



WINTER 2008

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THE 2008 AGM HELD AT BURLINGTON HOUSE ON 10TH JUNE 2008, AT 4.10PM

ANNUAL REPORT FOR 2007-2008

During the year 2007, the Group planned its usual two scientific meetings. The first meeting was to be on 'Going Paperless,' in Manchester on June 29th. Unfortunately, although an excellent programme had been arranged, this had to be cancelled for lack of interest.

The second meeting, on November 1st at Burlington House, was to cover the area of data mining. This also had to be cancelled as we were unable to complete organising the programme in time.

However, our first meeting of 2008 has already been held, on May 22nd at Burlington House. This dealt with 'Open Access Publishing in the Chemical Sciences,' and was very successful with an attendance of nearly 50.

The second meeting of 2008 is planned for November 1st and will be a rerun of the successful training day on 'An Introduction to Chemical Information,' run in conjunction with the CSA Trust.

During the year the Committee met three times in person. No electronic meetings were held. The new CICAG committee was elected at the 2007 AGM, held on May 16th at Burlington House. The AGM was followed by a talk by Philip Stewart of the University of Oxford on "The Chemical Galaxy" which was very well received.

During 2007 we decided to issue the Group Newsletter electronically and distribute it by email, with a copy posted on the Group website. We produced two printed Newsletters, in the summer and autumn of 2007, which were circulated to all members. Thereafter, we have used electronic

distribution. We are grateful to Dot Parker for her help in producing the Newsletters and to Don Parkin for his work on distributing the electronic versions and on maintaining the Group website.

The process of merging the finances of the two Groups is still in hand, using the existing CIG bank account. As of February 2008, membership of the combined group was just over 400.

Doug Veal, Secretary

MINUTES OF THE 2008 AGM

- Apologies Were received from Keith White, Jan Davies, Lindsay Battle, Chris Evans, Alan Tonge, Don Parkin and Martin Cadman.
- Previous minutes Minutes of the 2007 CICAG AGM were approved.
- Matters Arising The merging of the Chemical Information and Computer Applications Group accounts was still awaiting action by the bank, but this was in hand. No progress had been made in getting increased committee representation from the old CASG membership
- Annual report: The annual report, included in the newsletter was approved.
- Accounts: The 2007 audited accounts were tabled. The Group made a small surplus during the year and has approximately £38,000 in the bank. The accounts were approved and signed by the Chairman.
- Election of Officers
- | | |
|-----------|--|
| Chair | Keith White |
| Secretary | Don Parkin |
| Treasurer | Chris Evans continues |
| Members | Jan Davies, Lindsay Battle, Doug Veal, Martin Cadman, Alan Tonge, Bob McDowall, Diana Leitch |
- Subscriptions: Under new RSC arrangements (final details still to be clarified) it is understood that all members, for a fee of £5, will be entitled to membership of up to three Groups. Therefore, no Group subscription needs to be set, except for the unlikely circumstance of someone who wishes to join the Group in addition to three existing memberships. It was agreed that, should that situation arise, a Group subscription of £2 would apply.

Note

Barry Dunne who was originally voted in as chair, stood down from the committee shortly after the AGM, due to the increased responsibilities of starting a new long term strategic assignment within CAS. We would all like to thank Barry for his long standing support of the CIGAG and his knowledge and experience in encouraging people to speak for us will be sorely missed. We are certain that all of you will wish him good luck for his future.

CAS is currently recruiting an additional Regional Marketing Manager for the UK & Ireland. In the interim, Yvonne Pope will be taking on Barry's previous responsibilities. Yvonne has worked at CAS for 5 years supporting CAS customers in the biotechnology, consumer health, chemical and government areas. Yvonne's background is in Biological Chemistry and she is also a graduate of the Department of Information Studies in Sheffield. Prior to joining CAS, Yvonne worked as an Information Scientist both at GSK and ArQule. She cites her interests as walking, climbing, cycling, baking and Sudoku. Some of you may know Yvonne by her maiden name of Yvonne McCormick.



This picture shows Barry, Yvonne (right) and Diana Leitch on the occasion of her retirement from the John Rylands University Library at the University of Manchester on 4 July 2008. As Diana joins the committee we may even see more of her as she enjoys "retirement"!

