

NEWSLETTER AUTUMN 2010

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Chemical Information and Computer Applications Group Website:
<http://www.rsc.org/CICAG>

Linked in® <http://www.linkedin.com/groups?gid=1989945>

Chemical Information and Computer Applications Group (CICAG)

CICAG aims to keep its members abreast of the latest activities, services, and developments in all aspects of chemical information, from generation through to archiving, and in the computer applications used in this rapidly changing area through meetings, newsletters and social networking.

RSC CICAG Meeting Autumn 2010

A Celebration of the History of Chemical Information

Monday 29th November, RSC, Burlington House, London, 10.30am

The RSC Chemical Information and Computer Applications Group, the RSC Historical Group, and the CSA Trust are organising a joint one-day meeting celebrating the history of chemical information. A superb panel of speakers is being assembled for this very special meeting which will provide a unique opportunity to hear from some of those who have contributed to the very significant developments which have occurred in the last few decades. The meeting will be held on **Monday, 29th November 2010, at Burlington House, starting at 10.30am but with a lengthy registration time/coffee time from 9am to welcome early arrivals and enable attendees to see the exhibition in the Chemistry Centre.** The exhibition of historical material related to chemical information will be held alongside the meeting.

Programme

- 0900 - 1030 Coffee and Registration; viewing of exhibitions in Chemistry Centre.
Chairman for the day Dr. Diana Leitch, Information Consultant.
- 1030 - 1100 *The Contribution of the RSC* Dr. Doug Veal, CICAG
- 1100 - 1130 *The Language and Symbolism of Chemistry* Dr. Bill Town, President, Kilmorie Consulting
- 1130 - 1200 *The Chemical Literature* Dr. Engelbert Zass, Head of the ETH Zurich Chemistry Biology Pharmacy Information Centre
- 1200 - 1330 **LUNCH** Time available too for exhibition viewing
- 1330 - 1400 *Chemical Structures* Dr. Phil McHale Vice president, Market and Corporate Communications Elsevier MDL
- 1400 - 1430 *Databases* Dr. Helen Cooke, Business Consultant, Proprietary Information Access, GlaxoSmithKline, Philadelphia
- 1430 - 1500 *Data* Prof. Alexander Lawson, Director of R&D, Elsevier Properties SA, Neuchâtel
- 1500 - 1530 **TEA**
- 1530 - 1600 *Chemoinformatics :historical development of database methods* Prof. Peter Willett, Dept. of Information Studies, University of Sheffield
- 1600 - 1630 *The Future* Prof. Bobby Glen, Unilever Centre for Molecular Science Informatics, University of Cambridge.
- 1630 - 1700 *Discussion and Conclusions*
- 1700 Close of Meeting

We have managed to arrange that the fee for the whole meeting, including the exhibition, tea, coffee and forked buffet lunch is only £30.

We expect a high level of interest in this meeting and those who wish to attend are advised to get their applications in as soon as possible.

A booking form is appended to the end of this newsletter, and further details can be obtained from Dr Diana Leitch at: diana.leitch@googlemail.com

A limited number of student bursaries are available. These will cover UK travel costs and the meeting fee, to enable selected students to attend the meeting at no cost whatsoever.

Please contact Dr Keith White, Chair of RSC CICAG at: keith.white@matthey.com.

RSC CICAG Spring 2010 Meeting Report

Contributed by Keith White, RSC CICAG Chairman

RSC CICAG/CSA Trust Training Course: “Chemical Information for the Chemist and Non-Chemist”

Location: RSC, Burlington House, London; **Date:** 19th May 2010

The RSC CICAG/CSA Trust Training Course, “Chemical Information for the Chemist and Non-Chemist”, consisted of a series of presentations providing an impartial and critical overview of Chemical Information products, given by specialists from academia, industry and vendors. There were over 30 attendees from academia and industry.

The presentations are available on the CICAG section of the RSC website.

The training course started with “What Makes Chemical Information Different?”, by David Walsh (Information Scientist, Pfizer). Walsh stated that a chemist would need to read over 2000 articles per day to keep up to date with all the newly published chemistry research.

“ChemSpider: Building a Community Platform to Support Chemistry”, by Jan Davies (ChemSpider Community Specialist, RSC) and Richard Kidd (Manager, Informatics, RSC), was very relevant to RSC CICAG members. ChemSpider is a free access online structure-based community for chemists to research data and information. The database of over 25 million chemical structures and associated data has been derived from depositions by well over 300 contributing data sources, including chemical vendors, commercial database providers, web-based ‘scraping of data’ and individual scientists looking to share their information with the community. Text-mining and conversion of chemical names and identifiers to chemical structures has made an enormous contribution to the availability of diverse data on ChemSpider and includes contributions from patents, open access articles and various online resources. The presentation provided an overview of the present state of development of ChemSpider and described the harvesting, deposition and curation of large datasets derived via text-mining and conversion.

