NEWSLETTER Winter 2014

CICAG meeting **What's in a Name?** was held on 21st October 2014 in the RSC Chemistry Centre. See page 3 for a full report.

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 professional networking.

Chemical Information & Computer Applications Group: http://www.rsc.org/CICAG

http://www.linkedin.com/groups?gid=1989945

http://my.rsc.org/groups/cicag

https://twitter.com/RSC_CICAG

QR Code

Contributions to the CICAG Newsletter are welcome from all sources - please send to the Newsletter Editor: Lindsay Battle, email: lindsay.battle@chem.ox.ac.uk

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Chemical Information & Computer Applications Group Chair's Report

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

It's now nearly six months since I became Chair of the CICAG back in May 2014, a few weeks after leaving GlaxoSmithKline, and I have greatly enjoyed the role so far. Getting involved with the CICAG Committee has allowed me to reconnect with my chemical information roots after my career had recently taken me in the direction of IT programme management (primarily involving the roll out IT solutions for R&D staff). Before taking on the role of Chair, I had been familiarising myself with the activities and scope of the CICAG as well as getting to know my fellow Committee members. It was particularly rewarding in my first few months on the Committee to have had my first involvement with the organisation of a successful scientific meeting for CICAG, "What's in a Name? The unsung heroes of open innovation: nomenclature and terminology", the inspiration for which originated from Professor Jeremy Frey, our Vice-Chair (a report from this meeting appears later in this Newsletter).

Chemical data and information, both published in the public domain and proprietary primarily in the private sector, underpin the work of chemists in all areas, as do the IT tools needed to manage them. We are all users of information and data, and it's hard to imagine any chemist, at whatever stage of their career or role they have, not being impacted, and potentially overwhelmed, by these on a daily basis. As such, I believe the CICAG has an important role in supporting the wider chemistry community (not just information professionals), particularly RSC members.

Therefore, one of my missions while in the role of CICAG Chair is to broaden our outreach by forming partnerships with other RSC interest groups, and outside organisations with whom we share common interests. Key to this will be organising meetings of relevance to the broader RSC membership, and we will be looking to do this in 2015. I also hope that we can work more closely with RSC staff, particularly those involved with the Global Chemistry Network. I hope too that we can have greater engagement with staff within SMEs, in support of Dominic Tildesley's vision for the role of the RSC.

I also am keen to recruit more members to the CICAG Committee. I hope that younger RSC members, and perhaps those who are on a career break but looking for ways to re-engage with their profession, might see becoming active in our group as a development opportunity. I'd be happy to talk informally to anyone with an interest in joining us.

Finally, I'd like to express my sincere thanks to our Committee members for their continued dedication to the work of the CICAG, and for welcoming me to the team.

Current CICAG Committee Members

Chair: Dr Helen Cooke
Vice Chair: Prof Jeremy Frey
Secretary: Dr Alan Tonge
Treasurer: Dr Diana Leitch
Other Members:
Mrs Lindsay Battle
Miss Hannah Morgan
Mr Stuart Newbold
Dr Stephanie North
Mrs Yvonne Pope
Dr Doug Veal
Dr Keith White

A full list of RSC CICAG Committee Officers and Members, with their affiliations and contact details, is provided on the CICAG website: http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/committee.asp

Report from the RSC's 2014 General Assembly

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

Every autumn the RSC holds a General Assembly, and this year it was at the Midland Hotel in Manchester from 7-8 November. All interest groups and local groups are invited to send a representative from their Committee, and I was very pleased to be able to participate on behalf of the CICAG. The overall theme of the Assembly, introduced by Domenic Tildesley, RSC President, was "Supporting professionalism in our community".

Day 1 was comprised of plenary talks and break-out discussions on the RSC's priority activities. The discussion sessions were:

(1) Professional skills and recognition
(2) Embedding diversity in activities
(3) Connecting scientists to data and tools – building the global chemistry network
(4) Barriers to engagement

Each attendee could join two discussion sessions, and I opted for (3) and (4).

(3) is core to the interests of our group. RSC staff introduced the topic by telling us about several tools and resources which are contributing to the development of the Global Chemistry Network initiative, e.g. KUDOS, Chemical Sciences Article Repository and the National Compound Collection. Group discussions revealed the problems chemists are facing with managing ever-increasing quantities of data, information and IT tools, and participants put forward ideas around how the RSC could help. The CICAG's next planned meeting entitled "From Big Data to Chemical Information" on 22nd April 2015 will be an important forum for further discussion which could potentially influence development of strategy in this area for chemists.

The RSC's membership survey had revealed that only 12% of RSC members are active in outreach activities, and participants in discussion group (4) were asked to explore what can be done to encourage more members to become involved, and/or inspire those already involved to do more. Several approaches were discussed, including building on the government-funded STEMNET initiative (targeted at school students) and organising repeatable regional events. The preferred level of involvement of RSC Outreach team staff was also discussed.

A member of RSC staff was present at each discussion group table, and feedback will be consolidated and analysed to identify common themes. Day 1 concluded with dinner and the annual prize-giving ceremony.

Day 2 was a session for attendees to share their groups' experiences and ideas. Suggestions were made around how to recruit younger members to committees, and encourage those on career breaks to become involved. There were also ideas around use of technology to enable Committee meetings to be run by teleconference, and using social media for publicity and to communicate with interest group members (I'm pleased to say the CICAG is making use of most of the social media channels already).

Overall, this was a very worthwhile event, with lots of lively discussion (more than in most previous years I was told).

Please feel free to get in touch if you have any questions about the General Assembly and its outcomes.

Notice of Future Meeting: From Big Data to Chemical Information

To be held on Wednesday 22nd April 2015 at RSC, Burlington House, Piccadilly, London

Large and complex data sets, often referred to as "Big Data", can be difficult to manage and analyse using conventional processes and software tools. Such data sets exist in many disciplines, and chemistry is no exception. Most chemists are familiar with the huge growth in the number of compounds registered in databases in the public domain, the majority of which have data associated with them. Many will also have struggled with increasingly large data sets generated through their work, often stored in spreadsheets with limited analytical capabilities. The CICAG, in partnership with the EPSRC's Dial-a-Molecule Grand Challenge Network, is therefore organising a scientific meeting to explore the challenges presented by big data in chemistry.

More details and registration form available at: http://www.rsc.org/events/detail/16591/from-big-data-to-chemical-information

Meeting Report: What's in a Name?

What's in a Name? - The unsung heroes of open innovation: nomenclature and terminology
21st October 2014 at RSC, Burlington House, London

Report by Colin Bird, University of Southampton

Introduction
This event was co-sponsored by the RSC Chemical Information and Computer Applications Group (CICAG) and the ITaaU Network+, which is one of the four sub-themes of the RCUK Digital Economy programme. The meeting brought together a diverse group of attendees interested in the communication of chemical knowledge, the efficient exchange of ideas, and the way in which computers and the Internet can most appropriately advance chemical understanding and innovation.

In his welcome, Richard Kidd remarked that standards have become more important over time. Jeremy Frey then noted that the UK makes a significant contribution, valued elsewhere, to nomenclature, which, together with terminology, is important for international business.

Emergent themes
The increasing significance of nomenclature theme was perhaps "a given" for this meeting, and certainly came to life from the first presentation onwards. The two themes of relevance to communication and the attention given to mitigating difficulties became apparent during Richard Hartshorn's presentation and continued to arise during the rest of the meeting. The importance of curation theme emerged gradually, became progressively more apparent, and became a key aspect of Mat Todd's presentation.

