

The future of the CICAG Newsletter

This newsletter is the main vehicle by which members of the CICAG are kept in touch with the Group's activities. It is therefore a vital channel of communication. However, since the merger of the CIG and CASG, the task of distributing the newsletter to the larger combined membership has also increased significantly, as has the cost of postage, especially with the new regulations on the size of postal items. The folding, stuffing and posting of several hundred hard copy newsletters is now a marathon task performed entirely voluntarily. We are most grateful to Dot Parker (and the long-suffering Geoff!) for her efforts to date, but recognise that the task is now becoming too burdensome.

Alongside this, an increasing proportion of our members have an email address and the vast majority, if not all, have access to the Internet. We have therefore agreed that in future the newsletter will only be distributed electronically. For those of you who have supplied an email address, future issues will be sent to you via email. If you have an email and have not yet let us or the RSC know, please do so now.

For other members, each issue will be posted on the Group's website, and can be accessed at: www.rsc.org/CICAG

These changes do mean that it will be easier to produce issues more frequently, and information will reach members quicker than would otherwise be the case, especially for our overseas members.

So, please note: **THIS WILL BE THE LAST PRINTED ISSUE OF THE CICAG NEWSLETTER.**

Doug Veal, CICAG Secretary .

RSC Chemical Information and Computer Applications Group – Future meetings

The 8th International Conference on Chemical Structures

The CICAG will again be sponsoring the highly successful International Conference on Chemical Structures. The 8th conference in the series will once again be held in Noordwijkerhout, The Netherlands from June 1st to 5th, 2008. The scientific program has not yet been finalised but anyone wishing to attend or present a paper should start preparing now as places are limited and it has previously been oversubscribed.

For further information, please keep an eye on <http://www.int-conf-chem-structures.org/> where information on the new conference should appear.

Information about previous meetings can also be found at this address.

Some items of interest from the literature and internet

U.S. Department of Energy (DOE) and the British Library

U.S. Department of Energy (DOE) and the British Library, along with eight other participating countries, recently opened an online global gateway to science information from 15 national portals. The gateway, WorldWideScience.org, was developed and is maintained by the DOE Office of Scientific and Technical Information. It gives researchers and anyone interested in science the capability to search science portals not easily accessible through popular search engines such as Google and Yahoo! British Library Research and Innovation Newsletter, July 2007

Find out more: <http://www.worldwidescience.org/>

Structure-recognition software unveiled

08 August 2007 Ned Stafford/Hamburg, Germany
A software tool which automatically converts old pictures of chemical structures into computer-readable format promises to solve the most tedious problem plaguing chemical bibliographers. But it's got competition.

For years, the images contained in old scientific journals and patents have had to be redrawn digitally and entered manually into databases, so that computers can search them. Now, Germany's Fraunhofer Institute for Algorithms and Scientific Computing (SCAI) says it has developed software that automates this process.

This article comments on both SCAI and CLiDE (Chemical Literature Data Extraction), marketed by Toronto-based SimBioSys Inc.

Richard Kidd, who leads the RSC's Project Prospect, has analysed a demo version of CLiDE. He agrees that it is hard to develop consistently accurate chemical structure recognition software, partly because structures in publications often include other information crammed on to the

image. Unless software can do the work with a minimum of human supervision and double-checking, it would usually be less time-consuming to simply draw the images from scratch, Kidd said. He believes the results of even the best recognition software in the future will need some human supervision: 'It would never be 100 per cent, I don't think. But it could get good enough to be worthwhile

Full item: Chemistry World | News, August 2007
<http://www.rsc.org/chemistryworld/News/2007/August/08080701.asp>

Scientific publishing stagnates in the US

US scientists and engineers have not increased the rate at which they publish papers in peer-reviewed journals since the 1990s despite rising research and development funding, reports the National Scientific Foundation (NSF).

Meanwhile, the total number of papers published across Asian nations and the European Union has increased.

The findings are published in 'Changing US Output of Scientific Articles: 1988 – 2003' and is part of a larger study of trends in scientific publication by NSF's Division of Science Resources Statistics (SRS).

