



The Royal Society of Chemistry

**Chemical
Information
Group**

NEWSLETTER Spring 2003

Future meetings:

The Future Of Chemical Information In The UK

To be held at Burlington House, London Tuesday, May 27th 2003.

What is the future of access to chemical information in the UK? This meeting aims to discuss this and other related issues by holding talks in the morning followed by an informal brain-storm session and discussion in the afternoon. Discussions will be lead by Nigel Lees, Manager, Library and Archival Services, Royal Society of Chemistry. Other speakers include Julia Stocken (Head of Science, Technology & Innovation, The British Library), Dr Gillian Sinclair (Resource Guide Adviser for the Physical Sciences) and Joanne Yeomans (Faculty Team Librarian, University of Leeds) We hope you will attend, share your views, come up with new ideas and have some fun!

A BOOKING FORM IS ATTACHED TO THE END OF THE NEWSLETTER

Royal Society of Chemistry CIG - AGM

The 2003 AGM of the Group will be held on Tuesday, May 27th 2003, at Burlington House, Piccadilly, London, commencing at 2.00pm.

AGENDA

1. Apologies for absence
2. Minutes of the 2002 AGM
3. Matters arising
4. Annual report
5. Election of Officers and Committee Members
6. Nomination of auditors
7. Annual subscription 2004
8. Any other business

Annual Report for 2002-2003 - Doug Veal, Secretary

During the year 2002-2003, because of logistical difficulties, the committee held one scientific meeting, rather than the normal two. The meeting was held on November 20th in Burlington House, on the subject of 'Information at the Chemistry/Biology Interface.' This was a successful meeting, attracting over 30 attendees. Liaison with the Chemical Structure Association (CSA) has continued to benefit members of both organisations, and a joint committee meeting took place at IOLIM on Dec. 3rd. We agreed to hold a joint meeting this autumn. This will be at Burlington House on October 30th, and will take the form of a Training/Workshop previously run with great success by the CSA. Further details will be circulated nearer the time.

We continue to support the three-yearly International Conference on Chemical Structures held in the Netherlands at Noordwijk. This year's meeting made a small surplus so no financial liability was incurred by the Group.

During the year the Committee met three times in person and once electronically. At last year's AGM Doug Veal stood down as Chairman, having served his 3 years, and Don Parkin, previously Vice-Chairman, took his place. Dot Parker resigned as Secretary and from the Committee, having served the Committee in various roles for many years. Doug Veal took over as Secretary. Peter Rhodes resigned as Newsletter Editor and from the Committee. We thank Dot and Peter for their services to the Group. Dot will continue to help produce the Newsletter, in conjunction with Don. Lindsay Battle and Barry Dunne joined the Committee. The Group's finances remain sound.

Annual Accounts are available and will be included in the next Newsletter

PATMG Patent Jamboree, British Library Conference Suite, London June 10-11th

Following successful events in 1998, 2000, and 2001, the Patent and Trade Mark Group will host a "Jamboree" at The British Library in London on Tuesday-Wednesday June 10-11th 2003. The programme, presently being finalised, will include workshops, technical presentations and demonstrations, designed to attract and inform information professionals dealing with intellectual property.

PROVISIONAL PROGRAMME (from the Website - 10th April 2003)

Tuesday Afternoon, June 10th from midday - Pre-Conference Workshops

Value-added Patent Searching - Magister Ltd., Stephen Adams

DOLPHIN - the database of all pharmaceutical inventions - Thomson Current Patents

Tuesday evening, June 10th from 6pm

Opening Address - A patent office speaker (to be announced)

Sponsored Reception and PATMG Chair's address

Exhibition open until 8pm

Wednesday June 11th, Plenary Sessions - The Diversity of Intellectual Property Rights

- Trademark Image Searching Technology - John Eakins (University of Newcastle)
- Protection of Computer Software - Patrick Lloyd (Reddie & Grose)
- Utility Models and Petty Patents - (to be announced)
- The British Maritime Technology WISPER Project - (to be announced)
- Certification of Patent Searchers - Aalt van de Kuilen (WON, Netherlands)
- The European Patent Office's User Survey - Nigel Clarke (EPO)

Also - Information Consultants' and Vendors' presentations, including:

- British Library
- Derwent / Delphion
- Dialog
- MicroPatent
- Minesoft Ltd
- Questel*Orbit
- RWS Group
- STN Agency UK / CAS
- Thomson Current Patents

Conference closes 5pm - updates to the Programme will be available on the PATMG website - <http://www.patmg.org.uk/Events/events.html>. Delegate registration forms will be mailed from the beginning of April.

