

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

SPRING MEETING - JUNE 6th 2006 ELECTRONIC LAB NOTEBOOKS

The spring meeting of the Chemical Information Group will be a **joint meeting with the Computer Applications Subject Group**. This one-day meeting will be held on Tuesday, June 6th, at The Royal Society of Chemistry, Burlington House, Piccadilly, London.

The subject of the meeting is 'Electronic Laboratory Notebooks,' a topic of great current interest. An international team of expert speakers will present a comprehensive overview of the current state of the art of electronic laboratory notebooks, including what ELNs are, why you should consider moving to them if you have not already done so, and guidance on how to plan and manage the implementation of an ELN project.

This meeting represents extremely good value for money, as the cost is only £30 for CIG and CASG members, and £40 for non-members, including coffee, tea and lunch. Further details and application forms are available from:
Chris Evans – (please see back page for details)

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CHEMICAL INFORMATION GROUP AND THE COMPUTER APPLICATIONS SUBJECT GROUP

In recent years, following the unfortunate loss of two of its key officers, the Computer Applications Subject Group (CASG) has been somewhat moribund. The lack of activity has caused concern within the Royal Society of Chemistry, particularly at the Science and Technology Board to which CASG reports. The possibility of closing the group has been mooted on more than one occasion. Nevertheless, the continuing healthy membership of the group (currently about 350) indicates a strong continued interest in the subject area covered by the group.

The other group most closely related to the CASG in terms of subject matter is the Chemical Information Group (CIG), which also reports to the STB. Therefore, in order to avoid the closure of the CASG and to continue to cater for the interests of its members, discussions have taken place between officers of the two groups, which have led to a proposal to merge to two groups.

The CIG currently has about 150 unique members, the CASG about 300, and there are about 50 people who are members of both groups. It appears that the simplest way of achieving this merger is to amend the constitution of the CIG to broaden its remit to cover the computer applications area.

A joint meeting organised by the two groups is being held, on the subject of Electronic Laboratory Notebooks, on Tuesday, June 6th, 2006 at Burlington House. Further details of the meeting appear elsewhere in this newsletter. This meeting will also include the AGMs of the groups, where a formal proposal for the merger and a constitution for the merged group will be presented. It is important that as many members as possible come along to the AGMs to present their views on the proposed merger.

(Cont...)

Whilst there is a modest fee for attending the scientific meeting (£30 for members of either group) attendance at the AGMs is free. They will be held immediately after lunch, starting at 2pm in the Council Room at Burlington House.

The key parts of the proposed merged constitution are as follows:

1. The Subject Group shall be called the "Chemical Information and Computer Applications Group" of The Royal Society of Chemistry, affiliated to the Science and Technology Board. The Group shall be deemed a Charitable Trust.

2. Aims

To keep chemists and other users of chemical information and of computer applications for gathering, storing, retrieving and using chemical information aware of relevant activities, services and developments by means of organizing meetings and lectures, promoting newsletters and publications of interest, and representing members' views to information and computer applications providers.

A proposal to this effect has already been discussed by the STB, which met in March. STB agreed the merger in principle, subject to the approval of the memberships of the groups.

It is clearly vitally important that the views of the members are made known. If you are unable to attend the June meeting, please let us have your views in writing. These should be sent as soon as possible to one of the following:

Dr Barry Dunne
Chairman, CIG
SII/CAS
34 Worsall Road
Yarm
TS15 9DF

Bob McDowall
Chairman, CASG
73 Murray Avenue
Bromley
Kent
BR1 3DJ

bdunne@cas.org

R_D_McDowall@compuserve.com

**Royal Society of Chemistry
Chemical Information Group
2006 AGM**

The 2006 AGM of the Group will be held on Tuesday, June 6th 2006, at Burlington House, Piccadilly, London, between 2.00 and 2.30pm.

AGENDA

1. Apologies for absence
2. Minutes of the 2005 AGM
3. Matters arising
4. Annual report
5. **To approve the following motion:** To agree that the Chemical Information Group merges with the Computer Applications Subject Group and that the CIG constitution be amended by modifying clauses 1 and 2 – full details shown in left hand panel marked in **Purple**
6. Election of Officers and Committee Members
7. Nomination of auditors
8. Annual subscription 2006
9. Any other business

**Royal Society of Chemistry
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AGENDA

1. Apologies for absence
2. Minutes of the 2005 AGM
3. Matters arising
4. Annual report
5. **To approve the following motion:** To agree that the Chemical Information Group merges with the Computer Applications Subject Group and that the merged Group operates under the CIG constitution suitably amended – full details shown in left hand panel marked in **Purple**
6. Election of Officers and Committee Members
7. Nomination of auditors
8. Annual subscription 2006
9. Any other business

Note. The AGMs are being held TOGETHER in conjunction with the joint Group's spring meeting. Whilst there is a charge for that meeting, members are entitled to attend just the AGM free of charge.

ACS News and New Journals

(Mrs Lindsay Battle – Chemistry Inf. Officer – Chemistry IT Centre – Univ. Oxford)

Citation Manager

<http://pubs.acs.org/journals/citation/index.html> The new Citation Manager feature allows researchers to download an ACS journal reference into citation management software such as EndNote. This feature is available on all ACS journal full-text and abstract html pages and is located at the top of the page. **N.B.** Only one reference can be downloaded at a time, and abstracts are not included.

