Chemistry Update

Newsletter 289, 29th September 2017

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Calendar of Events

Research Seminar
Speaker: Dr Luisa Ciobanu, French Alternative Energies and Atomic Energy Commission (CEA)
Date: Wednesday 4 October
Time: 1pm—2pm
Location: C/B101

KMS Seminars
Date: Wednesday 4 October
Time: 2pm—5pm
Location: C/A101

Green Chemistry Seminar
Speaker: Dr Florent Bouxin, Joint BioEnergy Institute (JBEI)
Date: Thursday 5 October
Time: 3pm—4pm
Location: C/F106

Industry Mini-Symposium
Speakers: Professor Tim O'Riordan, Sygenta and Peter Lindsay-Scott, Lilly
Date: Wednesday 11 October
Time: 12.30pm—2pm
Location: C/B101

Inorganic Seminar
Speaker: Dr Joy Farnaby, University of Glasgow
Date: Wednesday 18 October
Time: 1pm—2pm
Location: C/B101

Date of Next Issue: 27th October 2017

Leading National Education Conference Held in Department of Chemistry

The Variety in Chemistry Education and Physics Higher Education Conference (ViCEPHEC) is the leading national conference for chemistry and physics education at tertiary level in the UK. This year the conference was held in the Department of Chemistry at the University of York between 23 and 25 August.

Delegates ranged from academic staff at universities to schoolteachers, outreach officers, laboratory specialists, technicians, students, industrialists and publishers. The event, attended by over 175 delegates, provided opportunities to share best practice within the disciplines of chemistry and physics by discussing cutting edge educational research and practice.

New for 2017 was 'Labsolutely Fabulous', chaired by Dr David Pugh, which was an opportunity for conference delegates to present lecture demonstrations, experiments and outreach activities. This addition to the programme complemented the interactive workshops, oral presentations and five minute oral bytes. A poster session at the National STEM Learning Centre provided further opportunities to discuss aspects of teaching and scholarship.

Professor Andy Parsons and Dr Glenn Hurst both gave presentations at the meeting. Andy talked about his online course 'Explaining Everyday Chemistry' and the way in which this demystifies organic chemistry to a wide range of different learners. Glenn presented the variety of ways in which, working alongside Louise Summerton, Avtar Matharu and James Clark, he has been embedding Green Chemistry principles into a range of different learning environments – from schools in Brazil to undergraduate labs here in York.

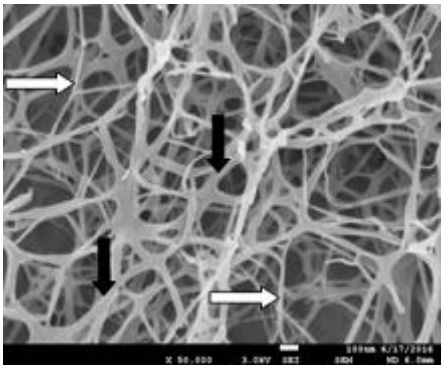
Professor John Holman gave a thought-provoking plenary lecture in which he explored the transition made by students (and himself) between school and university chemistry education. A number of York alumni also came back to the Department and made great contributions to the meeting: Dr Dan Cornwell (ex-Smith group, now Kings College London) described a new introductory 'sweet' experiment to spectrophotometry and Dr Russ Kitson (ex-Taylor Group, now University of Warwick) presented a brilliant example of how students can be motivated with monopoly money via 'game-based learning', in which they must work in teams to spend their money wisely on analysis in order to determine molecular structure as efficiently as possible.

A highlight of the meeting was the conference dinner held at the National Railway Museum – a spectacular venue, which made a real impression on conference delegates and showed off York at its very best.

Dr Glenn Hurst, Chair of the conference organising committee said: "The many great discussions over dinner and throughout the rest of the meeting attest to the healthy state of education in the physical sciences at university level and the strong sense of community that exists."

Smith Group Mixes it Up

New research from the Smith group has reported innovative new materials that successfully 'mix up' four different components, each of which performs a different job in the final gel.



Making materials that do multiple different things can be a challenging task yet has the potential to unlock exciting new biological applications. In this recent research paper Vânia Vieira, PhD student, Laura Hay, MChem project student and Professor David Smith, employ a multi-component approach, gaining an understanding of how different active ingredients can be simply mixed together yet still retain their individual activities.

The first component is a soft self-assembling gel, which is highly responsive to pH. This weak gel is physically reinforced by mixing in a robust polymer gel, agarose. Heparin, a key biomolecule that plays key roles in controlling both cell growth and blood coagulation can then be incorporated, with the two different gel networks each playing different roles in controlling the release of heparin from the overall material. Finally, a self-assembling heparin binder can also be mixed into the materials – this binds strongly to the heparin within the gel and completely prevents its release until the whole material has been broken down.