Reports on Past Meetings

Information at the Chemistry / Biology Interface

A one-day meeting organised by the RSC Chemical Information Group looked at new initiatives being developed to stimulate information exchange between chemists and biologists, as the boundaries between the two disciplines are becoming increasingly indistinct. The meeting was held at Burlington House, London, the headquarters of the Royal Society of Chemistry, on 20th November 2002.

Following a welcome by Don Parkin, the first speaker, Stephen Baker, gave a paper entitled "Are you a chemist or a biochemist?" Stephen is working at the chemistry/biology interface in the Centre for Chemical Biology at Leicester University, and the title of his paper related to a question posed by a potential sponsor of his work. The aim of the department, which started in 1988 as the Centre for Research in Molecular Recognition, is to promote collaborative research which bridges the two disciplines of Chemistry and Biology, and to be identified as an international centre of excellence. The group does not have its own building, but has a committee with representatives in computer modelling, protein interaction, molecular enzymology, structural biology and synthetic chemistry. Further details about the department can be found at <http://www.le.ac.uk/chemistry/chembiol/index.html>.

Thomas Oldfield, who works at the European Bioinformatics Institute in Hinxton, near Cambridge, then discussed the Macromolecular Structure Database (MSD). Protein data is collected from many different sources, and thoroughly checked before it is stored as a relational database, so that complex search queries can be carried out on the data. The MSD is one of three groups which collect macromolecular structural data, but is the only one which goes through detailed cleaning of the data, and storing it as a relational database. Information on the MSD can be found at <http://www.ebi.ac.uk/msd/index.html>.

The next speaker, Simon Edwards, is the Life Sciences Manager at the RSC. His role involves looking at the interface between chemical sciences and biosciences, and he works closely with the chemical biology community. Simon discussed the problem of the reduction in numbers of undergraduates in the UK who are studying chemistry, whereas medicine and related subjects are showing an increase. Chemistry requires new marketing initiatives and the RSC is trying to broaden its remit, by extending the interests to cover key interfaces between chemistry and other subject areas, such as biomedical, biomaterials, pharmacology. Workshops have been set up in priority areas, and the key challenges include identifying the people who constitute the chemical biology community; forming partnerships with Research Councils and Learned Societies; and developing a programme of activities in the chemical biology area. For further details see <http://www.rsc.org/science/lifescience.htm>.


The last speaker of the morning was Lesley Thompson, the Programme Manager of the Life Sciences Interface Programme within the EPSRC (Engineering and Physical Sciences Research Council). In the UK, research funding is organized through Research Councils, and the Life Sciences Interface was formed in 1999 to fund high quality research and to provide training at the Life Sciences/ Physical Sciences interface. The work involves collaboration with other EPSRC programmes and other Research Councils. More information at: <http://194.66.183.26/website/default.aspx?CID=5605&ZoneID=3&MenuID=410>.

After an excellent lunch, the afternoon started with a very different lecture from Denise Harrison (Sheffield Science Librarian), who had recently moved the Sheffield University Chemistry Branch library into the main library. Anyone planning to do the same would be well advised to contact Denise for some advice, as she managed to overcome a large number of hurdles and the antagonism of all the staff, students, secretaries, other librarians and porters, to achieve her aim (which was forced upon her by a change of use of the original Chemistry library building). The last two lectures of the day were from Derwent and CAS, respectively. Simon Alcock (Product Development Manager of the Life Sciences Division) talked about the Derwent Biological databases on STN, including GENESEQ and BIOTECHABS. An interesting statistic was that the number of sequences added to the GENESEQ in 2001 more than doubled the size of the database. Details of the two databases can be found at <http://www.derwent.com/geneseq/> and <http://www.stn-international.de/stndatabases/databases/biotecha.html>