Keynote Introduction: What's in a Name? Possibly Death and Taxes! *Richard Hartshorn*
Richard captivated us with the title of his keynote presentation, but duly made the link via Benjamin Franklin to Lavoisier, who developed chemical nomenclature. Richard then showed that nomenclature is vital for communication, by linking the importance of finding the right information (to avoid death) to regulation (think taxes), following up with three examples. If his list of hazards for DiHydrogen Monoxide is anything to go by, it's dangerous stuff. The Ethylene Diamine example illustrated how nomenclature issues had hampered easy access to its MSDS. Copper (II) acetate monohydrate has a more complex structure than its name might suggest, demonstrating that the level of nomenclature can matter. Richard then appraised some of the means by which naming issues can be

mitigated, starting with PINs (Preferred IUPAC Names) and InChIs. PINs are preferred for legal and regulatory purposes, but other nomenclatures are still allowed for general purposes. InChIs are coded in layers, enabling the same identifier to represent substances at all levels. The ability to barcode InChIs will become increasingly important. Richard exemplified kappa grammar with a ruthenium cobalt complex and a deca-nickel wheel, showing how the need for kappa terms to define the coordination of bridging ligands in multinuclear complexes can lead to excessively long names, but that a new variation on the convention can mitigate the issue. In answer to a question, he commented that beyond two lines, people turn away. Richard certainly showed that there is more to names that death and taxes!

Nomenclature Challenges for the 21st Century

The three speakers in this session were all discussing their experiences "at the coal face", dealing with nomenclature issues that arise with regard to communication within their specific domains.

Extended Structures, Crystallography and Polymers – Challenges. ***Clare Tovee***

Clare gave us an overview of some of the challenges that the Cambridge Crystallographic Data Centre faces with the names given to crystal structures, of which, at the time of her presentation, the CSD held 744,232.

She outlined the characteristics of searches of the database: the majority are by sub-structure; common names are used when they exist; generally the IUPAC name is used; semi-systematic names can ease searching. With regard to name sources, they extract them from CIFs when possible, but full systematic names often not given in the CIF. Clare also presented some of the challenges that the Centre experiences which include: bond types and unusual valencies; molecular symmetry; polymers; and cluster compounds. She concluded by listing useful future improvements.

Naming Polymers - buy one get one free. ***Richard Jones***

In introducing Richard, who is the UK National Representative of the IUPAC Polymer Division, Jeremy Frey remarked that polymers are one of the areas of difficulty for nomenclature.

Richard began by contrasting source-based and structure-based names, the former being derived from the monomer and the latter adopting the rules of IUPAC organic nomenclature for naming constitutional units. Although source-based names are most commonly used and include traditional polymer names, not all of the latter are acceptable, for example, the name polyphenylene oxide was rejected because it omits the 2 methyl groups in the monomer structure. When they have been synthesized by a different route, some polymers are named after an apparent rather than a real monomer. Source-based names can, however, lead to ambiguity, for example when monomers can polymerise in more than one way. Structure-based names avoid such problems. Richard illustrated the process of determining the structure-based name, poly[oxy(1-bromoethylene)] by identifying its preferred constitutional repeating unit (CRU) by reference to the rulebooks, thereby selecting it from a number of alternative CRU names. The rules for naming polymers and their corresponding monomer units/CRUs are found in the IUPAC Purple Book and Blue Book respectively.

The importance of chemical identifier standards in the pharmaceutical industry. ***Colin Wood***

Colin is an Enterprise Information Architect (not a chemist) with GlaxoSmithKline (GSK) with responsibility for Master Data Management (MDM). The development roadmap starts with some 4 million compounds, from which about 30 late stage assets emerge. Less than 1000 compounds have gone right through in GSK history. The essence of MDM is to maintain one identifier across the organisation, enabling the organisation to understand what a substance is, remove duplicates, and to standardise. It is important always to use the full identifier, to avoid ambiguities. Data integration becomes particularly important if a patient has an incident, in which case they need to able to trace back through history.

Colin raised the issue of standards at several points during his talk. He presented a long list of terms that, depending on context, could mean the same thing, or something entirely different. Pistoia Alliance has shown that pharmaceutical companies are using different terms to mean the same thing, so there is clearly an issue with semantics. It is also important to understand what a given term identifies: is it a single active compound or a combination? Trade and brand names are part of the picture, as are product families.

When asked about buying another large company, Colin described the process as "painful". It involves not only sorting out identifiers but also integrating business practices. In reply to a question about Open PHACTs, he said that GSK were trying to get internal consistency to enable integration with such organisations.

Discussion
An exchange of views flowed from Egon Willighagen asking whether systematic names were still relevant, given that databases could bring together different identifiers. The consensus was that the answer depends on who or what you are communicating with. Systematic names are still relevant but from a computer science perspective, the InChIs are superior because:

- InChIs can contain chemical information that is not found in a systematic name. Hence, there are strictly more InChIs than there are systematic names.
- It is always possible to convert an InChI to a systematic name for human consumption, however, the reverse not always the case, as the systematic name may not contain sufficient chemical information to "perfectly" identify the substance.

The impact of Computers and the Web
The five speakers in this session were all dealing with specific issues. The first three presentations related to solutions that rely specifically on computers and the Web, the last two focusing on aspects of nomenclature and/or terminology whose feasibility is dependent on computer technology.

The Web – What is the Issue? ***Egon Willighagen***
Egon proffered a selection of techniques that could be used to present chemical information in a web browser, beginning with the proposition that an alternative to a name is not a 2D depiction but a 3D structure. The techniques ranged from RSS feeds through microformats to Semantic Web technologies and the use of Semantic MediaWiki. He concluded by offering an answer to his question: the issue is that we're not using these innovative solutions enough.

Health and Safety and the Semantic Web. ***Mark Borkum***
Mark began by outlining the background to his development of a software system that assists with the completion of COSHH risk assessment forms. In the context of a chemistry laboratory, the COSHH regulations (Control of Substances Hazardous to Health) require the prior assessment of the risks associated with the substances to be used in an experiment and identification of steps to be taken to mitigate those risks. Mark's system for completing COSHH forms consumes the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) – CLP (Classification, Labelling and Packaging) in the EU - as the source of safety data. As Mark explained, aggregation and transcription of chemical information from safety data sheets is inherently prone to error, which could result unintentionally in dangerous situations.
Mark's solution uses the Semantic Web technologies RDF (Resource Description Framework) and SKOS (Simple Knowledge Organization System), both of which he explained briefly, with examples. Using example data, drawn from the Sigma-Aldrich product catalog, he illustrated the use of a web application to generate COSHH forms, and other documents, including product order forms, automatically.
Automation raises issue nevertheless, such as the concern that the chemist will not think carefully enough about what they are doing if they can perform their risk assessment with minimal personal involvement. Information leakage is also a potential problem: how many risk assessments would enable an agent to infer the research agenda? Mark also posed questions about whose legal responsibility it might be if information were misused or misinterpreted.

Defining Chemical Classes in OWL-based English for ChEBI. ***Janna Hastings***
Janna has been working for a number of years with the ChEBI database and ontology (Chemical Entities of Biological Interest). She began by outlining the evolution of ChEBI from a nomenclature database to its present form. The database requires a primary ChEBI name but synonyms that are in use are within scope. The ontology, however, is mainly structure-based: the example Janna presented showed a very apparent diamond-like poly-hierarchical classification.
The ontology is implemented using OWL (Web Ontology Language), which is a knowledge representation language comprising classes; relationships; axioms (quantified relationships). Essentially, if a molecule has a certain structural part, it is a member of the ChEBI class for that part. The definitions are chemically meaningful, human-readable, and can be used to match currently unknown structures. There are some limitations, such as expressing only binary relations and the exclusion of polymers. The entry criteria for ChEBI are that the molecule should be small and biologically interesting (to any user).