Most-Accessed Articles

http://pubs.acs.org/journals/promo/most_accessed/ Provides lists of the 20 most-accessed articles from each of the 33 current ACS journals for 2005 and 2004.

Articles on Request

<http://pubs.acs.org/reprints/policy.html> Articles on Request expands on the existing ACS policy of allowing up to 50 free electronic PDF downloads (e-prints) of each authors final published ACS articles during the first 12 months after publication. Access is permitted via links that ACS provides to authors, then authors provide to interested colleagues. Now, the access limitation is removed after 12 months, thereby allowing unlimited free e-prints via the same author-directed links. The author may distribute a link to the final version of the article at his or her own discretion. The link may be posted on the author's website or sent via e-mail from the author to interested colleagues.

ChemMedChem (Wiley)

<http://www3.interscience.wiley.com/cgi-bin/jhome/110485305> Launched in January 2006, this journal will publish a mix of peer-reviewed full papers, short communications, reviews, mini reviews, highlights and concepts covering drug design and discovery, drug

development and delivery, molecular modelling, combinatorial chemistry, target validation, lead generation, PCADMET studies and related topics.

Geochemical Transactions

<http://www.geochemicaltransactions.com/> From January 2006, this is published by BioMed Central as an Open Access journal. Chemical Biology (RSC) <http://www.rsc.org/Publishing/ChemicalBiology>. A supplement highlighting the chemical biology content of RSC journals and providing a snapshot of the latest developments in chemical biology.

News from Chemical Database Service, Daresbury

CDS are planning to run trials of a number of different databases. These include the structures and reactions database SPRESI from InfoChem, the ACD/Labs ILab (ACD Interactive Lab) web-based gateway to spectroscopy information, compound name generation and property prediction programs and the Science of Synthesis database from by Georg Thieme Verlag KG.

The CDS are currently working with these suppliers on the best way to coordinate trial access to the system. These trials will only be open to UK academics and it is hoped that they will commence soon after Easter 2006.

For more information, watch the CDS website at <http://cds.dl.ac.uk/cds> or contact cdsbb@dl.ac.uk if you have any immediate queries.

Leadscope Inc and Lhasa Limited Announce Collaboration on ToxML

Leadscope Inc, Columbus, Ohio, and **Lhasa Limited**, Leeds, England, are pleased to announce their joint support for ToxML, a public domain communication standard for chemical and toxicological data exchange. In order to promote the standard and to extend its coverage to new end-points, the companies will work together and collaborate with Leadscope customers, Lhasa Limited members and the wider scientific community.

Working to the ToxML standard will mean that users can move data not only between database management systems from the two companies but also across all platforms that support it.

For further information, please contact:

Lhasa Limited

22-23 Blenheim Terrace
Woodhouse Lane
Leeds LS2 9HD
United Kingdom

Tel: +44 (0)113 394 6020

Fax: +44 (0)113 394 6099

Web: www.lhasalimited.org

Email: marketing@lhasalimited.org

Second German Conference on Chemoinformatics

The CIC division of the German Chemical Society is proud to announce the Second German Conference on Chemoinformatics (<http://www.gcc-cic.de>) to be held in Goslar, Germany, November 12-14, 2006.

The conference language is English.

They will honour the life-time achievements of one of the founders of CIC and a pioneer of chemoinformatics, Johann Gasteiger.

They are now inviting the submission of abstracts for talks and posters in the following areas

- * Chemoinformatics and Drug Development
- * Chemical Information
- * Molecular Modelling
- * Computational Material Science

The conference website at <http://www.gcc-cic.de> has links to the abstract submission interface, a PDF version of the first circular as well as additional information.

eCheminfo Advanced Training Workshop

A Hands-on 5 Day eCheminfo Advanced Training Workshop Week will be held on 3-7 July 2006 at the Chemistry Research Laboratory, Oxford University, Oxford, UK

This 'Latest Advances in Drug Discovery Design & Planning Methods' workshop will cover Virtual screening, structure-based drug design, reaction

planning and predictive toxicology supporting decision making for chemists in drug discovery

Workshops will be held at the Chemistry Information Technology Center with exercises supported by leading drug discovery software including OpenEye, Schrodinger, ChemAxon, CAChe, Scitegic, Lhasa and Umetrics. More information and online registration available at... http://echeminfo.colayer.net/COMTY_training/

NEW from CAS – (Paul Peters – Marketing Manager, Europe and Middle East)

World-leading databases in chemistry bigger and better than ever

CAS databases continue to grow and add value for chemistry-related research.

- CAS RegistrySM is enhanced with the addition of experimental NMR and IR spectra from Wiley and Japan's National Institute of Advanced Industrial Science and Technology.
- Nearly 1.1 billion predicted and experimental properties, tags that refer to additional data, and spectra have been added to CAS Registry records for 19 million substances.
- CASREACT[®] now contains over 10 million reactions: over 4.2 million single-step, more than 5.8 million multi-step. More than 981,000 abstracts were added to CAplusSM in 2005, bringing the total to more than 24 million records for scientific journals and patents from around the world. In addition, CAplus has now exceeded 150 million citations.