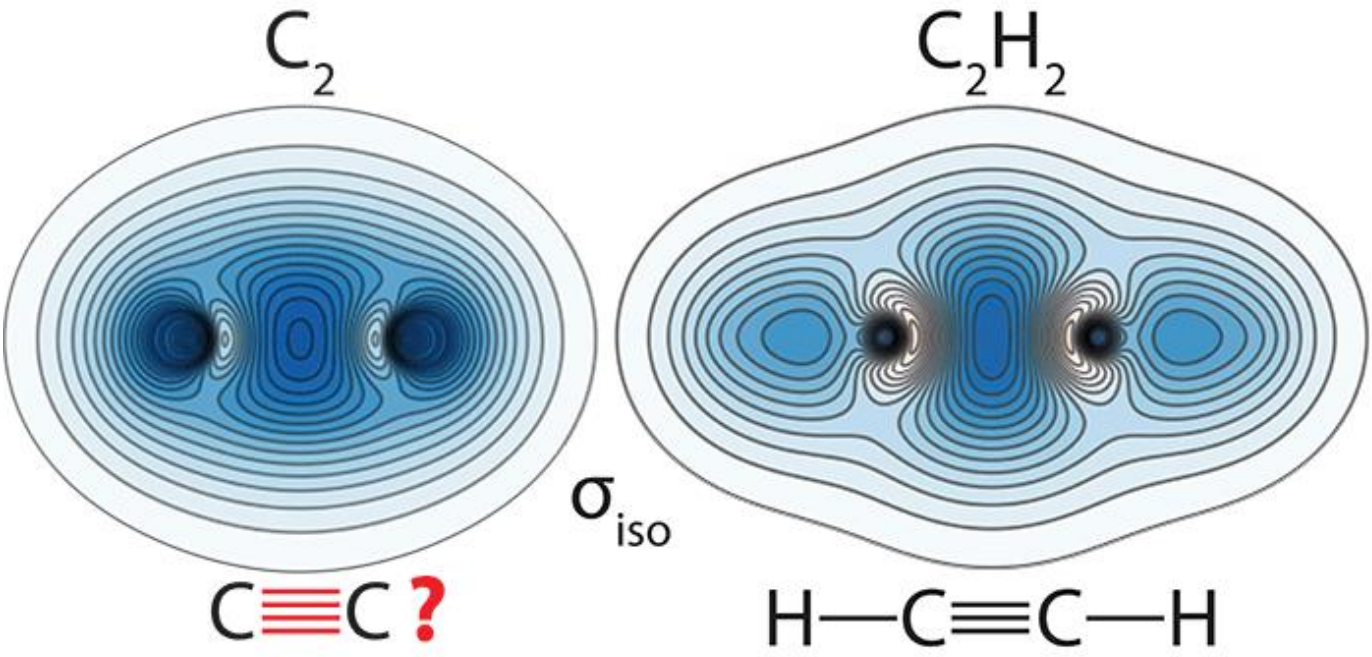
Materials such as these have potential biological applications where controlled release of heparin is desirable. Ultimately, this could lead to systems for slow sustained release of heparin, useful in a hospital setting, where a daily injection of heparin is often required to prevent blood clotting. Alternatively, these materials could be useful as scaffolds for growing cells, where controlled heparin release can help direct tissue growth. Research towards these important applications is currently ongoing in the Smith labs.

Professor Smith said: "Understanding complex self-assembled materials, which contain mixtures of nanoscale systems, is a difficult job. This paper is an important step forwards with multiple functions being programmed into a single material in a simple and rational way."

The researchers are a part of the Molecular Materials research grouping in the Department of Chemistry.

Towards the Quadruple Carbon-Carbon Bond

New theoretical studies support the view that C_2 has partial quadruple bond character.



All chemists are well-acquainted with alkanes, alkenes and alkynes, which have single, double and triple carbon-carbon bonds respectively. But what happens in dicarbon C_2, a molecule which only exists at high temperature in the gas phase? Should the bond be considered as a double bond, a triple bond or perhaps even a unique quadruple bond? This intriguing question has been the subject of much speculation in the field of quantum chemistry.

Recent research from the theoretical chemistry group of Dr Peter B Karadakov uses magnetic shielding studies of C_2 and C_2H_2 to provide new insight into this problem. Off-nucleus shielding calculations indicate that the carbon–carbon bond in C_2 is more shielded than the triple carbon–carbon bond in the alkyne C_2H_2, and, therefore, has higher than triple bond multiplicity.

Intriguingly, however, the authors find the carbon–carbon bond in C_2 is bulkier than in C_2H_2, and, although it has partial quadruple bond character, it is actually weaker than the corresponding triple bond in C_2H_2.

This study makes use of a new approach developed in Karadakov's group based on the analysis of changes in the off-nucleus magnetic shielding tensor within the space surrounding a molecule, which has been shown to reveal more information about chemical bonding than simple variations in electron density.

The paper, 'Magnetic Shielding Studies of C_2 and C_2H_2 Support Higher than Triple Bond Multiplicity in C_2' is published in *Chemistry A European Journal*, where it was selected by reviewers and editors as a Hot Paper.

An App for Applicants

An interdisciplinary team of staff and students from the Departments of Chemistry and Theatre, Film and Television (TFTV) combined their expertise to design and produce the first mobile app to support admissions at in the Department of Chemistry.

The team consisted of Dr Glenn Hurst, Lecturer; Professor Andy Parsons, Admissions Tutor; Katrina Sayer, Undergraduate Student Experience Manager; Dr Jonathan Hook, Lecturer in Interactive Media in TFTV; and Chris Fulford, TFTV undergraduate student.

The work was completed as part of a 10-week summer project in 2016 with the aid of a grant from the Student Internship Bureau.

Chris designed the app for prospective applicants and visitors to the Department of Chemistry, with features including a campus map, promotional videos, news feed, links to resources to aid the school-university transition, employability information, life as a student and details about admission days.

Approximately 250 applicants downloaded the app ahead of their UCAS interview in the Department of Chemistry, with the total number of downloads exceeding 500.

Feedback from applicants has been very positive: “I must thank you for introducing me to the Chemistry@York app, which is a service I haven’t seen any other university employ. It has given me insightful information about York as a university, the students that study with you and the Department of Chemistry.”

This project aligns with the institutional internationalisation strategy by providing an additional technological resource for prospective applicants from both the United Kingdom and overseas - 49% of app downloads are from outside the United Kingdom.

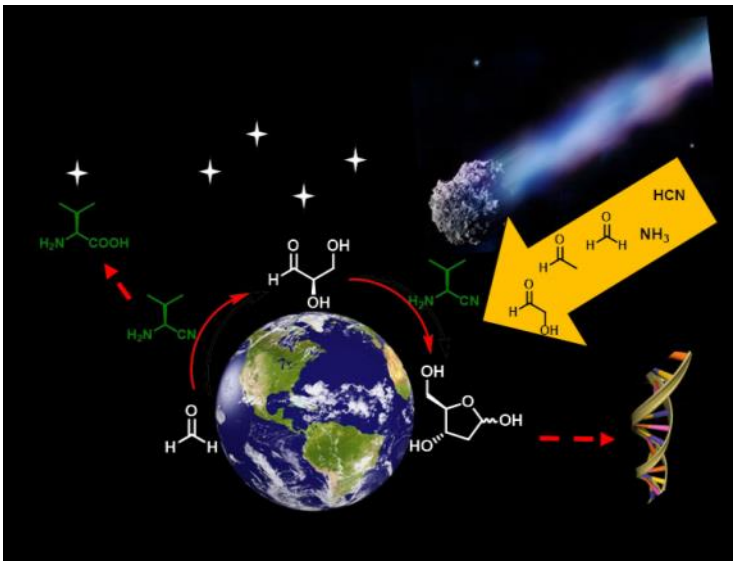
The app has been designed so that the framework can be re-populated with appropriate content, allowing the resource to be easily updated but also making the app translatable for use in other departments within the institution.