Yvonne Pope, Regional Marketing Manager, CAS, gave two presentations: “An Introduction to SciFinder, the Chemical Search Tool for Scientists” and “Overview of Structural Databases on STN”. The first presentation was a short overview on the web version of SciFinder. The second presentation was aimed at helping the attendees to access the most appropriate database for their particular information requirements.

“Chemical Structure Drawing Packages”, by Don Parkin (Chemical Database Manager, Chemical Database Service, Daresbury), gave detailed information on the available chemical structure drawing packages to allow attendees to make a direct comparison of the resources available.

Prof. Dr. Alexander J. Lawson, Director R&D, Elsevier Properties SA, Neuchâtel, Switzerland, in his presentation “Reaxys: Making Sense of Chemistry Information”, focussed on examples illustrating the general Reaxys strategy to tackle the major tasks facing all chemistry information systems. The web-based system “Reaxys” is the successor to the well-known CrossFire suite based on the Beilstein, Gmelin and Patent Chemistry databases.

Nazma Masud (Chemical Information Specialist, RSC) described “The RSC Virtual Library”. The Virtual Library is “a collection of full-text e-books and journals from various publishers and sources which can be accessed 24/7 from any internet-connected PC anywhere in the world”.

The closing presentation by Dr Jonathan Goodman (Department of Chemistry, University of Cambridge), “Choosing Information Resources: An Academic User’s Viewpoint”, helped generate further thought. His main concern for academics is “Which chemical information resources give the best value from the limited funds that are available?”. The UK higher education funding is in contract; academics are facing hard choices with regards to their chemical information resources. Goodman stressed the importance of peer review (organised by publishers).

General feedback comments included:

- “Great event, really useful to me as a new librarian supporting chemistry.”
- “Remarkable that a consensus emerges from all of the different speakers. Well done.”

RSC CICAG AGM Spring 2010

AGM held at Burlington House on 19th May 2010

The meeting was attended by 16 CICAG members. The annual report for the group in RSC format appears on the CICAG web site. A report on the year was handed around and read out by Don Parkin (see below).

The 2009 audited accounts were tabled. The treasurer, Chris Evans, explained that the finances had been hit by the fall in interest rates and now had to pay for events and committee meetings at Burlington House. Despite this, the Group still showed a healthy balance due to two very successful meetings and this balance actually went up by £55.

Chris Evans stood down from Treasurer and the committee due to work commitments. The chair thanked him for the sterling work as Treasurer for the last 10 years and as a committee member – a sentiment echoed by all committee members. Diana Leitch was elected as the new Treasurer. Due to the change in Treasurer, the appointment of the auditor will now be left to Diana.

Stuart Newbold, Information Manager, Astex Therapeutics, Cambridge, was elected to the committee. Jan Davies also stood down from the committee following a move from STN to ChemSpider. Again the chair thanked her for her efforts as a committee member.

It was noted that an all-inclusive membership subscription will be introduced in 2011. This will enable all members to join up to 3 Interest Groups as part of the annual subscription. Additional groups will cost an extra £10.

CICAG Annual Report 2009

Contributed by Don Parkin, RSC CICAG Secretary

RSC Chemical Information And Computer Applications Group: Annual Report for 2009

During the year 2009, the Group held its usual two scientific meetings. The first meeting on 20th June 2009 at Burlington House was “Scientific Text and Data Mining” and was attended by 45 people. Speakers represented practitioners from both academic and commercial areas. The second meeting, held on 28th October 2009 at Burlington House was “Should I Really Be Searching Patents” and was also well attended (46 participants). Speakers were drawn from a wide variety of scientific, industrial, commercial and legal organisations. A meeting report and copies of the PowerPoint presentations given are available on the Group's website.

Two meetings are planned for 2010. The popular 'training' day on chemical information for chemists and non-chemists, organised jointly with the CSA Trust, will be moved from the usual autumn date to a spring date (19th May).

The second meeting of 2010 is planned for 29th November and will cover “Celebrating the History of Chemical Information”. This event is a joint meeting with the Historical Group and the CSA Trust.

During the year the Committee met three times in person and held an AGM on 20th May 2009 at Burlington House. During the year the committee welcomed Yvonne Pope as a new committee member.

Two Newsletters were produced during the year and made available on the group website then links circulated to all members. Committee member Lindsay Battle took over the role of Newsletter production editor from Dot Parker, who was thanked for the sterling work done over many years. Don Parkin remains the technical editor.

The CICAG have set up a group on LinkedIn where we have Discussions and Jobs. You can find us at <http://www.linkedin.com/groups?gid=1989945> or by searching Google for: LinkedIn RSC CICAG. LinkedIn users can request to join the RSC CICAG LinkedIn group.