The IUPAC Green Book - Unit's Dictators Source Book? ***Jürgen Stohner***
Jürgen chairs the IUPAC Commission on Physicochemical Symbols, Terminology, and Units. He began his talk by saying that it would *not* be about nomenclature, although there would be some terminology. Illustratively, he noted that computer code usually does not distinguish

between quantities and units. The names of quantities and units are the business of ISO, not the Green Book.
Jürgen gave three examples where flawed conversions between units had led to problems: the loss of the Mars Climate Orbiter; the bridge between Germany and Switzerland, the two parts of which differed in height by 54 cm; and the confusion over an instrument's units that could have made the difference between a patient being diagnosed as hyperglycaemic and hypoglycaemic. Fortunately, the problem was noticed so the patient did not die.
The Green Book provides advice without enforcement. However, as UN, UNESCO, and EU have all adopted the IUPAC Green Book. Customs officials now have to decline any documents that don't comply, which add extra pressure for the Green Book to be more prescriptive. The Commission is currently working on a Green Book Light, a 4-page summary, and is consulting about changes to SI definitions and the redefinition of the mole that would follow from the redefinition of the kilogram.

Reaction InChI - Distilling the Essence of a Chemical Transformation. ***Jonathan Goodman***
Having admitted that Reaction InChIs (RInChIs) were to some extent a solution looking for problems, Jonathan reviewed some tasks for which a RInChI could be useful. If different people were doing the same reaction, the identifier should be the same, so the RInChI could be used to find duplicates. RInChIs could also be used to combine reaction lists. RInChIs are very likely to be valuable in Electronic Laboratory Notebooks (ELNs) and non-chemists have a need for reaction identifiers.
Jonathan used the Grignard reaction between EtMgBR and CO_2 to illustrate the RInChI, noting that the additional information includes a direction, thus "d+" means the reaction goes left to right.
The website http://www-rinchi.ch.cam.ac.uk/ provides information about RInChIs and has a service for generating reaction identifiers from reaction files, and for creating a long and/or a short RInChIKey, which are hashed forms that enable users to check whether they are doing the same reaction as someone else. There is also a service for reading a RInChI and generating an rxnfile. One of the tests of the RInChI had found different products from the same starting materials, which suggests that the reaction conditions were different.
When asked about fuzzy searches, for example to find one class of reagent working with another, Jonathan said that it was feasible in principle, but there were probably not enough RInChIs available yet.

Discussion
Richard Hartshorn raised two topics during the discussion, both of which related to RInChIs. Firstly, the addition of Health & Safety information might enable researchers to recognise either that the reaction was making something dangerous, or that the reaction itself is dangerous. Secondly, acknowledging the difficulty with recording failed reactions and/or experiments, could the RInChI help? Jonathan's response was that one could match the RInChIKey: one wouldn't know what the failed reaction was but if the keys were the same the match could still be useful.s were the same the match could still be useful.

Final Keynote: From Chaos Comes Order - Managing Data in Open Source Drug Discovery. ***Matthew Todd***
Explaining the title of his keynote presentation, Mat said that there is a lot to be gained from openness but with it comes an element of chaos, because you don't know what's coming. However, he now has experience of three open projects. He drew distinctions between open source (with which you can see everything that's going on), open access, and open innovation. Open projects are not necessarily open source, because some have no real responsibility to do anything with the data that they put out in the open.
Mat believes in leading by example, so he and his group adopted the LabTrove ELN [http://www.labtrove.org/], put his notebook out in the open and committed to going paperless. The objective of the first open project was to get rid of extremely bitter enantiomer of praziquantel, a drug used to treat schistosomiasis. Being open with this work led to a lot of input from the chemical industry to the effect that the group's first approach would not work. Most of the inputs that led to finding the solution came from the chemical industry, not academe.
Mat illustrated several characteristics of open projects, after noting the advantage that having the experiments and data already in the public domain means that the project may be continued by anyone.
Molecules that have been made can be tested in other labs, and the community can vote for molecules that are needed the most for a given purpose. In one case, being open had established that a candidate molecule had already been excluded.

Data management requires care, in part because people have different approaches to calculating the same thing. For example, solubility is one of the selection criteria for candidate molecules, but putting in 'H's in ChemDraw can alter ClogP, so it is necessary to be aware of that and guide the community to ensure standards in the methods used. Manual curation is required, for example to record all the attempts to make a given molecule: curation involves inserting links to all the relevant entries. Also links from images of compounds to the relevant entry have to be curated.
In concluding, Mat remarked that curation and standardisation are essential, especially with data and information coming from different sources, but curation is hard and needs to be automated, which is also hard.

Matthew Todd, University of Sydney, giving the Final Keynote talk.

Discussion and RSC/CICAG role
This discussion focused on what the RSC and CICAG might do or get done to improve communication, leading to the following suggestions, observations, and questions:

- A young scientists meeting, with young presenters but a broad audience! Such a meeting could be in partnership with other organisations.
- As CICAG is more interested in data and information than other groups, should it look at what could be got out from the large volume of data coming in? This topic will be addressed in the April 2015 Big Data meeting.
- There is a need for a book of definitions, rationale and best practice … luminous pink is still available!
- There is still a lot of work to be done regarding, for example, standards of representation and identifiers. There is also still a gap between existing solutions and what is coming along.
- Students could make two-minute videos for other students, showing how they had solved particular problems.
- Bring academics and people from industry together, for example to consider formulation, aiming to identify some areas where small steps could start making progress.
- Interest other areas of RSC, perhaps with a poster competition for the best use of nomenclature.
- Is there scope for UK journal of cheminformatics and chemical information?

Jeremy concluded by asking for comments, volunteers for the April 2015 meeting, and suggestions for any other things that CICAG should be doing.

A student point of view
Ed Duesbury (PhD Student in Chemoinformatics, Information School, University of Sheffield) was awarded a **CICAG student bursary** to attend the above meeting and describes his experience:

As someone from a non-chemistry background, this CICAG meeting introduced me to a number of issues resulting from nomenclature that I would never have even contemplated. In particular, concerning changes in systematic notation as well as applications and problems of nomenclature in database searching, as well as the problems in computational nomenclature for complex molecules and inorganic molecules, and what problems arise when companies merge. Although the meeting will not have a direct impact on my research (which concerns graph-based similarity), I have used InChI and InChIKey in past projects and was interested to see how it was used by other researchers and associated problems that have arisen since its release(s). The use of directed graphs in documentation and ontology was also of interest and it was enlightening to see their uses in ChEBI and in health and safety documentation.

Speakers' presentations, along with the meeting programme, speakers' biographies and abstracts of talks, can be downloaded at:
http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/meetings.asp

Student Bursaries

A number of Undergraduate Research Bursaries, funded by the Royal Society of Chemistry, will be available to students in UK and ROI Chemistry and related departments from June-September 2015. The purpose of the awards is to give

experience of research to undergraduates with research potential in the middle years (i.e. 2/3, 2/4 or 3/4) of their degree and to encourage them to consider a career in scientific research. Applications relevant to the interests of the CICAG will be welcomed in the areas of cheminformatics, chemical information, chemical data management, chemistry data analytics, chemistry IT solutions and applications. Further information can be found here:
http://www.rsc.org/Education/HEstudents/undergraduate-bursary.asp, and we will publicise further via the CICAG MyRSC group, Twitter and other channels as appropriate.

Sponsorship

CICAG sponsored the Noordwijkerhout: 10th International Conference on Chemical Structures (ICCS) and 10th German Conference on Chemoinformatics (GCC) held in June 2014 in Noordwijkerhout, Netherlands.
Selected presentations and posters are available:
http://www.int-conf-chem-structures.org

A day in the life .....

"**A day in the life of a retired librarian**" was written by Dr Diana Leitch, CICAG Treasurer, and published recently in **Insights: the UKSG journal,** which is now fully open access with no article processing charges.

Those approaching retirement and expecting a quiet life will see that the reality may turn out to be very different!

The PDF of the article is appended to this newsletter (with kind permission of Diana and the Insights editors), and can also be found here:
http://dx.doi.org/10.1629/2048-7754.199

To show life at the beginning, as well as at the end, of a career in library and information work, we asked our youngest committee member to write about a typical day in her working life. Hannah Morgan's "**A day in the life of a Senior Library Assistant in an Oxford College Library**" is also appended to this newsletter.