Research Information, 2 August 2007

http://www.researchinformation.info/news/news_story.php?news_id=99

eMolecules and Wiley Announce ChemGate, the Spectroscopy Search Engine

With 700,000 Spectra for 500,000 Chemicals

Full item:
<http://www.marketwire.com/mw/release.do?id=766397&sourceType=3>

Scholarly publishers snub Microsoft

11 August 2007 - Microsoft's latest Word release has caused chaos in scholarly publishing circles, earlier this year the software giant launched the latest version of Office, with Word 2007 and its new XML-based file format, DOCX. Unfortunately online publishing systems cannot accept these files. Full item: Research Information, 11 August 2007

http://www.researchinformation.info/news/news_story.php?news_id=106

Chemgate

DEL MAR, CA and WEINHEIM, GERMANY-- (Marketwire - September 4, 2007) - eMolecules, Inc., provider of the world's largest chemical structures search engine, and Wiley-VCH, a leading publisher for the scientific, technical, and medical communities worldwide, announce the release of ChemGate at

www.chemgate.emolecules.com.

The search engine containing high quality NMR, IR and MS spectra allows chemists to search by chemical structure and access spectra for a given structure by a single click. For full details see

www.emolecules.com.

ChemSpider

ChemSpider - a web service containing a database of almost 20Million compounds now provides access to methods to manipulate InChI Strings and InChIKeys, including conversion to and from the MOLfile format, checking the validity of the InChI identifiers and searching ChemSpider using InChI inputs.

See <http://www.chemspider.com/inchi.asmx> for more details.

Chemical-Information-Sources-SNS

Chemical-Information-Sources-SNS is a global Facebook group intended to serve a forum and venue for the presentation, consideration, and discussion of any and all matters relating to Chemical Information Chemical-Information-Sources. SNS is dedicated to Eugene Garfield, PhD.

<http://iastate.facebook.com/group.php?gid=6035271802>

U.S. Department of Energy Launches New Patent Web Site

The U.S. Department of Energy (DOE) announced the launch of a Web site, DOepatents, which allows search and retrieval of information from a collection of more than 20,000 patent records (www.osti.gov/doepatents). The database represents a growing collection of patents resulting from R&D supported by DOE. DOepatents consists of bibliographic records, with full text where available via either a PDF file or an HTML link to the record at the U.S. Patent and Trademark Office.

European patents set to get cheaper

Patents valid across many European countries will soon be much easier and cheaper to register, with the coming into force of the so-called London Agreement.

The agreement simplifies the translation requirements for patent applications filed with the European Patent Office. It was negotiated by EU member states in 2000, but has been in limbo ever since because of France's refusal to ratify it.

Chemistry World, 14 September 2007

<http://www.rsc.org/chemistryworld/News/2007/September/14090701.asp>

Search giants offer new features

Yahoo and Microsoft have announced upgrades to their search engines in efforts to gain ground on rival Google.

Yahoo's makeover will include features that allow users to refine searches as well as offering links to photos, music and video on the results page.

Microsoft's new-improved Live Search represents a "quantum jump in search results" according to the company.

There has been a rise in so-called metasearch engines which trawl through a variety of other search engines to find results.

Items on this can be found on the BBC webpages on

<http://news.bbc.co.uk/1/hi/technology/7023757.stm>

and

Technology Review, Tuesday, October 02, 2007

<http://www.technologyreview.com/Wire/19467/?nlid=580>

Computational Organic Chemistry

Steven Bachrach announced the publication of his book, "Computational Organic Chemistry" through Wiley. This book surveys the field of computational organic chemistry, presenting case studies of the application of ab initio and DFT computations to organic chemistry problems, along with interviews of six major figures in the field.

He is also providing two services on the web that augment the book. First, the book's web site (<http://www.trinity.edu/sbachrac/coc/>),

And the blog that serves as a mechanism to update the book, <http://hackberry.chem.trinity.edu/blog>.

Both the book's auxiliary web site and the blog are operational and can be accessed for free. Enjoy!

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The Online Information Conference is the world's no. 1 conference for the information industry. The conference attracts over 800 delegates from over 45 countries across all continents, providing a forum dedicated to learning, debate, professional development, technology reviews and assessments, expert discussion as well as case-study presentations and the sharing of research results and opinion.

