

NEWSLETTER Winter 2014

CICAG meeting K \Uhg]b`U'B Ua Y3 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>

MyRSC <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:

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

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 extend my thanks to our Committee members for their continued dedication to the work of the CICAG, and for welcoming me to the team.

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>

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.

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>

Unsung heroes of open innovation: nomenclature and terminology
21st October 2014 at RSC, Burlington House, London

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 "agiven" for the first time 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. The importance of curation theme emerged gradually, became progressively more apparent,

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:

- x InChIs can contain chemical information that is not found in a systematic name. Hence, there are strictly more InChIs than there are systematic names.
- x 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 "perfect

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 **c o n f u s i o n o v e r a n i n s t r u m e n t ' s u n i t s t h a t c o u l d** 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 **d o c u m e n t s t h a t d o n ' t c o m p l y , w h i c h a d d e x t r a** 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

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' 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.

MatthaTD Alo-2(islo)5(-td)-9f)-3(o)4(k)U-13(y -(a)-55(l)-9 -17)4(k)U-13(yysnio)ls)-3snio)lsM7Gypsb0*14 ()Tj0-5(uto)5(

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.

CICAG sponsored the Noordwijkerhout: 10th International Conference on Chemical Structures

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>

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 **t h i s y e a r ' s w i n n e r o f t h e T o n y K e n** 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,

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.

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

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

databases: CASM/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:

- x Unique access points. Many CPCs only appear as part of a combination set in the record
- x 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
- x 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.

2015

January 6-8: 4th IEEE International Symposium

which you may have missed, but can follow up
online

May 19-21 2014: ChemAxon European UGM,
Budapest 2014 (report by Wendy Warr)

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 librarians chat 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%: Fol 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

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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.

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. I received an e-mail from the RSC on 10th July 2014 and I replied to it on 11th July 2014.

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’.

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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 24 hours a day, though as we do not have a self-issue machine borrowing is restricted to during staffed hours. Dhout 1ilcfTht 1i7

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