Many thanks to Diana and Hannah for providing these very interesting glimpses into their daily lives. It would be good if we could make this a regular feature of the CICAG newsletter, and cover a wide range of jobs, career stages and employment sectors. So if anyone would like to contribute a description of a day in their working life (anything from a couple of paragraphs to a couple of pages), please get in touch with the Newsletter editor (contact details on cover).

Catalyst Science Discovery Centre

Contributed by Dr Diana Leitch

The RSC Special Interest Groups, CICAG and the Historical Group (HG) have both been involved with support for the Catalyst Science Discovery Centre and Museum in Widnes over the past two years and the Centre continues to provide much-needed educational provision in practical chemistry and the public understanding of science to local children and their families.
The RSC itself has also been paying during 2013 and 2014 for the salary of the Education Manager there, as an RSC Teacher Fellow. The original Manager, Phill Day, moved on at the end of October 2014 to become the Public Engagement Manager at the Science and Technology Centre at STFC Daresbury on the opposite side of the River Mersey, but hopes to work, in his new role, in collaborative ventures with Catalyst in promoting science.

Phill was replaced at the beginning of November 2014 by Dr Clare Hampson, a chemist with a BSc and PhD from Durham who had been teaching chemistry in a secondary school for the last 8 years. A new Education Assistant, Gemma Read, started in September 2014. Gemma is a graduate of the Centre for the History of Science Technology and Medicine (CHSTM) at the University of Manchester and has experience in science communication skills.
The money invested by the RSC, and the two RSC interest groups who provided the IYC Challenge Money which funded a project called ORIGINS and subsequently put their £10,000 winnings in to a new project called OUTBREAK, has been greatly appreciated by Catalyst and enabled it to carry on the work it has been doing since the mid 1980s. OUTBREAK, which was a project enabling children to use scientific experiments to tackle the outbreak of a mysterious disease following a meteorite strike, will be rolled out nationally from 2015 onwards and a teachers' pack has been created for KS2 and KS3 children. It is hoped that this will encourage children to investigate and do collaborative hands on science.

In July 2014 Nobel Prizewinner, Professor Harry Kroto, visited to do one of his famous 'buckyball' sessions with 100 local children which was inspirational. In September Gill Arbuthnott, an Edinburgh based children's science writer, came to talk about her book 'What Makes YOU you?' and to do a demo on DNA extraction from strawberries. The book had been nominated for the Royal Society Young People's Book Prize 2014 and the Glasgow Science Centre allowed Catalyst to use its DNA Bracelets Workshop which the kids loved.
The monthly SciBars have continued, as has participation in Chemistry at Work Week, National Science and Engineering Week, Cheshire Science Festival and many daily weekly workshops for children and adults. The centre's chemical industry archives are used by historians across the world.

So do come and visit in 2015. Catalyst, which is nearly 30 years old, enters a new phase as it also becomes the Visitor Centre for the new Mersey Gateway (new Bridge) Crossing with spectacular views from the fourth floor Observatory of the construction work.

Hopefully a new relationship with RSC will evolve in the next three years as final negotiations are being concluded, as I write, for Catalyst to be awarded some money under the Outreach grant scheme to undertake 11 Work packages promoting the public understanding of chemistry to the general public, enabling young people to pursue careers and in chemistry and sustaining those already in employment in chemically related roles. As a Trustee of Catalyst Diana Leitch, CICAG Treasurer, has been deeply involved in writing Catalyst's submission and will be involved with the staff in delivering all of these packages.

More about these projects in a subsequent Newsletter. There will be opportunities for other CICAG members to become involved if they wish to.

Photographs of Professor Sir Harry Kroto's visit can be found in Diana's "**A day in the life of a retired librarian**" article referred to above.
For more about Catalyst see:
http://www.catalyst.org.uk

Tony Kent Strix Award 2014

UKeiG, in association with the International Society for Knowledge Organisation UK and the British Computer Society Information Retrieval Specialist Group, is delighted to announce that this year's winner of the Tony Kent Strix Award is **Dr Susan T Dumais**, Distinguished Scientist and Deputy Managing Director as well as Manager of the Context, Learning, and User Experience for Search (CLUES) Group, Microsoft Research, Redmond, WA 98052 USA. A presentation took place on the second day of Internet Librarian International 2014:
http://www.cilip.org.uk/uk-einformation-group/awards-and-bursaries/tony-kent-strix-award

UKeiG Chair, Nicky Whitsed (left) presenting Susan Dumais (right) with the Strix Trophy
(c) Internet Librarian International

Susan Dumais' research interests include algorithms and interfaces for improved information retrieval, as well as general issues in human-computer interaction. Her current research focuses on gaze-enhanced interaction, the temporal dynamics of information systems, user modeling and personalisation, novel interfaces for interactive retrieval, and search evaluation. She has has published widely in the fields of information science, human-computer interaction and cognitive science. Dr. Dumais has had incredible practical influence within Microsoft where she is widely regarded as a

thought leader for tackling difficult technical challenges in search and retrieval.

Dr. Dumais is a worthy recipient of the 2014 Tony Kent Strix award. For over 30 years, she has been a well-respected leading light in information retrieval - both in terms of research and practice - with sustained contributions that are both innovative and practical. Her significant impact has a range of theoretical, systems, and empirical bases. Dr. Dumais has developed novel algorithms to help people to find, use, and make sense of information. Her research at the intersection of human computer interaction and information retrieval has broad applications for both understanding and improving searching and browsing from the Internet to the desktop. Dr. Dumais has made a number of significant contributions to theory, experimentation, and practice in information retrieval. Perhaps her most significant contribution to date is the co-invention of Latent Semantic Analysis and Indexing (LSI); a key feature of which is its ability to extract the latent conceptual structure from a large collection of texts by analysing the associations between terms that occur in similar contexts, thus enabling a search engine to retrieve using concepts rather than keywords.

The Tony Kent Strix Award is sponsored by the RSC Chemical Information & Computer Applications Group, and is offered annually; a further call for nominations will be published early in 2015. For further information about the award, and a list of past winners, see:
http://www.ukeig.org.uk/awards/tony-kent-strix

Other Awards - Recent Recipients

Neelie Kroes, the European Commission Vice-President for the Digital Agenda, presented with BioMed Central **Open Access Advocacy Award**
http://www.biomedcentral.com/presscenter/pressreleases/23072014

Herman Skolnik Award 2015 to be awarded to **Prof. Dr. Jürgen Bajorath**
http://bulletin.acscinf.org/node/655
The 2014 Herman Skolnik Award recipient, **Dr Engelbert Zass**, was recently honoured with an Award Symposium:
http://bulletin.acscinf.org/node/665
http://bulletin.acscinf.org/node/666

Jason Farradane Award
UKeiG has announced the winners of the 2014 Jason Farradane Award: Professor Blaise Cronin and Lucy Tedd. The presentations were made at Internet Librarian International 2014.
http://www.ukeig.org.uk/awards/jason-farradane

CINF Scholarship for Scientific Excellence
Spring 2014, co-sponsored by InfoChem and Springer, awarded to:

- Katrin Stierand, postdoctoral fellow at the Center for Bioinformatics (ZBH) at the University of Hamburg, Germany http://bulletin.acscinf.org/node/589

Fall 2014, sponsored by the Royal Society of Chemistry, awarded to:

- Alexander Geanes, Dept. Chemistry, Vanderbilt University, Nashville, USA
- Vinícius Alves, Faculdade de Farmácia, Universidade Federal de Goías, Goiania, Goias, Brazil
- Huifang Li, Vancouver Prostate Centre, University of British Columbia, Canada
- Katarzyna Odziomek, Laboratory of Environmental Chemometrics, University of Gdansk, Poland and Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, USA http://bulletin.acscinf.org/node/654