Once again the group helped to sponsor the Tony Kent Strix Award. This award is offered in recognition of individuals or groups for an outstanding contribution, practical innovation or achievement in the field of information retrieval.

The Group's finances remain sound and a very small increase of £55 was made over the year.

Further details of the Group can be found on its website at:

<http://www.rsc.org/Membership/Networking/InterestGroups/CICAG>

Committee Members

Contributed by Keith White, RSC CICAG Chairman

A full list of the current RSC CICAG Committee Officers and Members, with their affiliations and contact details, can be found on the CICAG website:

<http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/committee.asp>

Please see below for thanks to Chris Evans and Jan Davies, who both came off the RSC CICAG Committee at the last AGM. Don Parkin (Chemical Database Manager, Chemical Database Service, Daresbury Laboratory) continues as Honorary Secretary. Diana Leitch (Diana Leitch Information Consulting) has stepped up to be Treasurer. I would like to welcome Stuart Newbold (Information Manager, Astex Therapeutics Ltd) and Yvonne Pope (CAS Regional Marketing Manager) as new Committee Members. Lindsay Battle (Information Officer, Department of Chemistry, University of Oxford), Alan Tonge and Doug Veal continue as Committee Members. For our Newsletters, Lindsay is Production Editor and Don is Technical Editor.

We are always on the look out for new members to join the committee, so if you would like to volunteer, or just find out more about what is involved, please contact the RSC CICAG Chairman (Dr Keith White; email: keith.white@matthey.com).

Thanks to Chris Evans and Jan Davies

I would like to thank Chris Evans and Jan Davies for their contributions while serving on the RSC CICAG Committee. Chris did an outstanding job as Treasurer, which involved giving up much of his own time. Chris also played a full role in the organising of our events. Jan also supported these events by coming up with the names of potential speakers, and using her contacts to promote the events. Jan made informative contributions to the Newsletter.

Chris Evans originally joined the RSC Chemical Information Group (CIG) Committee at the 2000 AGM (at the behest of Dot Parker, the then Treasurer) and was Treasurer for the whole time. Chris currently works as an Information Specialist in the civil service, specialising in information management. Chris previously worked in both the pharmaceutical and textile industries, managing their library and information services, and trying to keep up with the constant pace of change..... (especially from print to electronic sources and tools).

Jan Davies started out in chemistry with a BSc from Nottingham Trent University and went on to start a career in chemical information working for RSC Chemical Information Services in Nottingham where she was involved in the applied chemistry team abstracting the UK published literature for the Chemical Abstracts Service.

When the RSC relocated its Publishing & Information Services to Cambridge, Jan joined the STN Marketing team where she was involved in providing support and training to UK customers of the online vendor STN International. It was during this time that Jan first became involved with the RSC CIG. 'My work brought me into contact with librarians and information professionals whom I could often persuade to be speakers for our group meetings'.

More recently Jan has moved to a new role within the RSC as support for the ChemSpider Community following the acquisition of ChemSpider by the RSC in June last year. 'This is an exciting time to be involved in cheminformatics. In particular, there is a lot of buzz within the community about ChemSpider and how such high-quality services that are provided for free to end users will change the cheminformatics landscape'.

Jan's move from STN to ChemSpider has also meant that she has withdrawn from the CICAG Committee. 'It is with regret that I stand down the CICAG committee, but I will still be an active participant in group meetings'.

Tony Kent Strix Award

Contributed by Doug Veal

The CICAG has been proud to be associated with this prestigious award for a number of years, and has sponsored the award financially. We are delighted to report that this year, the award has also received a donation of \$300 from one of the 'greats' of chemical information, Gene Garfield. The awards committee is always grateful to receive additional sponsorship. Potential sponsors should in the first instance contact Doug Veal, Chairman of the Awards Committee at dougveal@waitrose.com.

Call for Nominations for the UKeIG Tony Kent Strix Award

Nominations for the 2010 award are now being sought by the UK eInformation Group, who administer the award. The UKeIG Tony Kent Strix Award is given in recognition of an outstanding practical innovation or achievement in the field of information retrieval. This could take the form of an application or service, or an overall appreciation of past achievements from which significant advances have emanated. The Award is open to individuals or groups from anywhere in the world.

Nominations should be for achievement that meets one or more of the following criteria:

- a major and/or sustained contribution to the theoretical or experimental understanding of the information retrieval process;
- development of, or significant improvement in, mechanisms, a product or service for the retrieval of information, either generally or in a specialised field;
- development of, or significant improvement in, easy access to an information service;
- a sustained contribution over a period of years to the field of information retrieval; for example, by running an information service or by contributing at national or international level to organisations active in the field.