Although Barry Dunne was given the last slot of the day to discuss the CAS coverage of Biological sciences, he always gives a lively and stimulating talk. He described the biochemistry coverage, GenBank data, cell and other published biosciences information within Chemical Abstracts, STN, SciFinder and ChemPort. He also gave an interesting analysis of CAS sequence data from 3 major pharmaceutical companies, from which their relative research activities in this area could be compared. For information about CAS and the biological sciences see <http://www.cas.org>; <http://www.cas.org/stn.html>;

<http://www.cas.org/SCIFINDER/bio/index.html>; <http://www.cas.org/chemport/index.html>.

The RSC-CIG is to be congratulated on bringing together some interesting speakers, and providing an excellent day which, as always, was extremely good value for money (£25 including lunch, with a reduction for RSC members).

	<p>The Pharma Documentation Ring (P-D-R) held its 44th AGM in Newmarket, UK from the 8th - 11th October 2002. The associations members represent the scientific information departments of the leading R&D-based pharmaceutical corporations. The 23 companies represented account for approximately 60% of the total global turnover of ethical drugs., by far the majority of top 20 global pharmaceutical companies are corporate P-D-R members. Over 45 delegates from 11 different countries in Europe and North America attended this year's meeting, which was ably hosted by GlaxoSmithKline.</p>
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With limited space I have not included all the review of this meeting - but there is a complete review on <http://www.p-d-r.com/prensa/prensa.html>

Topics discussed included:

1. The continuing information explosion and the increase in CA registry numbers, CAS register a new substance every 5 seconds, approximately 6.7 million substances were added to the CAS Registry in 2002. and the CAS Registry File itself has now grown to more than 42 million substances
2. The availability of biosequence information which has increased dramatically in recent years e.g. it took Derwent 20 years to reach 1 million sequences but only 9 months to add the second million to Geneseq.
3. More than 40% of the 23 million references in the CA database now relates to bioscience topics, and the proportion of bio-molecules in the CAS registry growing from approximately 10% of all substances in 1995 to 45% in 2002.

Four strategic topics of particular interest to the P-D-R representatives were discussed in two parallel streams

Measuring what we are doing Data and Text Mining Marketing Information Services
Database Futures

The PDR web site can be found at <http://www.p-d-r.com>. On the website there are some useful, new publicly accessible features, including the Pharmaceutical Company ranking tables (2001 and 2002) from Wood Mackenzie, PharmaProjects, Current Patents as well as overview articles from Pharma Marketletter. In addition, a new daily web spider service from Reg123 is available, reporting on the very latest press releases from the P-D-R member websites. Additional functionality and content had also been added to the 'members only' area of the website.

The press release notes that this was a highly successful and interactive meeting and a survey conducted amongst attendees indicated there had been, a very high level of relevant and quality presentations by PDR members and invited speakers. The meeting continues to be regarded by most participants as the major annual event of its type for the international pharmaceutical industry.

The 45th P-D-R AGM will be held on 24th - 26th September 2003, near Thame, Oxfordshire, England and will be hosted by Wyeth.

News

Thanks to Lindsey Battle and others who have forwarded these items:

WIPO

A key decision making body of the World Intellectual Property Organization (WIPO) unanimously decided on Tuesday to recommend the appointment of Dr. Kamil Idris as Director General for a second six-year mandate. The Coordination Committee, meeting in Geneva on March 24 and 25, 2003, will now send its recommendation to WIPO's General Assembly, for endorsement at an extraordinary session on May 26 and 27, 2003. Dr. Idris' current mandate expires at the end of November 2003.

The WIPO Coordination Committee consists of 79 member states and under the terms of the "WIPO Convention" it is required, when the term of office of the Director General is about to expire, to nominate a candidate for appointment to such position by the General Assembly. Dr. Idris' candidature was the only nomination received for consideration by the Coordination Committee.