Updated Online Department Suggestion Box

The online Equality and Diversity suggestion box has been extended to be a suggestion box for the whole Department. You can submit your thoughts / suggestions / ideas for general Departmental matters as well as matters relating to Equality and Diversity. You can find the new Google form on the intranet homepage or at this link.

Could Interstellar Ice Provide the Answer to Birth of DNA?

Researchers in the Department of Chemistry have shown that molecules brought to earth in meteorite strikes could potentially be converted into the building blocks of DNA.



They found that organic compounds, called amino nitriles, the molecular precursors to amino acids, were able to use molecules present in interstellar ice to trigger the formation of the backbone molecule, 2-deoxy-D-ribose, of DNA.

It has long been assumed that amino acids were present on earth before DNA, and may have been responsible for the formation of one of the building blocks of DNA, but this new research throws fresh doubt on this theory.

Meteor shower

Dr Paul Clarke, from the University of York's Department of Chemistry, said: "The origin of important biological molecules is one of the key fundamental questions in science. The molecules that form the building blocks of DNA had to come from somewhere; either they were present on Earth when it formed or they came from space, hitting earth in a meteor shower.

"Scientists had already shown that there were particular molecules present in space that came to Earth in an ice comet; this made our team at York think about investigating whether they could be used to make one of the building blocks of DNA. If this was possible, then it could mean that a building block of DNA was present before amino acids."

Before life began

In order for cellular life to emerge and then evolve on earth, the fundamental building blocks of life needed to be synthesised from appropriate starting materials – a process sometimes described as 'chemical evolution'.

The research team showed that amino nitriles could have been the catalyst for bringing together the interstellar molecules, formaldehyde, acetaldehyde, glycolaldehyde, before life on Earth began. Combined, these molecules produce carbohydrates, including 2-deoxy-D-ribose, the building blocks of DNA.

DNA is one of the most important molecules in living systems, yet the origin 2-deoxy-D-ribose, before life on earth began, has remained a mystery.

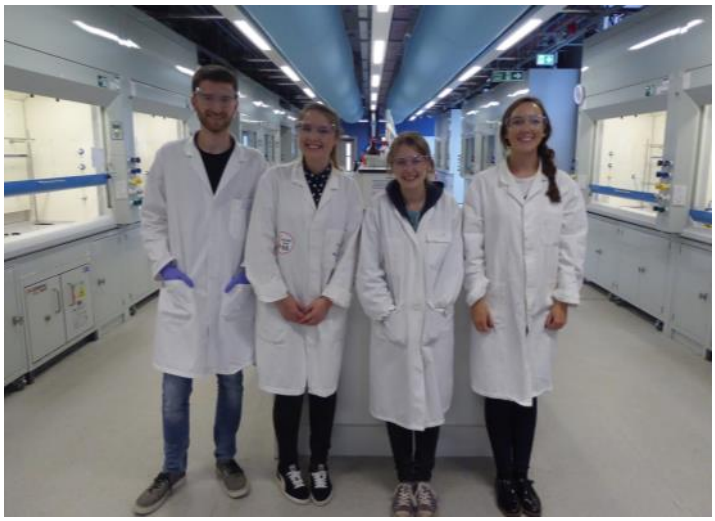
'One-pot'

Dr Clarke said: "We have demonstrated that the interstellar building blocks formaldehyde, acetaldehyde and glycolaldehyde can be converted in 'one-pot' to biologically relevant carbohydrates – the ingredients for life.

"This research therefore outlines a plausible mechanism by which molecules present in interstellar space, brought to earth by meteorite strikes, could potentially be converted into 2-deoxy-D-ribose, a molecule vital for all living systems."

This work is published in *Chem. Comm*. http://dx.doi.org/10.1039/C7CC06083A

Summer Student Development Work in Teaching Laboratories

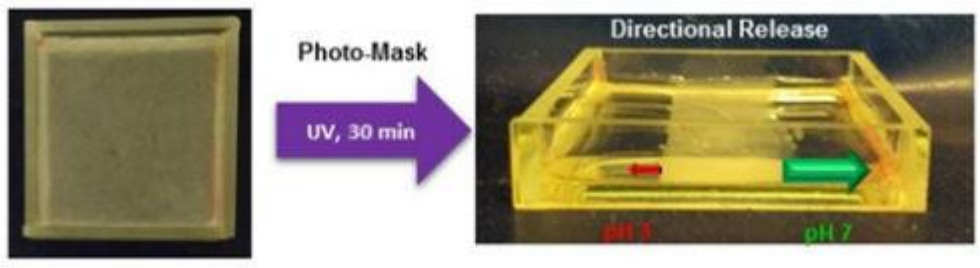


For the first three weeks in August, teaching laboratories hosted four summer students from the second year. The students worked on improving existing and introducing new undergraduate practicals, predominantly for the revised first year laboratory course. From left to right in the picture: Alex Brown worked on improving a number of recrystallisation steps, optimising solvent conditions to find the best conditions for purity and yield. He also worked on expanding the range of 'unknowns' in the determination of phosphate in water experiment and challenging his fellow students to see if they could determine his unknowns (which, thankfully, they could!). Ana Roberts worked on the development of a new two-step reaction to replace a problematic Friedel Crafts reaction (after spending a while seeing if this reaction could be fixed first!). She developed a Horner-Wadsworth-Emmons reaction which is performed in water, followed by a hydrolysis reaction to yield 3-nitrocinnamic acid and developed ⅓ of a metal-AcAc complex formation experiment with aluminium. Katie looked at the copper-AcAc ⅓ of the reaction and worked on the second year Advanced Synthesis course testing a new chromatography experiment developed by Chris Maddocks, which sees students separate 2 and 4 nitrophenols by choosing an appropriate solvent system and isolating both compounds. Abby Coulson worked on the iron ⅓ of the AcAc experiment and looked at other ligand-metal experiments with mixed success, discovering that some publications lack crucial information to allow experiments to be successfully reproduced! Once experiments were developed, the students would swap the experiments around to be tested by the others.