Key characteristics that the judges will look for in nominations are innovation, initiative, originality and practicality. The information to be supplied in the initial nomination should comprise:

- The name, institutional address and qualifications of the nominee
- A brief biography (not more than half a page of A4)
- A relevant bibliography (i.e. not comprehensive but including the key publications relevant to the nomination)
- A justification for the nomination, of not more than half a page of A4, showing clearly which of the Strix award criteria the nominee meets and how the criteria are met

Further details of the award, together with the full Call for Nominations and the address to which nominations should be sent, can be found at <http://www.ukeig.org.uk/awards>

The **deadline for nominations is Friday 24th September 2010.**

The Strix Award is presented in memory of Dr Tony Kent, a past Fellow of the Institute of Information Scientists, who died in 1997. Tony Kent made a major contribution to the development of information retrieval 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.

Past winners have been Carol Ann Peters (2009); Kalervo Jarvelin (2008); Mats Lindquist (2007); Stella Dextre Clarke (2006); Jack Mills (2005); Prof Cornelis Joost (Keith) van Rijsbergen (2004); Dr Herbert van Sompel (2003); Malcolm Jones (2002); Prof Peter Willett (2001); Dr Martin Porter (2000); Dr Donna Harman (1999); Prof Stephen Robertson (1998).

ChemSpider

Contributed by Jan Davies, ChemSpider Community Specialist



<http://www.chemspider.com>

ChemSpider website has had a makeover

With the new design, the ChemSpider website is now more visually appealing and easier to navigate with drop down menus from the top navigation bar. The layout of the info boxes and their content remains very similar, with a few additions. Here is a round-up of some of the new features:

Pillbox integration

Imagine your child has found a bottle of pills and mistaken them for candy. Worse still, the label is so old you have no idea what the pharmaceutical ingredient is. Pillbox helps you identify drugs by shape, colour and imprint. It's a great community tool and now [Pillbox is integrated to ChemSpider](#)

Better integration to PubChem

The PubChem database is a valuable community resource and a number of ChemSpider depositors put regular updates of their data into PubChem. To maintain links back to PubChem and expose data of interest via ChemSpider we've developed a background process to facilitate updating of specific PubChem datasets. The blog article [Scraping high quality sets of molecules from PubChem](#) tells you how this is being done.

New collaboration

We're excited to announce a new [software agreement with iChemLabs](#), the developer of the popular ChemDoodle chemical drawing program. ChemSpider will be integrating ChemDoodle Web Components into our service to provide you with a next generation HTML5 experience.

Infotherm data now integrated into ChemSpider

You can now search for additional thermodynamic and physical properties data on ChemSpider thanks to a recent [collaboration linking the INFOTHERM® database to ChemSpider](#). The database, produced by FIZ CHEMIE Berlin, provides information on 33,000 mixtures and 9,000 pure substances from a total of 12,000 compounds. If you are an RSC member, having identified the relevant data in ChemSpider, you can view the results for free via your Virtual Library login.

Links to ChemAxon's chemicalize

There is a new tab in the Properties Info Box where you can link to ChemAxon's chemicalize website to [Calculate properties at chemicalize.org](#) in addition to the predicted properties for ACD/Labs and EPISuite.

ChemSpider SyntheticPages continues to expand

Thanks to new authors depositing synthetic page articles online the ChemSpider SyntheticPages database is growing every week. We've improved the workflow for authors, enhanced the experience for readers and better integrated to ChemSpider with a reaction info box.

Chemical Database Service News

Contributed by Don Parkin, CDS

Trial of Symyx Databases

A free trial of the Symyx set of databases is available to all UK academics. Access is via DiscoveryGate and hopefully will also be via Isentris client software. Databases include organic synthesis, bioactivity, physical property, pharmacology, metabolism/toxicity, and chemical sourcing data.

ARChem Retrosynthetic Design Package Trial

ARChem is a revolutionary retrosynthetic route design package that automatically harvests reaction rules from common reaction databases, and employs them to generate full synthetic routes from commercially available starting materials to the target molecule. The system is web-based, and it comes with a large reaction database, covering close to 25 million reactions. CDS aim to run a trial starting in September for around 3 or 4 months.

For more information contact CDS at [cgsbb@stfc.ac.uk](mailto:cdsbb@stfc.ac.uk)

CAS SciFinder News

Contributed by Anne Jones, CAS Applications Specialist for UK & Ireland

The SciFinder web version has been enhanced with powerful new features to help SciFinder users:

Locate substance-related patent information easily

- **Markush searching.** Uncover additional disclosed chemistry in patents, previously unavailable to SciFinder users, with the new, simple-to-use Markush search capability. (*Available only to customers with substructure search module*)

Find information more easily

- **DOI search and display.** Search references by Digital Object Identifiers (DOI). DOIs are also conveniently displayed in the bibliographic detail for easier reference management and document look-up.
- **Transformation center highlighting.** Using the Get Similar Reactions feature, view transformation centers and adjacent bonds of reactants and products (contingent upon selected broad, medium, or narrow similarity). Users can see how a retrieved reaction is similar to the previous reaction and how all reactions in the answer set are related to a particular reaction.
- **Answer set ordering.** Prioritize answer sets in ascending and descending order.
- **Sorting options.** Sort substance answer sets by molecular formula and molecular weight to explore related chemical and literature information.