Delegations applauded Dr. Idris' leadership of the Organization since his appointment in 1997. Dr. Idris' candidature was formally presented by the Ambassador and Permanent Representative of South Africa to the United Nations in Geneva, Mr. Siphon Nene, on behalf of the African Group. In presenting the candidature, he said "We can all agree and appreciate that Dr. Idris has significantly transformed WIPO in breadth, clarity, simplicity and visibility of its activities. He has literally and figuratively pulled the Organization into a new century and a new millennium. Dr. Idris' efforts as Director General have injected a sense of motivation and increased interest in intellectual property issues. slowly, but surely, our countries are looking positively toward intellectual property as a potential tool for economic, social and cultural development" he added. "He has transformed WIPO into a forum where issues of interest and importance to all members, in particular, developing countries, can be addressed". Under his leadership, WIPO's contribution to the intellectual property system can truly serve to make our world a place rich in technological, economic, social and cultural development for the benefit of all peoples," the Ambassador said.

Speakers commended Dr. Idris for the efficiency, vision and dynamism with which he has led the Organization since 1997. This, they said, has enabled the creation of a modern, forward-looking and innovative intellectual property framework. Under his leadership, they said, the Organization has established itself as one of the leading UN specialized agencies in the knowledge-based economy. Member states commended his drive in successfully modernizing and streamlining the working methods of the Organization through, for example, the introduction of greater openness, transparency and results-based budgeting and the implementation of technology based solutions, such as the PCT automation or "IMPACT" project.

Many delegations expressed appreciation for Dr. Idris' emphasis on "deliverables" and the Organization's success, under his leadership, in advancing the traditional mission of the protection and promotion of intellectual property to the development of intellectual property systems as instruments of social and economic development for the benefit of all. Particular gratitude was expressed for his willingness to listen to and take into account the concerns and needs of developing countries and to mainstream the development dimension of intellectual property rights in the Organization's activities. Member states also commended Dr. Idris for the expansion of activities into such areas as public outreach, traditional knowledge, alternative dispute resolution procedures, the WIPO Digital Agenda and the WIPO Patent Agenda, for example.

Press Release PR/2003/341 (Geneva, March 25, 2003)

RSC Specialist Periodical Reports

Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research, and volumes back to 1998 will be made available electronically site-wide to print purchasers (of volumes bought during the last two years). Specialist Periodical Reports are published annually or biennially; titles are:

- Amino Acids, Peptides and Proteins
- Nuclear Magnetic Resonance
- Carbohydrate Chemistry. Monosaccharides,

Disaccharides and Specific

- Oligosaccharides
- Catalysis
- Chemical Modelling: Applications and Theory
- Electron Paramagnetic Resonance
- Organometallic Chemistry
- Organophosphorus Chemistry
- Photochemistry
- Spectroscopic Properties of Inorganic and Organometallic Compounds

Even non-subscribers can benefit from:

- Searching for chapters in Specialist Periodical Reports
- downloading PDF contents pages of individual books
- view individual chapters electronically, on a pay to view basis <http://www.rsc.org/is/books/spr.htm>

NanoTalk Email discussion List

<http://www.cla.sc.edu/cpecs/nirt/nanotalk.html>

There is a new email list called "NanoTalk: A discussion forum for issues related to nano-science." NanoTalk is hosted at the University of South Carolina and focuses on the exploration of philosophical, ethical, social and legal issues associated with nanoscience and technology. Topics for the forum include:-

- General summaries and reviews of current research in nanotechnology to inform participants about the status of the science.
- Identification and exploration of ethical, social and legal issues of current and future research in nanotechnology.
- Reflection on science studies issues such as the applied/pure distinction, the interface of classical and quantum effects, etc.
- Cultural and literary appropriations of nanoscience such as that found in art or science fiction.
- The relation between the community of nanoscientists and engineers and the communities of geneticists or cyberneticists and the many other areas of science.
- How should nanotechnology be best dealt with in legislation and politics?