Thanks to the Department for funding these three-week bursaries and we hope the changes are as successful when they run for real as they were in testing.

York Scientists Pioneer New Directional Drug Release Gel

Scientists in the Department of Chemistry have created a new smart gel that can be shaped by UV light and is able to control the direction in which drugs are released.



A drug-loaded gel that has been patterned into a stripe – if different sides of the stripe are exposed to solutions of different pH values, the drug is preferentially released in one direction (credit: Professor David Smith)

Assembled by carefully designed molecules, the goal of such hybrid hydrogels is to only release drugs when brought into contact with a target such as a tumour or inflamed tissue.

In this new innovative approach, chemists created a hybrid gel that combines two properties: a gel that interacts with the drug and controls its release depending on the acidity (pH) of the surrounding environment; and a polymer gel that when formed by light under a mask allows gels of any shape to be created.

Directional manner

Using the anti-inflammatory painkiller drug naproxen, researchers were able to release this drug in a directional manner. This new finding therefore paves the way for smart drug delivery for patients in the future.

David Smith, Professor of Chemistry and leader of the research team, said: “This is an important first step to showing we can make smart hydrogels that release an active agent depending on what they come into contact with.

Medical implications

“Future work will focus on developing systems which respond to a variety of biological stimuli so this directional release can be used to release drugs to important disease targets. For example, this might mean a gel could be tailored to only release a drug directionally towards skin it is brought into contact with.

“Alternatively if a shaped gel was implanted after tumour surgery, such as with brain or breast cancer removal, it could potentially be programmed to release its drug only in the direction of tumour cells, not healthy tissue. If implanted after general surgery, such gels could directionally release a drug into inflamed tissue to help with pain remediation.

"These kinds of targets are what we will approach next. Our simple pH driven system could not do such sophisticated targeting, but this research is the first stepping stone in proving the principle of directional release from shaped gels in response to an appropriate stimulus."

The research was carried out by PhD student Phillip Chivers, funded by the EPSRC, and is published Gold Open Access in *Chemical Science*.

To read, visit: http://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc02210g#!divAbstract

Tobacco-Smoke Residue that Lingers in Furniture, Curtains and House Dust Can Still be Harmful

Dr Jacqueline Hamilton, Reader in the Wolfson Atmospheric Chemistry Laboratories (WACL) has written a piece on the harmful effects of tobacco-smoke residue for The Conversation UK.

Each year about 600,000 people die from exposure to second-hand tobacco smoke (inhaling other people's cigarette smoke). Once the smoke clears, after a cigarette has been extinguished, nicotine and other harmful chemicals left behind can stick to surfaces and fabrics. This residue is known as third-hand smoke.

The idea of third-hand smoke has been around for a few decades, but came to prominence in 2009 after a study by Jonathan Winickoff, an assistant professor of paediatrics at Harvard Medical School, identified a link between parents' belief that third-hand smoke may cause harm and the likelihood they would prohibit smoking within their home.

There is growing evidence that third-hand smoke contamination is extensive and can linger for extended periods. Non-smokers can be exposed to third-hand smoke from breathing residual gases, touching surfaces and swallowing dust. Chemical reactions of nicotine stuck to surfaces can lead to an increase in the amount of carcinogenic chemicals over time.

Read the piece in full at:

https://theconversation.com/tobacco-smoke-residue-that-lingers-in-furniture-curtains-and-house-dust-can-still-be-harmful-84145.

Green Chemists of the World Come to York

Between the 3-6 September, the University of York hosted the 3rd EuChems Green and Sustainable Chemistry Conference (EuGSC3) which attracted ca 120 delegates from as far away as Australia, Japan, China, USA, Brazil and Chile as well as from most European countries. The event was the culmination of two years planning by staff within the Green Chemistry Centre of Excellence (GCCE).

We had been able to attract a stellar line up of plenary speakers to EuGSC3 including: Michael Gratzel (one of the three most highly cited scientists in the world with a h–index of 197), Paul Anastas (one of the founding fathers of green chemistry) and Ben Feringa (joint winner of the 2016 Nobel prize for chemistry). Other plenary speakers included our own James Clark, Nicholas Gathergood (president of the EuChems green and sustainable chemistry division) and Babette Petterson (Chief Business Development Officer at Capricorn Venture Partners) and they were supported by a strong line-up of keynote and offered lectures, including many from within the GCCE. In fact, we had so many offered lectures from the University of York that one whole parallel session was on 'Green Chemistry at York'. In addition, there was a poster session with prizes sponsored by the Royal Society of Chemistry (RSC) and Sairem.

Green and sustainable chemistry is a very broad discipline and this was reflected by the content of the lectures, especially the plenary lectures. James Clark opened the conference by surveying the work currently being carried out on sustainable chemicals production within the GCCE. The following morning, Michael Gratzel focussed on sustainable energy production and later that day, Babette Petterson discussed the commercialisation of sustainable products. The penultimate day started with Nicholas Gathergood discussing toxicology testing on ionic liquids and ended with Paul Anastas giving his RSC green chemistry award lecture and looking to the future, describing his vision of the future challenges for green chemistry. Finally, Ben Feringa discussed his work on catalysis using sustainable metals.

All feedback from delegates indicated that the event was a huge success in terms of the science, opportunity to network, conference venue (Ron Cook Hub), catering and conference dinner at the National Railway Museum.