Access information more conveniently

- **Automatic removal of duplicates.** Set a preference to automatically remove MEDLINE duplicates.
- **Monthly Keep Me Posted alert.** Stay current with a new monthly frequency Keep Me Posted alert.

If you are interested in SciFinder training or would like to know more about SciFinder then please contact Victoria Vowles at vvowles@cas.org

STN News from CAS and FIZ-Karlsruhe

Contributed by Anne Jones, CAS Applications Specialist for UK & Ireland

STN Fixed Fee Agreements Enhanced

The STN Fixed Fee Program provides customers with budget predictability and easy administration. Changes to the program this year are designed to make the program more appealing and inclusive for smaller organizations - expanding the pool of prospects to include organizations that may not be acquainted with STN. For more information on the STN Fixed Fee plan please contact your STN or CAS representative.

STN partners, CAS and FIZ Karlsruhe, are developing a new STN platform

Announced in April 2010, the new platform will provide a more modern interface and product architecture, while maintaining the critical search power and high quality content for which STN has become known. It will also have many advantages, such as:

- Better integration of analysis tools
- Improved database content consistency
- Higher system limits

The new platform will run in parallel with current STN services for a few years to provide a comfortable transition for users.

Our development activities are being supported by an advisory council of global information professionals and thought leaders. We will also reach out to additional customers to help us pioneer the development of the next generation of STN.

We will be providing additional information at various development stages. In the meantime, if you have any questions, please do not hesitate to contact your STN Service Center.

STN will continue to focus on delivering what customers expect: precision and comprehensiveness; premium, value-added content; and exceptional customer support.

STN Express Maintenance Release, Version 8.4.2, is Now Available for Download

A new version of STN Express, Version 8.4.2, is available for download. This is a maintenance release created to fix several software issues reported since the launch of STN Express, Version 8.4, and to ensure compatibility with Windows 7. Please visit the STN Software License and Download web site to obtain this release.

CAS Patenting Authorities Further Extended

On July 12, 2010, CAS enhanced its extensive patent coverage by adding patent and patent family information from the **Costa Rica** Registry of Industrial Properties. Also at this time, CAS expanded coverage of the **Argentina** National Institute of Industrial Properties. More information can be found at <http://www.cas.org/expertise/cascontent/caplus/patcoverage>

CAS Registry Number Crossover Limits Increased to 500,000 in Key STN Databases

Increase your STN search power by taking advantage of the expanded crossover limits for CAS Registry Numbers. Now you can crossover up to 500,000 CAS Registry Numbers at one time from CAS REGISTRY to six key STN databases instead of the previous limit of 300,000. The new limit applies to the following databases: BIOSIS, CA/CAPLUS, EMBASE, MEDLINE, USPATFULL, USPAT2

There is a charge to crossover each CAS Registry Number into non-CAS databases. Enter HELP COST in the CAS REGISTRY or ZREGISTRY databases for details.

EMBASE Adds Unique Records from MEDLINE, Expanding Coverage back to 1948

EMBASE has expanded its indexing collection to more than 7,000 journals and increased the size of its database by 8.4 million records going back to 1948 by adding unique records from MEDLINE.

Database	Years of Coverage
EMBASE	1974 to present
MEDLINE	1948 to present

MEDLINE records will now be included as part of the regular daily updates for EMBASE. The unique MEDLINE records retrieved from EMBASE differ from their counterparts in MEDLINE by having EMTREE indexing.

Enhanced Coverage of Citation Information in Inpadoc

As of July 9 2010, the coverage of patent citation data in the INPADOC files INPADOCDB and INPAFAMDB has been enhanced. The recent enhancements comprise new citation details and improved functionality supporting new and efficient ways for competitor analyses:

- publication dates available for cited patent numbers
- improved coverage of applicant citations
- sources of citation extended for PCT-applications
- search report office available for citations of PCT-applications
- cited patent assignee names are now searchable

ICSD now contains 132,526 crystal structures

The ICSD database now contains 132,526 crystal structures, including 117,389 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. These data are part of the legacy crystal structure data on metallic and intermetallic compounds added since 2008. During the update procedure 8,169 new entries were added, 2,413 entries were modified, and 27 entries were removed. The work on structure types has been expanded to the newly added and modified data. Thanks to the work by Professor Allmann, more than 95,000 ICSD entries have now been assigned to 5,159 distinct structure types.