SciFinder[®] 2006 and SciFinder Scholar[™] 2006 offer new features

- Similarity search tool based on the Tanimoto coefficient (SSM module) Variable Attachment Position tool and Repeating Group tool allows for powerful variation in substructure queries (subscription package)
- Query highlighting in reaction searching
- Easy access to additional reaction information
- Intermediate reaction steps in one single view
- New quick look-up of research references
- Duplicate detection and removal
- A Mac OS X version of SciFinder became available in 4Q 2005.

STN[®] AnaVist[™], version 1.1 offers new ways to share visualization results

- Users can share their visualization results with others in their organization through new Login IDs for Shared Projects.
- Create project reports as either .rtf or .pdf documents
- Create multiple versions of visualization projects

STN Express[®] V8.01 now available, featuring important capabilities

- Increased security to STN via SSL VPN
- Enhanced results analysis in VGAT
- Access to Questel-Orbit's Merged Markush Service
- Easy Access to REGISTRY spectral images

AA

Richard A. Kurt

We are sad to report the passing of a distinguished patent search practitioner and long time member of PIUG, Richard A. Kurt.

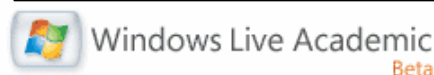
Richard passed away last night after a 9 month spirited battle with cancer. Those of you that know him will not be surprised to learn that in January he attained the highest technical level ever achieved by a patent information professional at 3M. He demonstrated excellence in all areas of IP information research and has a long history of significant contributions to the patent positions obtained and defended by 3M. In addition to thousands of IP information research projects, Richard designed or consulted on over 100 IP assessments, using visualization and analysis tools to help researchers and laboratory management evaluate new technology and business opportunities. His information solutions, including the development of new internal tools and the evaluation and introduction of new external resources, contributed to stronger patent foundations and better business decisions for 3M.

Richard was born June 2, 1950 in NYC, but spent most of his teen years and young adulthood in Austria. He graduated with Honors in Chemistry from Exeter University. The sheer body and breadth of his work over his professional lifetime, including at Derwent, Orbit,

Questel and finally at 3M had a lasting impact on how patent information is collected, indexed, packaged, researched and evaluated.

Richard leaves behind his wife Lesley, their three sons, David, Tim and Simon and numerous friends and colleagues. We miss him already. Memorials in lieu of flowers can be sent to the American Cancer Society.

Taken from emails distributed to PIUG-L@derwent.co.uk and Piug-discussion@piug.org



From <http://academic.live.com/default.aspx>

Windows Live Academic is now in beta. We currently index content related to computer science, physics, electrical engineering, and related subject areas.

Academic search enables you to search for peer reviewed journal articles contained in journal publisher portals and on the web in locations like citespace.

Academic search works with libraries and institutions to search and provide access to subscription content for their members. Access restricted resources include subscription services or premium peer-reviewed journals. You may be able to access restricted content through your library or institution.

We have built several features designed to help you rapidly find the content you are searching for including abstract previews via our preview pane, sort and group by capability, and citation export. We invite you to try us out - and share your feedback with us.

....and just to fill in the last space – from
<http://library.thinkquest.org/C004607F/humour.html>

Soccer Match

When Hydrogen Tech played Oxygen U, the game had just begun,

When Hydrogen racked up two fast points, and Oxygen still had none.

Then Oxygen scored a single goal, and thus it did remain,

At Hydrogen two and Oxygen one, game called because of...RAIN!

Neutron

A Neutron walked into to a bar and said: "How much for a drink?"

And the bartender said: "No charge!"



Chemical Information Group/Computer Applications Subject Group

One-day meeting – “**Electronic Laboratory Notebooks**”,
 Tuesday 6th June 2006, Royal Society of Chemistry,
 Burlington House, Piccadilly, London

BOOKING FORM

I/We* would like to attend

Name:	Mr/Miss/Mrs/Ms/Dr/Professor
Organisation:	
Address:	
	Postcode:
Phone:	
E-mail:	
Fax:	

Please tick boxes below. We regret we CANNOT ACCEPT CREDIT CARD bookings.

Cost of the meeting: Member of the CIG/CASG (£30.00)

Non-Member of the CIG/CASG (£40.00)

Payment by cheque enclosed:

Payment by bank transfer

(Lloyds TSB, Sort code: 30-92-76 Account: RSC Chemical Information Group Trust Account No. 0589218)

Invoice to address as above **Invoice to contact as shown here:**

Name: Mr/Miss/Mrs/Ms/Dr/Professor*

Organisation:

Address:

.....

..... Postcode

Please return the booking form by the 26th May 2006 to:

Chris Evans, RSC-CIG Treasurer, INVISTA Textiles (UK) Limited, Ermin Street, Brockworth, Gloucester, GL3 4HP tel. +44

(0)1452 633390 e-mail: chrisevans72@btinternet.com

Details will be sent upon receipt of this form 1-2 weeks before the event