The conference finished at lunchtime on 6 September, but we were delighted that Ben Feringa agreed to stay on to meet members of the Department of Chemistry in the afternoon and then to deliver a public lecture, 'The art of building small' in the evening. His public lecture attracted an audience of ca 140 and focussed on his Nobel prize winning work on the design and synthesis of molecular motors which can be turned in a single direction (clockwise or anti-clockwise). His work on 21st century molecular motors contrasted well with the 19th and 20th century motors which had featured at the conference dinner the night before at the National Railway Museum.

Overall this was a very enjoyable and productive four days that will have further raised the profile of the GCCE within the green chemistry community. I would like to once again thank everyone with the GCCE who helped to make this conference such a success: the organising committee, the speakers and poster presenters, the student helpers and most of all the admin team who did the bulk of the organising. EuGSC4 will be held in 2019, though the venue has not yet been finalised.

- Professor Michael North

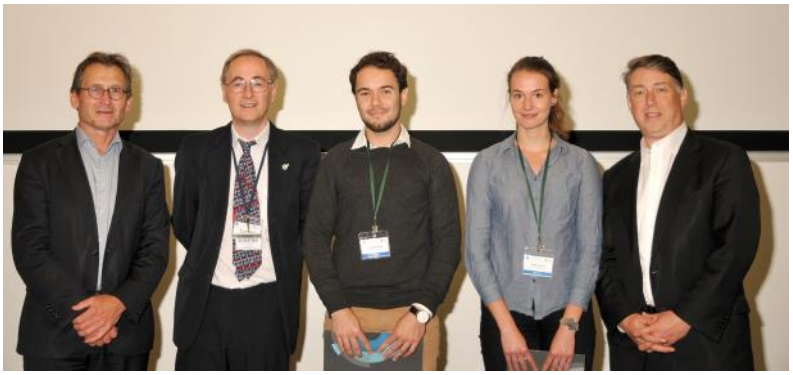
The official conference photograph

Ben Feringa's plenary lecture

Paul Anastas' plenary lecture

The conference dinner

Michael Gratzel's plenary lecture



Two of the poster prize winners along with Ben Feringa (left), Michael North (next along) and Paul Anastas (right)

Iodine in Japan by Professor Duncan Bruce

I suppose I'd never thought too hard about iodine before. Yes, I've taught some of its chemistry; yes, it is a key component of our work on halogen bonding and yes, we have also used hypervalent iodine compounds to oxidise metal centres. And, of course, I have some experience of iodine contrast reagents.

Yet despite all that, it was a little surprising to find that Japan has a Society for Iodine Science (SIS) and that every year it holds a scientific meeting on the subject at Chiba University, not far out of Tokyo. Turns out that Japan and Chile are the world's biggest producers of iodine (ca 90% between them) owing to the huge deposits that exist in Chiba Prefecture, found in the salt solutions (brine) pumped to the surface when recovering the huge reserves of natural gas. These contain 100 ppm of iodine, which is some 2000 times that found naturally in sea water.

So I was invited to take part in the 20th SIS conference – a meeting featuring speakers from Chile, the USA, Germany, Japan and yours truly from the UK. For the first time, the meeting was to have simultaneous translation and so the first job on the day of the meeting was to meet with the translators, to whom we had sent our presentations a week before. None were specialist chemists, but all had great command of English and soon got used to the particular vocabulary associated with the subject. The flip side of this was that the Japanese speakers spoke in their own language and so non-natives were given a headset through which they could hear the translation. It was then that I really appreciated the skill of the translators.

With iodine as the single common thread, the subject matter was particular diverse and the meeting heard accounts of the history of iodine production in Chile where it is found in caliche, a hardened, sedimentary rock mined for its deposits of saltpetre which in this area also contains appreciable amounts of iodine. There were two talks on applications of hypervalent iodine compounds in synthetic organic chemistry, one each on its applications in polymers and in solar cells, and my own presentation on halogen bonding. Then there was a talk on povidone-iodine formulation – an antiseptic used to disinfect the skin before and after surgery and which is used by people in Japan as a tincture, and another on iodine contrast reagents, which are used in medical X-ray imaging. These latter compounds contain a very high percentage of iodine by mass and are injected into the vascular system in very significant quantities where they show up in X-rays and CT scans owing to the interaction of their high electron density with the diagnostic X-rays. It is testament to the chemical design of these compounds that the iodine is chemically inert and that the compounds are excreted very quickly from the body.

After a long day of talks, any good Japanese conference closes with a banquet of beautifully prepared food washed down with copious amounts of beer, wine and sake, during which old acquaintances are renewed and new friendships formed. Truly an excellent day.

Now of course Japan would be a long way to go for a one-day meeting and so it proved possible to organise seminars and research discussions with academics at the University of Tokyo (hosted by Professor Takashi Kato) and Chuo University (hosted by Professor Youichi Ishii who visited Jason Lynam last year) as well as a visit to a former collaborator in Osaka. All was most enjoyable and a

highlight was the trip from Osaka to Tokyo on the Nozomi Shinkansen, which takes 2 h 20 mins to complete the 320-mile trip travelling just short of 190 mph and running to the minute. Now that's train travel.

Some of those at the symposium will be passing through the UK next summer, so watch out for more iodine chemistry here in the not-too-distant future.

Photo left: Duncan with members of Takashi Kato's group outside the famous Red Gate of the University of Tokyo.

York Chemistry Retains 4th Position in The Times University League Table

Chemistry at York has once again been recognised in the 2018 University League Table published by The Times, with the Department retaining its 4th position.

The Times League Table contains scores for 53 chemistry departments across the UK. The table scored departments for teaching quality, student experience, research quality, entry points and graduate prospects.

York achieved an impressive **total score of 94.3** with high scores across all areas, including **89% for student experience** and **88.6% for teaching quality**.

Professor Duncan Bruce, Head of Department said: "It is very gratifying to see the dedication, talent and professionalism of all of the Department's staff recognised in this way, reflecting the high-quality research and teaching that characterises what we do."