Diana Leitch who was formerly the Deputy University Librarian and Associate Director of the John Rylands University Library at the University of Manchester has joined the CICAG committee. She retired from the University of Manchester on 4 July 2008 and this photo with Barry and Yvonne was taken at her leaving do. Diana is a chemist by profession and was elected a Fellow of the Royal Society of Chemistry in 2005 in recognition of the work she had done in the development of chemical information in the academic sector over the previous 30 years. She is the only librarian in Higher Education ever to be accorded this honour. Diana is a former trustee of the Chemical Structure Association and Chair of the CSA and a current member of the RSC Publishing Board.

THE FUTURE OF THE NEWSLETTER

Technical Editor Don Parkin. Don can be contacted on donald.parkin@stfc.ac.uk. Any queries concerning the webpage should be sent to Don.

Production Editor Dot Parker. Dot can be contacted on blueclouds@btinternet.com any queries concerning the content of the newsletters or information to include can be sent here.

We intend to issue two Newsletters each year, approximately one month before each Event. (May and October) IF ANYONE HAS ANYTHING TO PUT INTO THE NEWSLETTER – OR ANY COMMENTS ABOUT HOW IT SHOULD BE CHANGED, PLEASE LET US KNOW. For many members this is the only contact we have with them and we would like to improve the newsletter to reflect better the interest of the group.

PREVIOUS MEETINGS

OPEN ACCESS PUBLISHING IN THE CHEMICAL SCIENCES

The RSC CICAG held a one-day meeting on “Open Access Publishing in the Chemical Sciences” in the Council Room of the RSC offices, Burlington House, on May 22nd, 2008. The meeting topic had stimulated interest from publishers, academics, university librarians, scientific information providers and the chemical industry; with all these groups being well represented in the forty plus delegates. The meeting involved eight presentations. All of these generated questions and some heated debate. [PDF's of the presentations](#) can be downloaded from the RSC/CICAG website, including a full summary document with links to examples of relevant blogs, articles and websites. Shown here are summaries from three of the speakers:-

SPEAKER SUMMARIES

Open Data - why it must become universal

Peter Murray-Rust, University of Cambridge

<http://wwmm.ch.cam.ac.uk/blogs/murrayrust/?p=1110>

<http://wwmm.ch.cam.ac.uk/blogs/murrayrust/?p=1113>

<http://wwmm.ch.cam.ac.uk/blogs/murrayrust/?p=1114>

<http://wwmm.ch.cam.ac.uk/blogs/murrayrust/?p=1115>

Also a fuller account in Nature Proceedings (preprint at:
<http://precedings.nature.com/documents/1526/version/1>)

Designing data repositories to support preservation & publication for the chemistry community

Simon Coles, University of Southampton

This presentation begins by outlining the changing nature of the exchange of chemical information and the new opportunities that are provided by the new generation of tools and services available on the World Wide Web. It then goes on to demonstrate the clear need for a new and structured approach to storing, managing and disseminating such information, given the current data deluge and approach to publishing. The Institutional Repository approach is presented as a solution and models, prototypes, policies and financial case studies are presented. The concept of using Blog technology to collaborate and exchange information relating to chemical experiments is discussed and an example of Open Notebook Science presented. Finally the concept of implementing the OAI-ORE protocol to wrap up heterogeneous data types from different sources and analytical experiments to produce an exchangeable complex digital object

package that is self describing and may be shared using new social networking approaches (in particular the my Experiment project) is outlined.

Growth of support for Open Access, and its spread from biomedicine

Bryan Vickery, Deputy Publisher and Chris Leonard, Associate Publisher, BioMed Central

The traditional publishing model relies on subscription charges invariably paid by libraries to recover the costs of the publication process, thereby creating a barrier to access content. In contrast, an Open Access (OA) model requires all articles to be made freely available immediately upon publication. Benefits of OA include retention of copyright for authors and free and immediate availability of the full text version of articles, allowing redistribution and use of research for derivative works, such as course materials.

