeley; Dublin; and currently (for nearly 20 years now) at the University of Glasgow. Another factor in the spread of his ideas is his supervision of a stream of high-quality research students, many of whom have made their own mark on the field in a variety of ways. His influence has been felt far and wide in the field of information retrieval.

The award will be presented during the October meeting of the CIG at Burlington House.

The BA Festival of Science

I found this through the link on the BBC website and although I am sure the BA would prefer more serious advertising, readers may be interested in the BA -

The BA (British Association for the Advancement of Science) is the UK's nationwide, open membership organisation dedicated to connecting science with people, so that science and its applications become accessible to all. The BA aims to promote openness about science in society and to engage and inspire people directly with science and technology and their implications

<http://www.the-ba.net/the-ba/Events/FestivalofScience/>

The vote, launched on 20 July by bbc.co.uk/cult and the BA, tied in with the theme of this year's [BA Festival of Science](#), 'the responsibility of being a scientist'. Voters took part

online at www.bbc.co.uk/cult/scientists where they chose from a top ten list of screen scientists including Mr Spock, Dana Scully, Q and Dr Strangelove.

Mad Muppets top cult science poll

Don't tell the health and safety people but Dr Bunsen Honeydew and his trusty assistant, Beaker, have topped a poll of the UK's favourite cult TV boffins.



Dame Julia Higgins, is the current president of the BA. "I'm not sure that Dr Honeydew is quite the role model we would be looking at for a responsible scientist," she said.

"His treatment of his faithful assistant Beaker is rather alarming, though admittedly also rather amusing."

The festival dates back to 1831, when the first meeting was held by the newly formed British Association for the Advancement of Science.

Its purpose is to act as a forum for publicly presenting and discussing developments across many different areas of science. Members of the public, journalists and school students are among the thousands of visitors who attend every year.

In the past, the festival has been the stage for some major clashes between leading academics.

The best known occurred at the meeting in Oxford in 1860 when the Bishop of Oxford, Sam Wilberforce, launched a bitter attack on Charles Darwin. Thomas Huxley and JD Hooker hit back in a series of legendary exchanges. Years later, when Bishop Wilberforce died after falling off his horse, Huxley remarked: "For once, reality and his brains come in contact and the result was fatal."

Another row started in 1836 with an attack on a young upstart railway engineer, Isambard Kingdom Brunel, by Dionysus Lardner, who refused to believe a steamship could carry enough fuel to travel from Bristol to New York.

The dispute continued into the 1837 meeting, but by the following year Brunel had won the argument. The Great Western took 15 days to cross the Atlantic to New York, with 25% of her coal unused.