STN Training and Help In the UK & Ireland

There will be a series of public workshops conducted in London and Manchester this year on the following dates

- 28-30th September – London
- 12-14th October - Manchester

The program is the same for both London and Manchester and users are welcome to register for all three days or selected days, There is no cost for attending. The sessions will be run jointly with CAS and FIZ trainers. The workshops are

- Day 1 - STN Basics
- Day 2 - STN Intermediate
- Day 3 - Introduction To Chemistry Searching

To Register for any of these days please go to:

<http://www.stn-international.com/workshops.html>

If you have any queries with your STN searching then you are welcome to contact the STN Helpdesk based in FIZ Karlsruhe by emailing helpdesk@fiz-karlsruhe.de or by telephone on +49 7247 808 555.

Training can also be arranged either via FIZ-Karlsruhe or by contacting the Anne Jones who is the CAS Applications Specialist for the UK & Ireland on annejones@cas.org

More ACS/CAS News

STN/CAS/ SciFinder on Social Media

You can now follow CAS and STN on twitter simply by adding @caschatter and @stninfo to your twitter contacts.

There is also now a SciFinder User Group on LinkedIn and a SciFinder follower page on Facebook.

CAS Chemistry Research Reports

CAS produced two issues of a new series, CAS Chemistry Research Reports. The first report is called "40 Years of Biofuel Research Reveal China Now Atop U.S. in Patenting and Commercialization of Bioethanol". The second describes "A Decade Later Human Genome Discoveries Spur Growth of Cancer Treatments". Links to the PDF copies of these two reports can be found at <http://www.cas.org/newsevents/press/pressreleases.html>

ACS Mobile: <http://pubs.acs.org/page/tools/acsmobile/index.html>

ACS has introduced a mobile software application for users of Apple's iPhone and iPod Touch devices. ACS Mobile provides readers with an up-to-the-minute live stream of peer-reviewed research content published across the Society's portfolio of scholarly research journals, and is augmented by "Latest News" from Chemical and Engineering News.

People News

Brian Vickery 11 Sept 1918 - 17 Oct 2010

Contributed by Vanda Broughton, Dept. Information Studies, University College London

Brian Vickery was one of the most significant figures in the field of classification and information retrieval of the 20th century, and a major architect of the theory of that discipline. He was born in Australia as Brian McCay, but when his parents parted after an acrimonious divorce, and his mother later remarried, he took his stepfather's name, and did not see his father again. In his final years Brian had been researching his family history, and was able to find information about his father Adam McCay, a professional writer, a leading journalist in Sydney, and a minor poet.¹

Leaving Australia, Brian travelled with his family first to Egypt, and then to England, where he went to school in Canterbury. Afterwards he went up to Oxford to Brasenose College, where, like a number of other information scientists of his vintage, he read for a degree in chemistry. After taking his degree, during World War II he worked as a chemist in a large explosives factory, and it was there that his involvement in information began, when he took responsibility for this aspect of work in the large research laboratory. When he later became a librarian he retained an interest in the sciences, and his early writings on classification often make use of science as an exemplar.

Brian had a distinguished career as a librarian, holding senior appointments. After his first post at Imperial Chemical Industries, he moved during the 1960s to be deputy librarian at the newly created National Lending Library for Science and Technology, and subsequently became head of service at the University of Manchester Institute of Science and Technology (UMIST).

Nevertheless it is as a theorist and researcher that he is best known. He had begun to make his mark from his early days in the field, and this led to him being invited to attend the Royal Society Conference on Scientific Information held in 1948. The findings of the conference led directly to the formation of what became the Classification Research Group, one of the most influential

research collaborations of the twentieth century, and one whose impact on information science theory cannot be underestimated. Most of the group were advocates of the faceted classification theory of the Indian librarian, S. R. Ranganathan, and it was within the CRG that this theory was brought to a high level of sophistication in what may be regarded as the 'British' tradition of facet analysis. It is striking that, collectively, the group, which consisted mainly of practising librarians, created little in the way of documentary output, and their work was principally recorded in an occasional bulletin published in the *Journal of documentation*. Brian Vickery proved to be an exception, and from the beginning he produced a steady stream of publications. Two brief but influential monographs appeared at this time: *Classification and indexing in the sciences*,² and *Faceted classification*,³ both of which still stand as seminal texts in the field, and a number of articles on classification theory which were published in the *Journal of documentation*. It is perhaps less widely known that he was the author of the article on information retrieval in the *Encyclopedia Britannica* at that time.