Synthesis Reviews & Synthesis Alerts

The Synthesis Reviews database is provided free of charge by Thieme; it contains 15,348 English language review articles (from journals and books) of interest to synthetic organic chemists, updated to include articles from 1970 to mid-2002. The whole database can be downloaded as a text file (open in any word processor) or as an Endnote library, for either Mac or PC. See: <http://www.thieme-chemistry.com/thieme-chemistry/journals/info/news/synrev.shtml>

Synthesis Alerts An overview with graphical abstracts of new reagents, catalysts, ligands, chiral auxiliaries, and protecting groups which have appeared in the recent literature. This is published in each issue of 'Synthesis' and is free to all in PDF format: <http://www.thieme-chemistry.com/thieme-chemistry/journals/info/synthesis/online/index.shtml>

Organic & Biomolecular Chemistry

<http://www.rsc.org/obc>

This new RSC journal, covering organic, physical organic and biomolecular chemistry, replaces the two Perkin journals from January 2003. The first four issues are now available online.

IsoStar

The IsoStar client package from CCDC has been updated to version 1.5 IsoStar is the definitive database of experimental and theoretical information on non-bonded interactions. It has been designed to play a prominent role in the field of molecular invention and will be of special interest to anyone involved in rational drug design. UK academics can get access to the data from

<http://cds.dl.ac.uk/cds/datasets/crys/csd/isostar/isostar.html>

ACS Electronic Journal Archive

The Archive contains an electronic version of every article ever published in an ACS journal, dating back to 1879 when JACS started, up to and including 1998 issues, for ALL ACS journals. (ACS 'Web Editions' subscriptions now provide only 1999 to present year). For more details of the Archive content, and a Timeline dating back to 1876, see: <http://pubs.acs.org/archives>.

Organic Syntheses Online

<http://www.orgsyn.org/>

Searchable database of reactions and experimental methods that have appeared in Wiley's publication 'Organic Syntheses'. Needs the ChemDraw Plugin and only works with certain combinations of system and web browser, so check the 'System Requirements and Plugin Downloads page':

<http://www.orgsyn.org/sysReq.html>

NIST Chemical Kinetics Database

<http://kinetics.nist.gov>

Contains reported kinetics results for thermal gas-phase chemical reactions; designed to be searched for kinetics data based on the specific reactants involved, for reactions resulting in specified products, for all the reactions of a particular species, or for various combinations of these. The database contains in excess of 38,000 separate reaction records for over 11,700 distinct reactant pairs. There are direct links to the corresponding NIST WebBook page; this provides thermodynamic, spectral, and other data.

Novel Antibiotics Database

The Japan Antibiotics Research Association provides a 'Novel Antibiotics Database', which is a series of searchable indexes to substance names, organism names, and activity (e.g. anti-tumor, anti-fungal) for substances which have been first reported in the Journal of Antibiotics:

<http://www.nih.go.jp/~jun/NADB/search.html>

Faculty of 1000

<http://www.facultyof1000.com>

Faculty of 1000 highlights and reviews the most interesting papers published in the biological sciences, based on the recommendations of a faculty of over 1000 leading researchers. Coverage includes biochemistry, chemical biology and structural biology.

Four knovel Chemical References Free to Academe

Knovel have announced access to four new chemistry references for academic libraries - **free forever!** They wish to support the scientific education community that has supported them and has granted colleges and universities permanent access at no charge to the four titles listed below. Two of the four titles are "Interactive Deep Searchable" (IDS), numeric searches can be performed by field and the data manipulated in spreadsheet-like tables. IDS titles are indicated with an asterisk (*).

1. *International Critical Tables of Numeric Data, Physics, Chemistry and Technology, 7 volumes and index (first electronic edition).
2. *knovel Critical Tables.
3. Thermochemistry of the Chemical Substances.
4. Smithsonian Physical Tables (ninth revised edition).

To register your institution for the above four free titles, please contact Carolynn Fitzgerald at 607-337-5002 x516, or by email at cfitzgerald@knovel.com. Please include full contact details.

Marvin Applets and Marvin Beans

Marvin Applets and Marvin Beans 3.0 have been released. The packages contain software development tools and applications for chemistry. Marvin Applets and JavaBeans support drawing/displaying chemical structures and handling molecule objects. FREE: - Marvin Applets are free for free web sites.- MarvinSketch and MarvinView applications accessed from ChemAxon's web site

<http://www.chemaxon.com/marvin/jnlp/index.html>

- Locally installed MarvinSketch, MarvinView, and MolConverter applications.