ALPSP Awards

- ALPSP Award for Contribution to Scholarly Publishing 2014: award to Fred Dylla in recognition of his efforts to develop and implement creative solutions for broadening access to scholarly publications.
- ALPSP Awards for Innovation in Publishing 2014: awarded
- to Frontiers, the open science platform; IOP ebooks from IOP Publishing and JournalGuide from Research Square.

http://www.alpsp.org/Ebusiness/AboutAlpsp/ALPSPAwards.aspx

Other Awards - Calls for Nominations

CSA Trust Grants
The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program and is currently inviting

the submission of grant applications for 2015. Deadline: March 13, 2015.
http://bulletin.acscinf.org/node/590

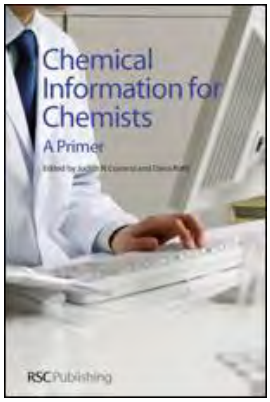
The Patterson-Crane Award - Call for Nominations
Sponsored by Dayton and Columbus Sections of the ACS. Nominees, who need not be ACS members, should demonstrate outstanding achievement in the field of chemical information. Deadline: January 31, 2015.
http://www.acscinf.org/content/call-nominations-patterson-crane-award

2015 Lucille Wert Scholarship - Call for Applications
Given by the ACS Division of Chemical Information to help those with an interest in the fields of Chemistry and Information to pursue graduate study in Library, Information, or Computer Science. The Scholarship consists of a $1,500 honorarium. Deadline: February 1, 2015.
http://www.acscinf.org/content/2015-lucille-wert-scholarship-call-applications

UKeiG Information Manager of the Year: for contribution to information management or the year's best exemplar of an information manager. UKeiG will issue a call for nominations early in 2015.
http://www.ukeig.org.uk/awards

Chemical Information / Cheminformatics Books

Chemical Information for Chemists: a primer. Edited by Judith N Currano & Dana L Roth. Royal Society of Chemistry, 2014. £24.99.
http://www.rsc.org/shop/books/2013/9781849735513.asp



Reviewed by Dr Helen Cooke, Chair of CICAG.

I was pleased to see a new book on this topic, as it's long overdue. Based on the title and notes on the back cover, I was expecting this to be a practical handbook to help practising chemists identify the most appropriate sources of chemical information for their research work. Although not a practising chemist, I also felt it would be helpful for me as a chemical information professional whose career has moved away from the area somewhat in recent years, so needing to be brought up to date.

Although the editors, and most of the chapter authors, are known to me as subject matter experts, a few questions and potential concerns sprang to mind when I discovered that all except one are from the United States (the one exception being from Canada). Why were there no authors from other countries where there is expertise in the area, e.g. Germany, Switzerland, UK? Perhaps the answer to this question, at least from the UK perspective, is that the number of academic librarians with a chemistry background is declining, so identifying authors may have been difficult.

My concern about the almost exclusive US authorship was realised in the first chapter, which has very few examples from outside the USA, and when practices and organisations referred to are almost exclusively US. I found this particularly worrying in the case of legal matters, and feel this would be misleading for practising chemists from outside the USA. There tends to be a US bias throughout the book, though some chapters are more balanced than others. Even RSC publications are under-represented – which I didn't expect.

Having been out of the field for a few years, there were some specific areas I wanted to learn about, e.g. open access journals, Google Scholar vs subscription services, big data and data quality, PubChem, ChemSpider, ejournal backfile availability, current awareness tools, latest developments in patent information, value or otherwise of Wikipedia, role of new technologies (e.g. mobile apps) in chemical information. I used these to test out the index, but found it to be lacking, and inconsistent in the level of detail of the index terms. Most (but not all) of my topics were discussed or mentioned somewhere in the text, but they were often hard to find. The stand-out chapter for me was Chapter 3, Chemical Patents, which is nicely structured, very readable, with tables and charts breaking up the text, and in my view written at the right level for chemists rather than information professionals.

Trying to put myself into the shoes of a practising chemist (perhaps a new research student), I feel that more practical examples and case studies would have been valuable, perhaps in a separate chapter, to bring all the topics together. This would help with prioritising information sources for different types of subject, determining the

right starting point for a search, and enabling researchers to develop the most appropriate information seeking strategy. A decision tree or flow chart would have been useful too.

Overall, I think this book would be most useful for information professionals or chemists moving into an information professional or publishing role, rather than practising chemists. It's a worthwhile addition to all libraries where chemistry is studied, however. At £24.99, the price is reasonable. It is possible to purchase most individual chapters in pdf format via the RSC's web site, but at £15 per chapter this wouldn't make economic sense for most potential readers. A Kindle edition would be helpful – as this would be fully searchable and would also overcome some of the deficiencies of the index.

Other reviews of the above book:

- by Bob Buntrock, published in the Chemical Information Bulletin: http://bulletin.acscinf.org/node/577
- by Robert E. Belford, published in J Chem Educ: http://pubs.acs.org/doi/abs/10.1021/ed500529k

See also:

The Future of the History of Chemical Information, ACS Symposium Series. Volume 1164, 2014. Edited by Leah R. McEwen and Robert E. Buntrock
http://dx.doi.org/10.1021/bk-2014-1164

Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment
ACS Symposium Series. Volume 1167, 2014. Edited by William G. Town & Judith N. Currano
http://pubs.acs.org/isbn/9780841229471

Chemical Poems: One on Each Element, by Markus, Mario. Dos Madres Press Inc. Loveland, OH, 2013. Reviews at: http://bulletin.acscinf.org/node/641 and http://cen.acs.org/articles/92/i7/Elemental-Amulets.html

RSC News

New RSC President: Professor Dominic Tildesley (Chemistry Views July 2014)
http://www.chemistryviews.org/details/ezine/5690851/New_RSC_President.html
See also: **Chemistry's Winning Formula** (FT Magazine, July 2014)
http://www.ft.com/cms/s/2/3f713c8e-0d41-11e4-bcb2-00144feabdc0.html
Chemistry World and Scientific American announce partnership (June 2014)
http://www.rsc.org/aboutus/news/pressreleases/2014/chemistry-world-scientific-american.asp

Jan Kuras: New manager to lead RSC open access strategy
http://www.rsc.org/news-events/rsc-news/articles/2014/sep/new-manager-to-lead-our-open-access-strategy/

RSC joins CrossMark
http://blogs.rsc.org/rscpublishing/2014/07/14/the-rsc-joins-crossmark/

National Chemical Database Service News

Shibboleth access to NCDS resources now available:
http://blogs.rsc.org/chemical-database-service/2014/08/29/shibboleth-access-to-ncds-resources-now-available/

CAS / SciFinder / STN News

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

CAS News

CHEMCATS® (Chemical Catalogs Online) on STN® Enhanced with New Search and Display Fields and More Frequent Updates

CHEMCATS on STN has been enhanced with new search and display fields based on additional information supplied by catalog providers. These fields allow for more efficient identification of suppliers that offer the desired quantity, purity and stock availability of chemicals. CHEMCATS is now also updated more frequently, whenever

new material becomes available, typically multiple times per week.

The new search and display fields are listed in the table below. The BULK field always has a value, based on information provided by the supplier, but the other new fields are optional.

Field label	Field name
SKAV	Stock Availability
QCAT	Quantity Category
SHIP	Shipping Time
PRCT	Purity Category
BULK	Bulk Availability
SCRN	Screening Compound

CAS Training in the UK 2015

In addition to the e-learning materials, we continue to offer training sessions for both STN® and SciFinder® in the UK.

We are also able to conduct 'in-house' training sessions or WebEx sessions on all aspects of CAS based STN or SciFinder searching. Also, if you wish to know more about any of the CAS products or would like further information or help with STN or SciFinder then please contact annejones@acsi.info

SciFinder News

New Substance Detail View in Latest SciFinder® Release Improves Readability and User Experience

A new layout and format greatly improves readability and user-friendliness of substance detail pages.