This completed a successful hat-trick of **top 4 places** for Chemistry at York in the **3 major University League Tables**, moving up to 2nd place in The Guardian University League Table 2018 and retaining its 4th position in the 2018 Complete University Guide.

Students' Experience of China

For the second year running students from the Department of Chemistry have attended the University Immersion Programme (UIP) at Sichuan University in China. Organised by Dr Alice Fan from the GCCE along with Dr Martin Cockett, seven students were offered the opportunity to attend the programme this year, doubling the number that attended in the summer of 2016.

This unique two-week programme was centred on a specially designed course that brought together faculties from all over the world to give a short lecture series to both domestic and international students. The course offered a number of chemistry-related activities, such as water sample analysis and creative chemistry experiments. However, it was by no means all work and no play. Throughout the course, significant opportunity was given to interact with Chinese students, academic staff, attend field trips and take part in sports activities; giving students profound access to China's beautiful culture, scenery and of course, food. Throughout the programme the students were immersed in a vibrant campus environment that ensured that their study experience was truly unforgettable.

One of this year's attendees, Darius Stankevicius, said: "The first thing that impressed me about the UIP was the hospitality which was shown to us all the way, from arriving at the airport to leaving. The indelible part of the experience was the Chinese student volunteers who became our greatest help in everything from buying ice cream to exchanging money. Nevertheless, the UIP program itself was incredibly stimulating and beneficial to our future careers. We have learnt to collaborate in a multicultural environment through experiments, like water quality analysis or the making of PVA jelly. Also, as part of the UIP programme, we have attended many fascinating lectures about the basis and modern applications of photochemistry given by Professor V. Ramamurthy from University of Miami. Moreover, we were given many university organised tours e.g. to the Jianxi archaeological site, that have allowed us to experience the historic and cultural aspects of Chengdu. Personally, I would say that UIP exchange programme was one of the best times of my life."

Another participant, Alastair Little said "Whilst there, we attended lectures on photochemistry and analysed water samples from local rivers to measure their contaminant levels. We were also given ample time to explore the city. Eager to improve their English, our Chinese classmates were happy to show us around, taking us to restaurants, museums, shopping complexes, markets, karaoke bars and the Chengdu panda reserve. Attending university in a foreign country was an experience I would highly recommend; it was really interesting to discover the similarities and differences between British and Chinese students' lives."

With the continued success of this course, Dr Fan intends to make this a permanent fixture in the

Department of Chemistry's calendar, giving more opportunities for students to experience this once-in-a-lifetime opportunity.

University Teddy Bear is Cover Model

The cover image on the current issue of *ChemComm* was inspired by the Parkin group's review of their recent advances in developing a transformative new technique for bioelectrochemistry.

Since arriving in York five years ago, Dr Alison Parkin and her research team have worked closely with their Australian collaborator, Professor Alan Bond from Monash University to develop his new electrochemistry methodology as a transformative technique for use in bioelectrochemistry; their *ChemComm* review paper details their recent successes.

Inspired by the wonderful wildlife around the University and the description of a classical voltammogram as a "duck", Alison's journal cover artwork was inspired by the idea of the children's fairytale 'The Ugly Duckling'. As shown, her picture captures how her electrochemistry technique has transformed their measurements of bio-electricity into a more complex, "swan-like" response.

This new approach developed by Alison and her team. enables far more sensitive, efficient and insightful measurements of the electron-transfer reactions, which control the biochemistry of life. In this way, turning an ugly duckling into a swan has provided a powerful addition to the toolkit of techniques, which help understand the electronic circuitry of life.

University of York teddy bears are available on campus but Alison makes the periodic table cushion covers herself.

Potatoes to Plastic

Staff from two different areas of the Department have been collaborating to raise the profile of science for primary children in York. CIEC (whose remit is to help children understand the potential of science for their future careers), worked with staff from the GCCE to produce a series of exciting activities, based around extracting starch from potato peel and using it to make bio plastic. The activities were then taken into school by Departmental ambassadors, after receiving training from the CIEC.

Scientists Today

Scientist swaps ski slopes for exciting medical research

Elizabeth Fear

Our scientist this week works in the cutting edge of medical research. She is working on ways to improve the accuracy of Nuclear Magnetic Resonance (NMR) which doctors use to look inside people's bodies. Being able to look in more detail at people's bodies will help doctors to diagnose illness earlier and more accurately. This will mean that life-saving treatments can be offered more quickly. Elizabeth told us how important this can be "The sooner the treatment begins the more likely it is that the patient will make a full recovery" she explained.

Elizabeth has a son who is 6 and a daughter who is 4.

Elizabeth told *Scientists Today* that before she took on her current role as a research scientist she worked for several years as a ski instructor in Italy. She lived there for 16 years and speaks fluent Italian. As energetic as ever she continues to enjoy yoga and walking.

We asked her if she regretted giving up her previous adventurous career. "Absolutely not!" said Elizabeth. "What I do now is very important and it is exciting to be at the forefront of this vital work. I know that what I do now will help to make a difference to people's lives now and in the future".

Scientists Today: Personality Profile

Each week we give our scientist a personality test. This is what we found out about Elizabeth...

Elizabeth is very organised and conscientious and is good at paying attention to the details which can make the difference between success and failure. She likes to help people, and is good at listening to them to find out what their needs are; she is then able to find creative solutions to their problems. She is also good at explaining science to people who are not scientists (from school children to politicians). She works well as a team and can get people to work together effectively.

Prior to the ambassador visit, children read articles from the fictitious publication 'Scientists Today' featuring the ambassadors they would meet. These articles helped to raise expectations and gave children time to formulate questions. Most importantly the articles showed that the ambassadors, despite being scientists, were humans who had much in common with people that the children knew. For example, they enjoyed hobbies such as making Lego models with their children, skiing, football, dancing and cooking!

So far three ambassadors; Andy Maneffa, Jenny Lewis and Liz Fear, have had the opportunity to work on the project with two local schools. The response has been extremely positive and out of 75 children involved, 57 have indicated that they would now consider being a scientist. Comments included:

"…. I found out that science was fun."

"… I learned new things. PS I also liked wearing the goggles and gloves."