There has been significant growth in the adoption of OA publishing since the first journals began in 2000, with ever more funding bodies and institutions supporting OA initiatives. Soon, 10% of articles in PubMed will be freely available immediately upon publication. OA is now spreading from biomedicine and physics to other disciplines, such as chemistry. However, while the Directory of Open Access Journals currently lists almost 3000 such titles, only 60 are categorised as "chemistry". BioMed Central - which publishes over 180 OA journals, launched Chemistry Central in 2006 to improve availability of peer-reviewed research on all aspects of chemistry and related fields.

"AN INTRODUCTION TO CHEMICAL INFORMATION "

The meeting was held on Wednesday 29th October 2008, at the Royal Society of Chemistry, Burlington House, London.

Suzanne Pears from the CSA Trust, thanked all those on the RSC CICAG Committee and at Burlington House, who helped to make the day such a successful event - it was a great team effort and she looks forward to working with them again in the future.

Suzanne was pleased to report that a lot of the attendees filled out the feedback forms and the vast majority of comments were very positive. She has now collated the information and has shared it with the group.

[PDF's of the presentations](#) can be downloaded from the RSC/CICAG website.

FUTURE MEETINGS

The AGM will be held during our Spring meeting on May 20th 2009. It is expected that the title of the meeting will be "**Scientific Text and Data Mining**".

The Autumn meeting will be 28th October 2009 and will possibly concern **Patents**.

2010 will see a joint meeting with the CSA Trust (a repeat of the training course meeting) and a joint meeting with the RSC Historical Group.

Note: CICAG are able to offer a subsidy to any students or young people that want to attend CICAG meetings.

CICAG BLOG

The CICAG has a blog to enable further discussion of CICAG meetings, Newsletters and other activities. It can be accessed from the [CICAG website](#) or directly from the [RSC Web Board](#)

OTHER MEETINGS WHICH MAY BE OF INTEREST

[42nd IUPAC Congress: Chemistry Solutions](#)

Glasgow, UK, Sunday 2 August Friday 7 August 2009

Email: [IUPAC 2009](#) Tel: +44 (0) 1223 432380

The Scottish Exhibition and Conference Centre (SECC) is Scotland's national venue for public events and is the UK's largest integrated exhibition and conference centre. Located on the river Clyde, just five minutes from Glasgow city centre, it has become an icon of Glasgow and a symbol of regeneration of the river.



IUPAC 2009 will use the 3,000 seat Clyde Auditorium, designed by Sir Norman Foster and affectionately known as the "Armadillo".

Themes

[Analysis & Detection](#)
[Chemistry for Health](#)

[Communication & Education](#)
[Energy & Environment](#)

[Industry & Innovation](#)
[Materials](#)
[Synthesis & Mechanism](#)

[Faraday Discussion 145: Physical Organic Chemistry](#)

Wednesday 2 September - Friday 4 September 2009, University of Wales Institute, Cardiff (UWIC),

Email: [RSC Conferences](#) Tel: +44 (0)1223 43225

Course: [Return to science, engineering and technology](#)

This Open University course is for anyone who has previously worked in the fields of science, engineering and technology and who wants to return to work. It will help you: look at what you really want from work; evaluate your skills and experience; blow the dust off your CV; make new contacts and revive existing ones; find out who is offering the kind of work you want to do; achieve that all-important work-life balance

The course is part time and on-line, allowing flexibility around your other commitments. May – July 2009 or October 2009 to January 2010.

Contact Samantha Haynes. Tel: +44 (0)1274 438910

If you would like to make any comments on this last few items e-mail rscgrapevine@rsc.org

MEET YOUR COMMITTEE

During "Online Information" at Olympia at the beginning of December

The committee meets every year around 11.00 am at the CAS stand before having a meeting but this would be a good time to come over and make yourselves known to us. Maybe you can suggest a meeting topic for next year?

235th ACS National Meeting and Exposition, New Orleans, LA, April 6-10, 2008

The contents list is on the Web at <http://www.warr.com/morepubs.html>.