<http://www.online-information.co.uk/online07/conference.html>

Chemical Information and Computer Applications Group - A Spiral Path from Atoms to Galaxies

At our AGM this year, Philip Stewart, retired Oxford Lecturer in Ecology and Economics, talked about the history of spiral representations of the Periodic system at the 2006-7 AGM. He has supplied the following note:-

After the Karlsruhe Conference of 1860, at which Canizzaro produced the first reliable list of atomic weights for the 60-odd then known elements, several chemists noted that chemical properties seemed to recur every eighth element. The first attempt to represent this graphically, by the French geologist Chancourtois, was in the form of a cylindrical spiral (1862). Another of the early pioneers, Hinrichs, a Danish American, produced a dislocated flat spiral (1867).

Mendeleev, who produced the first almost fully accurate representation in 1869, recognized that 'the series of elements is, in a certain degree, a spiral function', but he dismissed spiral

representations such as that of Baumhauer (1871) because ‘the number of radii and the formulation of the spiral are not dependent on anything’. I believe that the real reason why Mendeleev gave up active research on his ‘Periodic Law’ after 1871 was that he could make no headway in finding a mathematical function to relate atomic numbers to physical properties – but then nor could anyone before the electronic structure of the atom was worked out fifty years later.

Mendeleev’s prestige helped to make the table the normal representation, though it has the disadvantage of breaking the continuous series of elements. If he had experimented with a spiral, he might have seen that there were more wide gaps between atomic weights between the halogens and the alkali metals than almost anywhere else. His failure to predict this group was one of the reasons given for not awarding him the Nobel Prize in 1906, but another failure was his inability to fit the lanthanides into his 1904 table (in which he predicted the ether as element zero).

All these early attempts were marred by the authors’ fixation on the idea that the coils of the spiral or the rows of the table were seven or eight groups in length. It only became possible to see the strange form of the whole system, with pairs of coils or rows 8, 18 and 32 elements long, after Moseley had shown how to determine atomic numbers. The first spiral to show this was drawn by Hackh in 1914.

One of the most original designs was that of Von Antropoff (1926). He solved the problem of using an opened-out cylindrical spiral by making the width of the compartments progressively smaller, producing an architectural effect, but his most remarkable idea was that the element of atomic number zero would be neutronium, with the neutron as its atom. This was six years before Chadwick discovered the neutron, and 41 years before Bell and Hewish discovered the first neutron star, the core of which is thought to contain

neutronium with a density of about 300 megatons per cubic centimetre – surely the strangest of all elements!.

The all-time champion of periodic draftsmanship was Charles Janet, an engineer who married the boss’s daughter and obtained the wealth and leisure to indulge his passion for biology, producing beautiful illustrations. In his eighties he turned his attention to chemistry and produced an amazing series of images of the Periodic System (1929), including a very harmonious spiral. He anticipated Seaborg by 16 years in placing the actinides (of which only four were known) under the lanthanides, and foreseeing places for elements up to number 120. More controversial was his idea of ending the periods with the alkaline earth elements, at the head of which he place helium.

More spirals with neutronium followed: those of Emerson (1944), Scheele (1949) and Clark, but the most striking spiral was the mural painted by Edgar Longman for the Science Exhibition of the Festival of Britain in 1951. As an artist he saw the dynamic potential of giving his spiral an elliptical outline and tilting it up at an angle. Floodlit in the dark basement exhibition hall, with its brilliant colours running through the spectrum, this was my first encounter with the Periodic System. Aged twelve, I found it thrilling, and it reminded me of the M31 galaxy in Fred Hoyle’s book, *The Nature of the Universe*, which I had just read. I was filled with wonder at the idea that the elements had been forged in the heart of giant stars and blown into space by vast explosions.

Many years later, inspired by the memory of Longman’s mural and in honour of Hoyle - another great scientist denied a Nobel Prize - I returned to my boyhood love and designed my own Chemical Galaxy, hoping to inspire a new generation of chemists and to convey to non-chemists the excitement of our subject, which deals with the stuff of atoms, planets, stars and galaxies.