- Physical Property Data: list of commonly used properties at the top of the display makes it easier to find frequently needed property data
- Accordion Menu: the new layout's expandable/collapsible menu provides a quick, easy way to selectively display content of interest
- Content Area Tabs: collated tabs organize property information in scientifically meaningful ways
- Regulatory Information
  - Now conveniently accessed within a given substance's detail page
  - Reorganized in an easy-to-read format that allows users to quickly find information of interest, even by country
- Print and Export: Individually selectable content areas for print and export allow users to print only the data that matters to their research

Latest SciFinder® Release Marks Completion of the Non-Java CAS Structure Editor and Improved Access to Commerical Source Information

Non-Java CAS Structure Editor: The final non-Java editor enhancements include:

- User-defined templates: Select one or more .cxf files to serve as user-defined templates for quick access throughout your session. These templates can be placed on the canvas without clearing it.
- Eraser Tool Selection Enhancement: Erase part or all of a structure by clicking and dragging the mouse over the desired region.
- Flip Structure Tool Enhancement: Flip a selected structure 180° vertically or horizontally in one action, aided by improved visual presentation.

Commercial Source Table View: Provides easier and faster access to the commercial source data you need most, freeing up more of your time for lab work.

Makes popular existing features more prominent by bringing sought-after details to the forefront of answer set pages:

- Set Preference
- Chemical Name
- Country
- Purity
- Stock Status
- Ships Within

Provides many new sort options:

- Country
- Order from Source (previously known as Pricing and Availability)
- Purity
- Quantity
- Ships Within
- Stock Status

STN News

Cooperative Patent Classification (CPC) Combination Set Data Now Available in CAplus℠, INPADOCDB and USPAT Databases

As of September 28, 2014, CPC Combination Set data can be searched in the following STN®

databases: CA[SM]/CAplus, INPADOCDB and USPATFULL/USPAT2/USPATOLD.

CPC Combination Sets are groups of linked CPC symbols. Each CPC Combination Set identifies the technical features of a patent considered together. For example, a CPC Combination Set may include CPCs for the components of a new cement formulation, along with CPCs for reaction conditions for its manufacture.

Benefits of searching CPC Combination Sets include:

- Unique access points. Many CPCs only appear as part of a combination set in the record
- Precision. Searching for CPCs in the same CPC Combination Set may provide more relevant answers than searching for CPCs co-occurring anywhere in a patent record
- Value for novelty searching. The patents retrieved from a search for multiple CPCs in a single combination set are likely to be of interest to those assessing the novelty of an invention

Patents which most frequently have CPC Combination Sets relate to polymer chemistry, preparation of organic compounds, and compositions/mixtures, including pesticides and cements.

Forthcoming Meetings/Conferences

2015

January 6-8: **4th IEEE International Symposium on Emerging Trends and Technologies in Libraries and Information Services**, Noida, Uttar Pradesh, India
http://www.jiit.ac.in/lrcjiit/ettlis-2015

January 27th: **Keep Peddling: Libraries engaging in the student lifecycle**, ARLG West Midlands, Aston University
http://www.eventbrite.co.uk/e/keep-peddling-libraries-engaging-in-the-student-lifecycle-tickets-14625765057

February 9-12: **10th International Digital Curation Conference**, London
http://www.dcc.ac.uk/events/idcc15

February 16-17: **ASA Conference 2015: Research-to-Researcher**, London
http://www.subscription-agents.org/members-area/blogs/research-researcher

March 8-11: **International Patent Information Conference & Exposition**, Rome, Italy
http://www.ipi-confex.com

March 17-19: **UX in Libraries**, Cambridge
http://uxlib.org

March 26-27: **Information Tools for IP and Intelligence**, Singapore
http://www.infonortics.com/singa/

March 30-April 1: **UKSG 38th Annual Conference & Exhibition**, Glasgow
http://www.uksg.org/event/conference15

March 31-April 1: **Meeting the Reading List Challenge**, Loughborough
http://blog.lboro.ac.uk/mtrlc/

April 8-10: **LILAC: Librarians' Information Literacy Annual Conference**, Newcastle
http://www.lilacconference.com/

April 20-22: **emtacl15 - emerging technologies in academic libraries**, Trondheim, Norway
http://emtacl.com

April 22: **From Big Data to Chemical Information**, RSC CICAG Meeting, London
http://www.rsc.org/events/detail/16591/from-big-data-to-chemical-information

June 5: **USTLG meeting,** University of Bath
http://www.ustlg.org/?page_id=12

June 23-26: **5th Information: Interactions and Impact (i³)**, Aberdeen
http://www.rgu.ac.uk/research/conferences/i-2015

July 2-3: **CILIP Conference 2015: Bringing the information world together**, Liverpool
http://www.cilip.org.uk/conference2015

July 12-17: **European Summer School for Scientometrics**, Leuven
http://www.scientometrics-school.eu/index.html

July 20-22: **11th Northumbria International Conference on Performance Measurement in Libraries and Information Services**, Edinburgh
http://www.york.ac.uk/about/departments/support-and-admin/information-directorate/northumbria-conference/

Recent meetings

which you may have missed, but can follow up online

May 19-21 2014: **ChemAxon European UGM**, Budapest 2014 (report by Wendy Warr)
http://www.chemaxon.com/ugm-archive/2014-eu/ - report

March 16-20 2014: **Chemical Information and Computation 2014**, Number One. 247th ACS National Meeting, Dallas, (report by Wendy Warr) http://www.warr.com

October 12-15 2014: **26th ICIC International Conference for the Information Community (ICIC)**, Heidelberg, Germany
http://www.haxel.com/icic/2014/meeting

November 20 2014: **UKSG One-Day Conference,** London. Session videos now available to view.
http://www.uksg.org/event/NOVCONF2014

November 26 2014: **USTLG meeting: Supporting research**, Aston University. Presentations now available:
http://www.ustlg.org/?page_id=730

Other News Items

Johnson Matthey launches new journal of research exploring science and technology in industrial applications (Johnson Matthey July 2014)
http://matthey.com/media_and_news/news/2014/jmtr-launch

Open-access website gets tough: Leading directory tightens listing criteria to weed out rogue journals (Nature August 2014)
http://www.nature.com/news/open-access-website-gets-tough-1.15674

History of ChemDraw (ChemistryViews August 2014)
http://www.chemistryviews.org/details/ezine/6503101/History_of_ChemDraw.html
See also: **How did ChemDraw come into being?**
http://www.acs.org/content/acs/en/noteworthy-chemistry/2014-archive/october-13.html - nc5

Career: A Chemist Who Deals with Patents (ChemistryViews August 2014)
http://www.chemistryviews.org/details/education/6487251/Career_A_Chemist_Who_Deals_with_Patents.html

Garbage in, garbage out - the rise of low-quality and predatory open access journals and conferences (Chemistry World September 2014)
http://www.rsc.org/chemistryworld/2014/09/garbage-garbage-out-pipeline
See also:
Jeffrey Beall's **List of Predatory Publishers**
http://scholarlyoa.com/2014/01/02/list-of-predatory-publishers-2014/
Google Scholar is Filled with Junk Science
http://scholarlyoa.com/2014/11/04/google-scholar-is-filled-with-junk-science/

Can annotated articles help you? (RSC Publishing Blog September 2014)
http://blogs.rsc.org/rscpublishing/2014/09/19/can-annotated-articles-help-you/

The Academic Book of the Future: project to explore the future of academic books in the context of open access publishing and continuing digital change
http://pressandpolicy.bl.uk/Press-Releases/The-Academic-Book-of-the-Future-6bf.aspx

Kudos - Helping researchers explain, enrich and share their publications for increased research impact
http://blogs.rsc.org/technical/2014/07/15/kudos-helping-researchers-explain-enrich-and-share-their-publications-for-increased-research-impact/
https://www.growkudos.com