During the 1960s, Brian developed an interest in information retrieval theory more generally and later moved away from the CRG, who continued to focus on classification. Another influential book *On retrieval system theory*⁴ was published in 1961, and in 1966 he was appointed to a post at Aslib to take control of research activities there. He was successful in attracting external funding from the Office for Scientific and Technical Information (OSTI) and then from its successor body the British Library Research and Development Department (BLRDD). Consequently, this was a fruitful period, and he conducted a number of projects, including a major survey of existing classification schemes undertaken with a view to choosing one for the newly proposed British Library.

In 1973 he moved to the (then) School of Librarianship and Archive Studies at University College London, as Director of the School, and Professor of Library Studies. He was responsible for a number of important innovations: the word 'information' was added to the title of the School, computers were introduced, as were staff meetings, and a new MA in scientific information was instituted, as well as a contribution to the general BSc degree. His most significant achievement at UCL was undoubtedly the establishment of a lively research environment with funded projects and the recruitment of a number of able doctoral students. After his retirement from UCL in 1983, Brian continued to be active in his field. His second wife, Alina, whom he married in 1967, was herself a major player in the field of automated systems, and together they worked on a number of projects, including another book *Information science in theory and practice*.⁵

A few of Brian's major publications have been mentioned here, but his output was prodigious, and his writing elegant and incisive. A bibliography of his works to that date, compiled by Harry East and Amber Adams, was published as part of his eightieth birthday festschrift in the special edition of *Journal of documentation*,⁶ and another record of his writings, and the works in which he was cited can be found on Eugene Garfield's site at the University of Pennsylvania⁷. Here are to be found references for 173 items published between 1948 and 2006, and a database of over 38,000 references to and from his works, a truly astonishing measure of his significance in his field.

In his final years Brian attended several meetings of the newly formed UK Chapter of the International Society for Knowledge Organization, and was made an honorary member in 2008. On one memorable occasion he addressed the meeting, giving an overview of the development of information retrieval.⁸ His energy, lucidity, and mastery of his subject would have been impressive for a man half his age. It was an honour to meet at last the man who had so influenced my own work (for as a student at UCL, I had missed him by one year), and I was not alone in feeling that we were in the presence of a rare intellect, and a delightful person.

Brian Vickery died at home, shortly after his ninety-first birthday, after feeling mildly unwell for a day or two. He was active in writing, researching, and planning new projects right up to the end of his life.

1. Penelope Nelson "Under the influence? Adam McCay: journalist, poet, letter writer and influential friend". *Australian literary studies* Vol. 22 October, 2005
2. Vickery, B. C. *Classification and indexing in the sciences*. London: Butterworths, 1958
3. Vickery, B. C. *Faceted classification*. London: Aslib, 1960
4. Vickery, B. C. *On retrieval system theory* London: Butterworths, 1961
5. Vickery, B. C. and Vickery, A. *Information science in theory and practice* London: Butterworths, 1987
6. East Harry, and Adams, Amber. "B.C. Vickery: bibliography", *Journal of documentation*, 1998 44 (3) 205 - 215
7. <http://garfield.library.upenn.edu/histcomp/index-vickery.html>
8. http://www.iskouk.org/AgendaR_June2008.htm

Other Forthcoming Meetings/Conferences

2nd International Lhasa Symposium on New Horizons in Toxicity Prediction

15th - 16th September 2010

Leeds Royal Armouries Museum, UK

<http://www.lhasasyposium.com>

Seminar on Freedom to Operate

11th October 2010, 13.30 - 17.20

Organised by RSC Law Group; RSC, Burlington House, Piccadilly, London W1J 0BA

<http://www.rsc.org/ConferencesAndEvents/conference/alldetails.cfm?evid=106266>

PIUG Northeast Conference

11th - 15th October 2010

New Brunswick, NJ, USA

<http://www.piug.org/NorthEast/2010/ne10prog.php>

Internet Librarian International

14th - 15th October 2010

Novotel London West, London, UK

<http://www.ukeig.org.uk/trainingevent/internet-librarian-international>

Patent Information Conference 2010

19th - 21st October 2010

Lausanne, Switzerland

<http://www.epo.org/about-us/events/pi-conference.html>

ICIC 2010

24th - 27th October 2010

Vienna, Austria

<http://www.haxel.com/icic/2010>

Making Search Work - Course presenter Martin White

26th October 2010

CILIP, 7 Ridgmount St, London WC1E 7AE, UK

<http://www.ukeig.org.uk/trainingevent/making-search-work-course-presenter-martin-white>