The report includes:

1. News from more than 70 companies (including some not exhibiting)
2. Condensed press releases for the first six months of 2008
3. Accurate transcripts of presentations complete with color figures and literature references, with the following themes:
 - public cheminformatics resources
 - cheminformatics implications of collaborations between academia and industry
 - cheminformatics education
 - challenges in structure searching
 - open meetings of the ACS committees on ACS Publications and CAS
4. A report of a panel discussion on evolving use of chemical information, touching on topics such as networked biology, visualization, small molecules and properties, searching and Web 2.0, generating knowledge, search interfaces, serendipity, recommendations, text mining, data quality, data capture and data sharing.

wendy@warr.com

<http://www.warr.com>

RSC VIRTUAL LIBRARY



Members can browse, search and access the chemical sciences information they need, FREE of charge, 24/7, globally from premium resources provided by the RSC Virtual Library featuring:

- full text journals electronic reference books
- chemical and physical property data
- bibliographic abstracts databases
- chemical business information

Please email [Nazma Masud](mailto:Nazma.Masud@rsc.com) at library@rsc.com with any questions.

SANDY LAWSON GETS MIKE LYNCH AWARD

The Mike Lynch award is awarded by the CSA Trust. Its purpose is to recognize and encourage outstanding accomplishments in education, research and development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and properties.

Sandy Lawson was the 2008 award winner and received his award at the Eighth International Conference on Chemical Structures held in Noordwijkerhout, The Netherlands in June 2008. Just

before this he gave the plenary lecture entitled 'Challenges/Opportunities for chemical structure databases in the 21st century'.

Professor Dr Alexander (Sandy) Lawson held a number of positions including research fellowships at the Universities of Kent and Mainz, directorships at the Beilstein Institute from 1982 to 1994, and subsequently directorships at MDL.

He is currently Director of Research and Development at Elsevier Information Systems GmbH. Sandy has made major contributions to the fields of chemical information handling and chemical structure representation, in particular in the development of the Beilstein database and software (including the famous Lawson Number for indexing chemical structures).



[Sunday Telegraph highlights RSC views on exam standards](#)

29 September 2008 - CEO Richard Pike speaks of slipping standards in a Sunday Telegraph piece

"After the fiasco of the SATs we now discover that the process of question setting and marking is fundamentally flawed," said Michael Gove, the shadow children's secretary. "The regulator urgently need to take action to restore confidence in the rigour of the testing system."

Richard Pike, the chief executive of the Royal Society of Chemistry, said awarding marks to wrong answers was "indefensible."

"Not only is the paper very simple, it is being marked very, very leniently. To take answers that are demonstrably wrong is indefensible. It is further evidence of the breakdown of the regulatory structure. It cannot go on like this. We are not criticising the children in this but the system which allows them to gain grades which are purely illusory." See:-

<http://news.bbc.co.uk/1/hi/education/7750717.stm>

http://www.timesonline.co.uk/tol/life_and_style/education/article5240805.ece

LINKS TO OTHER ITEMS OF INTEREST

AN ONLINE CHEMICAL STRUCTURE DATABASE AND PROPERTIES GENERATION SERVICE

<http://www.chemspider.com/> is claimed to contain >10 million chemical structures... searched by Systematic Name, Synonym, Trade Name, Registry Number, SMILES or InChI or structure (which needs a plug-in and requires IE7+ or Firefox 2.0+).

This leads to the chemspider ID number, Structure, Empirical Formula, Molecular Weight, Monoisotopic Mass, Da, ACD/LogP, ACD/LogD, (pH 5.5), ACD/LogD (pH 7.4), # of Rule of 5 Violations, #H bond acceptors, #H bond donors, #Freely Rotating Bonds, Polar Surface Area, Molar Volume cm³, names, synonyms, FEMA numbers, EINECS numbers, CAS RN if available, and links to references in other chemical databases.

AWARD HELPS SAFEGUARD UK'S RESEARCH JOURNALS

Research Information, 20 July 2008

http://www.researchinformation.info/news/news_story.php?news_id=343

DOE ANNOUNCES INTERNATIONAL AGREEMENT ON GLOBAL SCIENCE ONLINE GATEWAY

Weekly News Digest, 16 June 2008

<http://newsbreaks.infotoday.com/wndReader.asp?ArticleId=49539>

HOUSE CLEANING: COPING WITH ERRORS, AMBIGUITY, AND FUDGING IN THE REALM OF CITATIONS

Chemical & Engineering News, 19 May 2008

http://pubs.acs.org/cen/science/86/8621sci1_web.html

LEVERAGING BRITANNICA'S CONTENT WITH WEBSHARE

NewsLink, 2 June 2008

<http://newsbreaks.infotoday.com/nbReader.asp?ArticleId=49388>

OLD NEWSPAPERS GET ONLINE LAUNCH

BBC NEWS | Technology, 9 September 2008

<http://news.bbc.co.uk/1/hi/technology/7605461.stm>

'ONLINE JOURNALS REDUCE CITATION COUNT'