"…we got to make plastic and learned what it's like being a scientist."

"…scientists make different things and they talk to each other all around the world."

"… [I learned] how to turn potatoes into plastic so you don't have to make it out of oil."

"… that there were such things as green scientists and waste can be reused."

We would like to make contact with more York primary schools who could benefit from the project so if you have any connections please do put us in touch (ciec@york.ac.uk)!

- Jane Winter, Professional Development Leader, CIEC

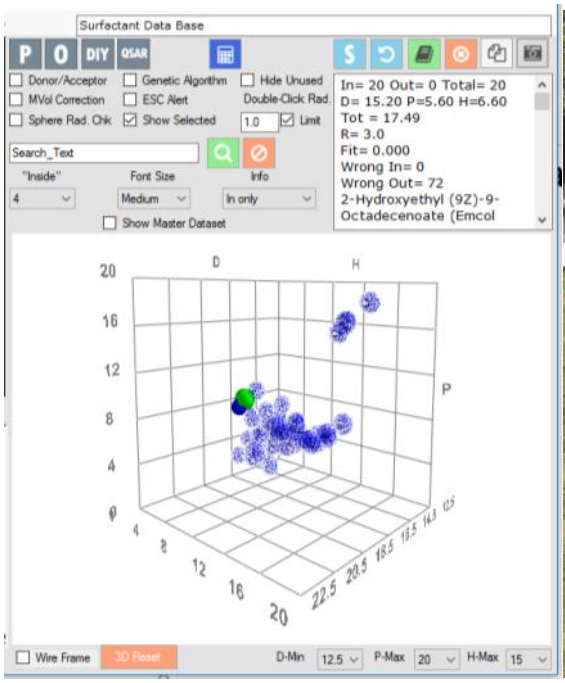
Computational Analysis of Surfactants using both HSPiP and Origin

Katherine Weddell, a third year chemistry undergraduate, has completed her six-week summer internship. Working alongside Dr Rob McElroy and Dr James Sherwood in the Green Chemistry Centre of Excellence (GCCE), Katherine was developing computational methods to analyse surfactants.

Currently, there are very few ways of accurately defining and classifying surfactants due to the complexity of their behaviour. Therefore, there is an obvious need for further research to be carried out in this area, as a breakthrough will prove valuable in both industry and research. The ability to predict the behaviour of novel surfactants will aid the development of safer, high performance products in the future.

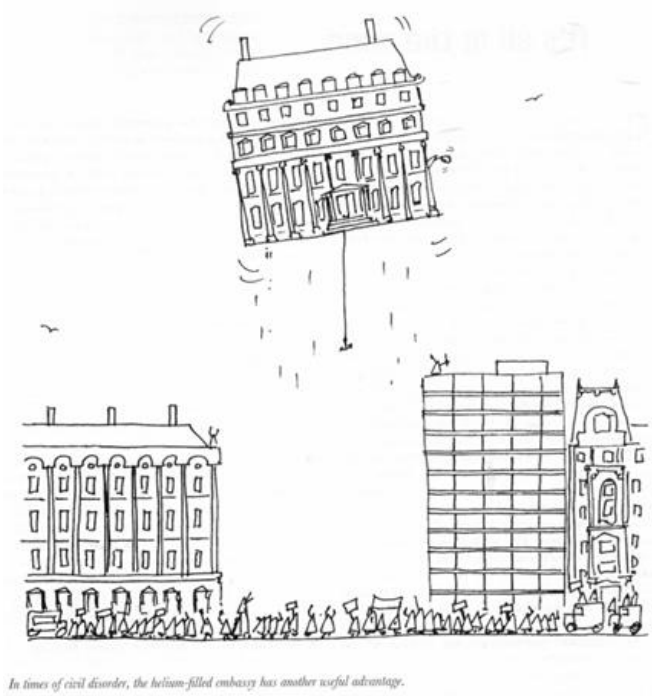
Katherine's summer project was based on the use of software able to predict the physical properties of compounds. The GCCE has a long running collaboration with Professor Steven Abbott, visiting Professor at the School of Mechanical Engineering at the University of Leeds. Using his software package HSPiP, the Hansen solubility parameters and molar volumes of surfactant molecules were calculated. The data generated by HSPiP as well as other characteristic properties of surfactants were then interpreted with a principal component analysis. This successfully classified groups of surfactants with similar properties together.

The aim of this process was to help aid the design and selection of surfactants for certain applications. By defining categories of surfactants based on their applications, the in silico design of new surfactants can be directed towards probable end-uses. At the end of her project, Katherine presented her findings to experts at Croda, who showed an interest in further developing this process.



An Unusual Scientific Mind

Daedalus produced more scientific ideas than anyone else I have ever known. He developed the ideas in his notebook, did some calculations to support his ideas, but did not put them to experimental test, not least because he intended the ideas to have a flaw! Daedalus was the pen-name of David Jones – David also had a fictional company, DREADCO. These ideas were published on the back page of *New Scientist* for many years, and later appeared in *The Guardian* and *Nature*. Just imagine doing this every week from 1964 to 2000. David's ideas often turned out to be possible after all – his greatest triumph was that it should be possible to close graphite sheets to form hollow carbon molecules. He even showed how Euler's theorem defines the number of pentagonal faces - and all this was long before Kroto, Curl and Smalley discovered C60. I first met David in 1970 when he came to a birthday party for his fiancée who was a student living along the corridor from my own girlfriend (later wife). He was then working in ICI's Corporate Laboratory, but he was far too eccentric to fit a place like that. Three years later, he arrived in Newcastle where I was a research student and we got to know one another better. It was then that I introduced him to Martyn Poliakoff and both Martyn and I kept up with David until his death in July of this year, aged 79. Because of this friendship, I was asked to write an obituary for *The Guardian*. That was an interesting experience – I was asked a string of questions by the editor, almost like dealing with the referees for a paper. Martyn and I also wrote letters about him to *Chemistry World* and *Nature*. Last week, we both took part in a film about David recorded for BBC Look North. The film centres on the fake perpetual machines that David built for science museums all over the world. I hope all this sparks enough interest that you investigate more through the links that I have provided.