Jean-Claude Bradley Memorial Issue in the Journal of Cheminformatics and Chemistry Central. to be published early 2015
http://www.chemconnector.com/2014/09/03/jean-claude-bradley-memorial-issue-in-the-journal-of-cheminformatics/

Developments in chemical education - how students are engaging in alternative ways of communicating and promoting science (Chemistry World September 2014)
http://www.rsc.org/chemistryworld/2014/08/developments-chemical-education

The digital toolbox - a new section of Nature examines the software and websites that make research easier (Nature September 2014)
http://www.nature.com/news/the-digital-toolbox-1.15810
http://nature.com/toolbox

ACS appoints New Editor-In-Chief For C&EN: Bibiana Campos-Seijo will begin her duties in December 2014. Currently, she is editor and publisher of the RSC 's magazine Chemistry

World and oversees the production of two additional magazines.
http://cen.acs.org/articles/92/web/2014/09/Chemical-Society-Appoints-New-EditorChief.html

Signing science: a project that's making sign language scientifically articulate (Chemistry World September 2014)
http://www.rsc.org/chemistryworld/2014/09/signing-science

The University Experiment - a Nature Special (Nature October 2014)
http://www.nature.com/news/universities-1.16123

The Human Element in Lab Informatics: Technology-savvy researchers will steer the laboratory toward digital integration (Chemical & Engineering News October 2014)
http://cen.acs.org/articles/92/i42/Human-Element-Lab-Informatics.html

Dana Roth: Reaching out from the library: Caltech's chemistry librarian chats about how librarians can support researchers. (Chemistry World October 2014)
http://www.rsc.org/chemistryworld/2014/10/interview-dana-roth-caltech-librarian

Spending on subscriptions to journals rises by up to 50%: FoI requests reveal substantial hikes in university outlay despite open access push (Times Higher Education October 2014)
http://www.timeshighereducation.co.uk/news/spending-on-subscriptions-to-journals-rises-by-up-to-50/2016635.article

Elsevier Enhances Pure, Providing New Research Analysis Functionalities through Direct Integration with SciVal (Elsevier October 2014)
http://www.elsevier.com/about/press-releases/science-and-technology/elsevier-enhances-pure,-providing-new-research-analysis-functionalities-through-direct-integration-with-scival

CES Selector 2015: Enabling materials decisions that solve real-world engineering problems
Updated software helps to improve product performance, reduce cost and risk (Granta Design October 2014)
http://www.grantadesign.com/news/2015/selector-2015.shtml

Dr Frank Allen, former Executive Director of the Cambridge Crystallographic Data Centre, and Herman Skolnik Award Winner 2003, passed away on 10th November 2104, aged 70.
http://www.acscinf.org/content/frank-allen-herman-skolnik-award-winner-2003-passed-away

The top 100 papers: Nature explores the most-cited research of all time (Nature October 2014)
http://www.nature.com/news/the-top-100-papers-1.16224

Gates Foundation champions open access (Chemistry World November 2014)
http://www.rsc.org/chemistryworld/2014/11/bill-melinda-gates-foundation-open-access-policy

Germany and Britain agree on closing 'patent box' loophole (Reuters November 2014)
http://uk.reuters.com/article/2014/11/10/uk-germany-britain-patent-boxes-idUKKCN0IU26920141110

Computational Chemistry in the Industry (ChemistryViews November 2014)
http://www.chemistryviews.org/details/news/6937261/Computational_Chemistry_in_the_Industry.html

Cost to Develop a Drug More Than Doubles to $2.56 Billion (Bloomberg November 2014)
http://www.bloomberg.com/news/2014-11-18/cost-to-develop-a-drug-more-than-doubles-to-2-56-billion.html

ACS announces new CEO: Thomas M Connelly, Jr (ACS December 2014)
http://www.acs.org/content/acs/en/pressroom/newsreleases/2014/december/american-chemical-society-announces-new-ceo-thomas-m-connelly-jr.html

And Finally…….

Contributed by Doug Veal

A few more entries for the Uxbridge Chemical Dictionary:

Angstrom	Romantic story bedevilled by anxiety
Cathode Ray	Girl in debt to boy
Esterified	Very scared Spaniard
Mannose	Socks
Methane	Declaration by Macbeth
Oxide	Leather
Tartrate	Escort agency price

[The Uxbridge English Dictionary is a compilation of new definitions of words contributed by team members of the comedy radio quiz series 'I'm Sorry I Haven't a Clue.' See last Newsletter for more examples]

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

APPENDICES

A day in the life of a retired librarian

Contributed by Dr Diana Leitch, CICAG Treasurer
Published in Insights 27(3), November 2014. Reprinted with kind permission of Insights editors.

A day in the life of a Senior Library Assistant in an Oxford College Library

Contributed by Hannah Morgan

A day in the life of *a retired librarian* Dr Diana Leitch MBE, FRSC

The sun was shining as my husband, David, and I woke up early in Didsbury, Manchester, on Thursday 10 July 2014 for what was to be a very intensive day and the culmination of over 18 months of planning.

Bolton-born Nobel Prizewinner for Chemistry, Professor Sir Harry Kroto, now based in Tallahassee, Florida, was taking time out of his intensive travel schedule to visit the Catalyst Science Discovery Centre and Museum in Widnes, Cheshire, where he was going to do one of his famous 'buckyball' presentation workshops with 100 primary school children. I had become involved with Catalyst (www.catalyst.org.uk), which is the oldest science discovery centre in the UK and the only one specializing in the promotion of chemistry and the chemical industry to children and the general public, about two years ago, and in early 2013 I became a Trustee of the Catalyst Science Discovery Centre Trust. So why was Harry Kroto coming?

Well, in May 2013 I had attended the 300th Anniversary of the Chemistry Department of the University of Edinburgh, my alma mater, for the award of Honorary Degrees to my former research supervisor, Professor Evelyn Ebsworth, later Vice-Chancellor of Durham University, and Professor Sir Harry Kroto, by Sir Timothy O'Shea, the Principal of Edinburgh and former Chairman of Jisc. So I was able to renew acquaintance with Sir Timothy and Harry, whom I had last met when the John Rylands University Library of Manchester (JRULM) was involved in the John Dalton 200th anniversary celebrations of his first paper on atomic theory, held in Manchester in 2003. I asked Harry if he would come to Catalyst. After several months of waiting, Harry's wife, Margaret, contacted me to say that they could come on the morning of 10 July 2014 between visits to Rome, the Galapagos Islands, Sheffield, Bolton, Sussex and Moscow!

After a speedy breakfast for us, our dog and cat, and arranging for a neighbour to take our dog on her usual three-mile run by the Mersey valley, we drove the 30 miles to Widnes to get there before the Year 4 children (from three primary schools) and 20 teenagers (from the Liverpool UTC), who were coming to the event. Planning beforehand had been going well

despite one of the Widnes schools having to pull out because of the threatened teachers' strike on 10 July. A substitute class was found at short notice from my own two children's former school, Didsbury C of E Primary School, and all the children arrived for Harry's demo and their opportunity to make a C60 buckminsterfullerene (buckyball) model.

Diana with Nobel Prizewinner, Professor Sir Harry Kroto (photographed by David Leitch)

Harry Kroto making C60 buckyballs with a group of children from Didsbury C of E Primary School (photographed by David Leitch)

I introduced Harry to everyone, told them a bit about Nobel prizewinners, and the children were thrilled by the whole experience. An up-and-coming Widnes Vikings rugby league star, Declan Hulme, who is a sports science student at Edge Hill University, turned up to present Harry with a 'C70' rugby ball. After lunch Harry departed for Sussex and the children had an exciting workshop on the 'Origins of the Universe' before leaving for their schools. This left me to breathe a sigh of elated relief and to have a brief fundraising meeting with fellow Trustees and the Outreach Manager from the Royal Society of Chemistry (RSC), who had come up from Cambridge. Fellow Trustee, Professor Alan Dronsfield, ex-Derby University, who was there, and I are members of the RSC Historical Group (RSC HG) and I am currently Treasurer of the Chemical Information and Computer Applications Group (CICAG) of the RSC, so we have been working closely with the RSC regarding support for Catalyst.