Digital Information Conference 2010

28th October 2010

Kings Place, London, UK

<http://www.cilip.org.uk/digitalinfo2010>

Library Management Systems Suppliers Showcase

5th November 2010

CILIP, 7 Ridgmount St, London WC1E 7AE, UK

<http://www.cilip.org.uk/lmslondon2010>

Pharma-Bio-Med

8th - 11th November 2010

Seville, Spain

<http://www.pharma-bio-med.com/>

Seminar on Recent Chemistry Case Law - Patents

16th November 2010, 12.30 - 18.00

Organised by RSC Law Group; RSC, Burlington House, Piccadilly, London W1J 0BA

<http://www.rsc.org/ConferencesAndEvents/conference/alldetails.cfm?evid=106279>

IBC Legal's 4th Annual Standards and Patents Conference

16th - 17th November 2010

London, UK

<http://www.informaglobalevents.com/event/standards-and-patents-conference-2010>

2010 CIPA Biotechnology Conference

18th - 19th November 2010

Bath, UK

<http://www.cipa.org.uk/pages/events/details?ED738335-0C01-44C1-8A5A-FD1433903375>

24th annual Pharmaceutical & Chemical Patent Practice Symposium

8th December 2010

New Jersey, USA

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

Online Information 2010

30th November - 2nd December 2010

Olympia, London

<http://www.online-information.co.uk/>

II-SDV

Search, Data Mining, Visualization

14th - 15th March 2011

Singapore

<http://www.infonortics.com/II-IDV/>

9th International Conference on Chemical Structures

5th - 9th June 2011

Noordwijkerhout, The Netherlands

<http://www.int-conf-chem-structures.org/>

NOTE: The Joint RSC CICAG/Law Group meeting on Competition Law and E-Publishing in Scientific Fields due to be held later this year has been CANCELLED

Other News Items

Digging into Data in New Ways

HPC Projects, 14 June 2010

http://hpcprojects.com/news/news_story.php?news_id=1200

DOE Launches Free Portal for Green Energy Research

Weekly News Digest, 26 April 2010

<http://newsbreaks.infotoday.com/Digest/DOE-Launches-Free-Portal-for-Green-Energy-Research-66786.asp>

Elsevier Introduces Chemistry Application That Helps Researchers Unravel Deep Layers of Information

PRNewswire-FirstCall, 20 July 2010

<http://www.prnewswire.com/news-releases/elsevier-introduces-chemistry-application-that-helps-researchers-unravel-deep-layers-of-information-98812184.html>

Open Access Uptake Plummetts

Information World Review, 10 June 2010

<http://www.iwr.co.uk/academic-and-humanities/3010277/Open-access-uptake-plummetts>

Free Journals Grow Amid Ongoing Debate

Science 20 August 2010: Vol. 329. no. 5994, pp. 896 - 898

<http://dx.doi.org/10.1126/science.329.5994.896>

Plagiarism Pinioned

Nature, 8 July 2010

<http://dx.doi.org/10.1038/466159b>

Chemical Information and Computation 2010, Number One

239th ACS National Meeting And Exposition; San Francisco, CA, March 21-25, 2010

Wendy Warr & Associates' 35th issue of their ACS report series is going to press. It has 40 transcripts of papers on visual analysis of chemical data, the future of chemical communication, chemical entity extraction, biochemical pathways and retrobiosynthesis, and Reaxys for finding synthetic methods, plus six months' worth of news from about 70 companies. Contents list and order form at: <http://www.warr.com/>

When Science Went International

Looking back 150 years at the conference that led to the assembly of the periodic table.

Chemical & Engineering News, September 3, 2010

<http://pubs.acs.org/cen/science/88/8836sci1.html>

And Finally

Scientists Discover New Element

Oxford University researchers have discovered the heaviest element yet known to science. The new element, Governmentium (symbol=Gv), has one neutron, 25 assistant neutrons, 88 deputy neutrons and 198 assistant deputy neutrons, giving it an atomic mass of 312.

These 312 particles are held together by forces called morons, which are surrounded by vast quantities of lepton-like particles called pillocks. Since Governmentium has no electrons, it is inert. However, it can be detected, because it impedes every reaction with which it comes into contact.

A tiny amount of Governmentium can cause a reaction that would normally take less than a second, to take from 4 days to 4 years to complete. Governmentium has a normal half-life of 2 to 6 years. It does not decay, but instead undergoes a reorganisation in which a portion of the assistant neutrons and deputy neutrons exchange places.

In fact, Governmentium's mass will actually increase over time, since each reorganisation will cause more morons to become neutrons, forming isodopes. This characteristic of moron promotion leads some scientists to believe that Governmentium is formed whenever morons reach a critical concentration. This hypothetical quantity is referred to as a critical morass. When catalysed with money, Governmentium becomes Administratium (symbol=Ad), an element that radiates just as much energy as Governmentium, since it has half as many pillocks but twice as many morons.

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Please send future items for the CICAG Newsletter to the newsletter editor:
Lindsay Battle, email: lindsay.battle@chem.ox.ac.uk