Research Information, 5 August 2008

http://www.researchinformation.info/news/news_story.php?news_id=348

PEER-TO-PATENT PILOT RELEASES REPORT ON PILOT PROJECT

Weekly News Digest, 19 June 2008

<http://newsbreaks.infotoday.com/wndReader.asp?ArticleId=49581>

FROM WIKIPEDIA – ALCHEMY OR CHEMISTRY?

In case you have ever wondered...

Chemistry (from Egyptian kēme (chem), meaning "earth") is the science concerned with the composition, structure, and properties of matter, as well as the changes it undergoes during chemical reactions. It is a physical science for studies of various atoms, molecules, crystals and other aggregates of matter whether in isolation or combination, which incorporates the concepts of energy and entropy in relation to the spontaneity of chemical processes. Modern chemistry evolved out of alchemy following the chemical revolution (1773).

Alchemy (Arabic) a part of the Occult Tradition, is both a philosophy and a practice with an aim of achieving ultimate wisdom as well as immortality, involving the improvement of the alchemist as well as the making of several substances described as possessing unusual properties. The practical aspect of alchemy generated the basics of modern inorganic chemistry, namely concerning procedures, equipment and the identification and use of many current substances.

A firework is classified as a low explosive pyrotechnic device used primarily for aesthetic and entertainment purposes. The most common use of a firework is as part of a fireworks display. A fireworks event (also called a fireworks show or pyrotechnics) is a display of the effects produced by firework devices. Fireworks competitions are also regularly held at a number of places. The biggest fireworks event in the world is held in Madeira, Portugal at the New Years' Eve celebrations, as documented in the Guinness World Records.

Fireworks (devices) take many forms to produce the four primary effects: noise, light, smoke, and floating materials (confetti for example). They may be designed to burn with colored flames and sparks. Displays are common throughout the world and are the focal point of many cultural and religious celebrations.

Fireworks were originally invented by the Chinese for entertainment purposes, as a natural extension of the Chinese invention of gunpowder. Such important events and festivities as Chinese New Year and the Mid-Autumn Moon Festival were and still are times when fireworks are guaranteed sights. China is the largest manufacturer and exporter of fireworks in the world. China is estimated to have exported over 6 million cases or 120,000 tons of fireworks to the US in 2005.

And finally to put you all (who eat them) off your Christmas dinners...Christmas pudding.

Although it took its final form in Victorian England, the pudding's origins can be traced all the way back to the 1420s, to two sources. It emerged not as a confection or a dessert at all, but as a way of preserving meat at the end of the season. Because of shortages of fodder, all surplus livestock was slaughtered in the autumn. The meat was then kept in a pastry case along with dried fruits acting as a preservative. The resultant large "mince pies" could then be used to feed hosts of people, particularly at the festive season. The chief ancestor of the modern pudding, however, was the pottage, a meat and vegetable concoction originating in Roman times. This was prepared in a large cauldron, the ingredients being slow cooked, with dried fruits, sugar and spices added.

The earliest reference to the "standing pottage" dates to 1420s, a dish of preserved veal, mutton or chicken, thickened with bread, reddened with sandalwood and full of currants. By the time of Elizabeth I, prunes were added to this basic concoction. This became so popular that the dish was known from this point forward as Plum Pottage.

Best wishes for a prosperous New Year!

"Be always at war with your vices, at peace with your neighbors, and let each new year find you a better man."
Benjamin Franklin

"May all your troubles last as long as your New Year's resolutions."
Joey Adams

"An optimist stays up until midnight to see the new year in. A pessimist stays up to make sure the old year leaves."
Bill Vaughan

"Cheers to a new year and another chance for us to get it right."
Oprah Winfrey