David and I arrived home by 4:30pm so, as the sun was still shining, we set off to the allotment to continue to pick the large quantities of redcurrants we had this year. These had to go straight in to one of my five freezers as there was no time that day to make any jams or chutneys, as I do most days, to raise funds for our 13th-century church. The apocryphal story in Didsbury since June is that I was awarded my MBE for the 'chemistry of jam making' not 'services to chemistry'. As we were picking, the mobile phone rang, and it was our granddaughter, Mhairi, aged two-and-a-half, wanting her usual chat with Grandma and Grandad, while being driven home from nursery in Glasgow by our surgeon daughter, Fiona. As we don't get to see them very often, for work reasons, phones and Skype are great assets in keeping in touch.

Daughter, Fiona, granddaughter, Mhairi and dog, Maisie (photographed in late July 2014 by Diana)

After dinner and a quick snooze in a chair, the day ended with my catching up with e-mails about various activities, including plans for the two RSC conferences in October 2014 for which I am acting as bookings administrator: one organized by CICAG, where I am working again with Helen Cooke (née Schofield), ex-UMIST Library and GSK, and the other organized by RSC HG on the chemicals of World War I. E-mails were also coming in about a meeting

with Manchester Literary and Philosophical Society Council members about the John Dalton 250th anniversary birth celebrations in 2016, an illustrated talk I was giving the following week to a U3A Group and thanks from former school friends for the highly successful 50th anniversary reunion four of us had organized on Saturday 5 July at our old school. (Was it really that long ago that we last saw each other and left Chester for pastures new and careers?) Sadly, 11 of our group of 60 have died already, which makes you determined to make the most of retirement whether in charitable activities, working on professional committees, doing consultancy work, undertaking grandparent duties or the other myriad of activities the retired are needed to undertake while also keeping their brains active. Carpe diem.

So finally, around midnight, to sleep "perchance to dream" about our forthcoming cruise in late July to Iberia and Morocco, an Edinburgh University dinner in September at Holyrood Palace and even a quick prayer that it might be possible for us retirees to have greatly reduced fees for a part-day's attendance at the UKSG Conference in Glasgow in 2015 to meet up with 'old mates'.

APPENDIX

A day in the life of a Senior Library Assistant in an Oxford College Library

Contributed by Hannah Morgan

I am a Senior Library Assistant in a small Oxford College Library. There are only four members of staff, three full-time and one part-time. The college is almost 500 years old and the current undergraduates still use the original library, though it has been extended over the years. The furniture in the first floor of the library dates from the early 17th century and some of the fixtures for chaining books to the shelves are still in place, though the chains themselves are long gone. Members of the college can access the library 24hours a day, though as we do not have a self-issue machine borrowing is restricted to during staffed hours. During term time we do employ students to staff the issue desk in the evenings and on weekends to extend borrowing hours.
As well as working full-time I am also studying part-time for my MSc in Library and Information Management via a distance learning course.

A typical Tuesday
Each morning when I get into work there is shelving to be done, both books that were returned the day before and those cleared from desks that morning. On Tuesdays I start work at 10am (and work until 6pm) so the clearing has already been done and the books for the English Room are waiting for me on their trolley. I notice with some dread that there are a few Dickens books to be shelved as this means I'll have to get out the really tall steps to reach the top shelf where they belong. Once the shelving is done I check through the CCTV footage to see if anyone set off the security gate alarm the night before. As the library is open 24hours, but the issue desk is not it's my job to check that no one has attempted to sneak books out overnight. Fortunately it was a quiet night and there is nothing to investigate. My next task is to count up the money taken at the library second-hand book sale held last Friday. We raised just over £160 for our missing books fund, from selling withdrawn stock or unwanted donations. There are still two boxes of books sitting under my desk waiting to be collected so the total should increase by the end of the week.
At 10.30am I cover the issue desk for 15 mins so the Library Assistant can have a tea break. After I've also had tea, the Library Assistant and I take some of the empty boxes from the book sale down to our closed stack for storage. We also take down a few fragile books that have just come back from the conservators. They have been put into custom-made archival boxes to help hold them together. The way down to the stacks is through four locked doors and two sets of stairs, the first of which is quite narrow and can be awkward to navigate when carrying a box full of books. We make our way down without accident and even manage to find space on the shelves for the newly boxed books, though it did take two of us to shuffle along the folios to make a gap for one volume.
When we got back to the library office I invoiced two urgent book purchases requested by readers, arrived them on our library management system (Aleph) and passed them to the Assistant Librarian for classification. We always prioritise the processing of acquisitions which have been requested by readers and one of the benefits of being in a small library is that a new book can be ready to borrow within a few hours of it's arriving. One of the books I invoiced had only been requested the day before and it was ready to be borrowed by lunchtime!
Whilst the Library Assistant was busy processing new books, I made a start on pricing the books we don't have in stock on an Old and Middle English Literature reading list. This would then get passed by the Assistant Librarian to the appropriate Fellows to decide if we need to make any new purchases. I also do a little basic cataloguing of journal offprints that have articles referring to items in our manuscript collection. These articles as yet only on a card catalogue, and I do some basic bibliographic cataloguing to get them onto a computer before passing the records onto the Assistant Librarian for checking and upgrading if necessary. It is a enjoyable project that I probably wouldn't have the chance to do in a larger library, and I get to practice the cataloguing theory I'm learning on my Masters course.
At 1pm we close the issue desk and library office for one hour head down to the college kitchens for lunch. In the summer we often take our trays out into the gardens to enjoy some fresh air and sunshine, but it is too cold to sit outside in November, so we head into the dining hall and eat amongst the portraits of past presidents of the college. I spend the rest of the lunch hour reading a journal article for my MSc.

As the Library Assistant only works mornings I staff the issue desk in the afternoons, and at 2pm I open it up and check our book bin for any returns during lunch. We have an external reader coming in to consult one of our modern books this afternoon and as I will need to supervise them I make sure I have all I need for the afternoon out at the desk. A large box of books arrived at lunchtime which should keep me busy invoicing for a while. A few of the books are replacements for damaged copies or are new editions and I make a note to withdraw the relevant titles later. My invoicing is interrupted a few times as readers come to the desk to borrow or return books, and a grateful reader borrows the requested purchase that we had rushed through processing that morning.

Throughout this I can hear organ music playing as the library is directly adjacent to the college chapel. This is unusual even for an Oxford College, and with only a large window separating us from the chapel we often have musical accompaniment of varying abilities!

The external reader leaves at 3.30pm and I go looking for the older editions that can be withdrawn to make room for the new stock, before having an afternoon tea break with the Librarian and Assistant Librarian in the library office. After discussing where to go for our Christmas meal I go back to the issue desk taking with me a pile of recently donated books from a retiring Fellow. These have to be checked against our current holdings to see if we already own a copy, and if so how many times it has been borrowed. Once I've done the initial assessment the Librarian and Assistant Librarian will use my notes to help decide which books will be of most use to our current readers and should be added into the library stock. As the Fellow donated two trolleys of books I am working through a pile a day and hopefully should have assessed all the books before Christmas! Once I've got through my allocated pile for today I finish pricing up the English Literature reading list, and email the Assistant Librarian the spreadsheet of those books we don't own that are still in print.

At five to six a reader comes rushing in to borrow a book before the issue desk closes, as they need it for an essay due tomorrow. As I lock up the issue desk I can hear the choir rehearsing in the chapel for evensong on Sunday and I walk across the quad to the sound of the theme tune from the Vicar of Dibley. Though I have finished work it is not yet home time as I am headed to another Oxford library to consult some reference-only items for my MSc.