Above illustration: a cartoon from one of David's books, drawn by the author. The caption reads "In times of civil disorder, the helium-filled embassy has another useful advantage". Reproduced from D. E. H. Jones, The Inventions of Daedalus,© Oxford University Press, 1982

- Robin Perutz

Links to the obituary and letters:

https://www.theguardian.com/science/2017/aug/18/david-jones-obituary
https://www.chemistryworld.com/opinion

http://www.nature.com/nature/journal/v549/n7670/full/549031d.html?WT.ec_id=NATURE20170907&spMailingID=54864391&spUserID=MjA1NzcwMjE4MQS2&spJobID=1244089361&spReportId=MTI0NDA4OTM2MQS2&foxtrotcallback=true

New Starters

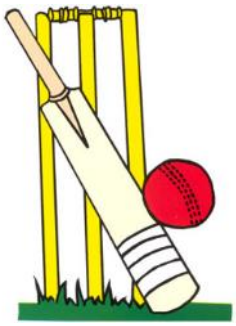
Sue Dunkerley, HR Administrator
Room: C/A121; Extension: 2716; Email: sue.dunkerley@york.ac.uk

Dr Stephen Andrews, returned to the Department as Instrument Engineering Manager in WACL
Room: C/G116, Extension: 4757, Email: stephen.andrews@york.ac.uk

June Forsyth, CIEC Administrator
Room: C/B016, Extension: 2523, Email: june.forsyth@york.ac.uk

Last Departmental Cricket Game of the Summer: Match Report

Monday 14-08-2017. Plongé 74 - 5 (16 overs). Chemistry 76 - 5 (14.1)



The nights are drawing in, so despite a punctual 5.45pm start and two full sides it was decided to play a 16 over game to avoid finishing in the gloom. 4 overs each for 4 bowlers, batsmen to retire on 30. For once Chemistry had Burns, Downes, Wade, Roy and Lynam all available. The final game of the 2017 season with Chemistry not having tasted victory since 30 July 2015, 12 matches and 24 months ago. Plongé chose to bat first. The new opening pair of Thornton and Jones looked worryingly experienced but Jones was LBW to Downes for 0 and in the first 8 overs against Downes (1-19) and Wade (1-19)and they struggled to score at more than 5 an over. Thornton was nicely caught by Lynam for 25 and Plongé were 43-2. Shan (16), Maltravers (10) and Newbold (9) were a sluggish middle order against Burns (1-14) and Roy (0-6) with the last 5 overs producing 17 runs. Plongé closed on 74 - 5 after 16 overs.

In reply, for the final game of the season, and their best chance of actually winning a game, the captain Tom Downes sent out his 'big guns' at the top of the order. Wade went in the 1st over for 1 but first Lynam and then, after Downes had gone for 11, Burns at no. 4, ensured the score kept ticking at 5 an over. Shan (2-12) and Nouman (0-16) meant just 33 off the first 8 but Thornton was expensive at 20 off 2 overs and Newbold (1-16) couldn't slow things down so with 4 overs to go Chemistry were 67 - 2. Adil created some last minute nerves with 2 - 2 off his first over with Burns (26 off just 18 balls) falling to an impossible catch from Newbold, Roy clean bowled for 0 and Murphy bowled by Newbold but Lynam (23 n.o.) and Lodi saw the chemists home in 14.1 overs. 11 balls to spare. A somewhat exuberant celebration from the boundary was surely understandable after two years of little to cheer about? 2018 is The 35th year of the Staff League. We can but hope.

- Dave Lindsey

Green Impact

Departmental Showers for Staff / Postgraduate Students

To all staff cyclists and pedestrians who travel to work by bike and on foot...

We have Departmental showers in D Block located in the disabled toilets on the ground, first and second floors.

We also have a shower on the ground floor of D block (D016A) located by the E014 labs / lifts (just beyond the wet labs).

Further showers are located in the WACL building (both ground and first floor) and the CHyM building (inside the main entrance, next to the disabled toilet, i.e. before you need Kaba access to get through into CHyM).

When using the showers, it would be really helpful if you could be careful not to leave water on the floor - if so, please mop up.

Discounted Bus Tickets!

Discount bus tickets – can use this for all First services in York (including Park and Ride!)

Students – travel on the 66 bus for only £200 for 12 months!

Staff – travel on the 66 bus for only £250 for 12 months!

https://www.firstgroup.com/york/more/your-bus-66-and-university-services/buy-tickets

Cycletowork Extra

https://www.york.ac.uk/admin/hr/employee-benefits/travel/cyclescheme/

You are able to make big savings on the cost of new bikes and related safety and security equipment under a Government initiative (Green Transport Plan) aimed at getting more people to travel to work on their bikes. The University of York has linked with a partner company, 'Cyclescheme', who provide cycle purchase vouchers that are accepted by a wide range of bike retailers. The University offers a scheme, Cycletowork Extra, whereby you can order a Cyclescheme voucher to purchase a bike and additional safety equipment, worth up to £1,000 in total, through a salary exchange agreement with the University over a 12 month period.

Bike Doctor Services and Registration

Bring along your bike to the regular free Bike Doctor services that take place between 10am—2pm on the below dates:

Thursday 19 October 2017	outside Vanbrugh
Thursday 16 November 2017	outside the Ron Cooke Hub
Thursday 14 December 2017	inside Your Space

Nearest Chemistry Cycle Storage

There is cycle storage by B block car park outside workshops and there is also additional storage next to the WACL building.

For other cycle storage areas on campus, see:

https://www.york.ac.uk/staff/travel/cycling-walking/ (new link)

New Arrivals

Lisa and Richard Douthwaite are delighted to announce the arrival of Jack Samuel, weighing in at 3.8 kg (8 lb 8 ox in old money!). All are doing well.

Laura and Nick Wood are delighted to announce the arrival of baby Christopher Jonathan (pictured with Rebecca and Alex). Mother and baby are both doing really well. Father is very tired.