Chemistry Update

Newsletter 351, 27 January 2023

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Calendar of Events

Research Seminar
Speaker: Dr Julia Westermayr, Universitat Leipzig
Date: Wednesday 8 February
Time: 1pm—2pm
Location: Virtual (Zoom)

UCAS Visit Days
Dates: 9, 14, 20 & 28 February
Time: 12pm—4pm

LGBTQ+ History Month event
Date: Friday 10 February
Time: 12.30pm—2pm
Location: C/B/102

ProteinTech Tabletop Exhibition
Date: Monday 13 February
Time: 10am—3pm
Location: Chemistry A block foyer

Research Seminar
Speaker: Professor Stuart James, QUB
Date: Monday 13 February
Time: 12pm—1pm
Location: C/A/101

Research Seminar
Speaker: Dr Adrian Chaplin, University of Warwick
Date: Wednesday 22 February
Time: 1pm—2pm
Location: C/A/101

Manchester Organics Tabletop Exhibition
Date: Tuesday 28 February
Time: 9am—5pm
Location: Chemistry A block foyer

Date of Next Issue:
24 February 2023

New study shows ‘self-cleaning’ of marine atmosphere

Scientists have shed new light on the ‘self-cleaning’ capacity of the atmosphere.

The team led extensive aircraft and ground-based observations in and around Cape Verde

This process of self-cleaning is essential to remove gaseous pollutants and regulate greenhouse gases such as methane from the atmosphere.

Researchers were already aware that the atmosphere had this ‘self-cleaning’ ability, but in a new study from the University York, experts have now shown a new process that increases the ability of the marine atmosphere to self-cleanse.

Using a combination of aircraft and ground-based observations, scientists were able to confirm the widespread presence of nitrous oxide in the remote Atlantic troposphere formed by so-called “renoxification”, whereby photolysis of aerosol nitrate returns nitrogen oxides (NOx) and HONO to the marine atmosphere.

Global scale

Scientists say the findings, published in *Sciences Advances*, could be highly significant for atmospheric chemistry and largely reconcile widespread uncertainty on the importance of renoxification.

With funding from the Natural Environmental Research Council (NERC), scientists from the Wolfson Atmospheric Chemistry Laboratories (WACL) led extensive aircraft and ground-based observations in and around Cape Verde in August 2019 and February 2020.

Recycling

Lead author, Professor Lucy Carpenter said: “Importantly, the observations showed that the efficiency of renoxification increased with relative humidity and decreased with the concentration of nitrate.

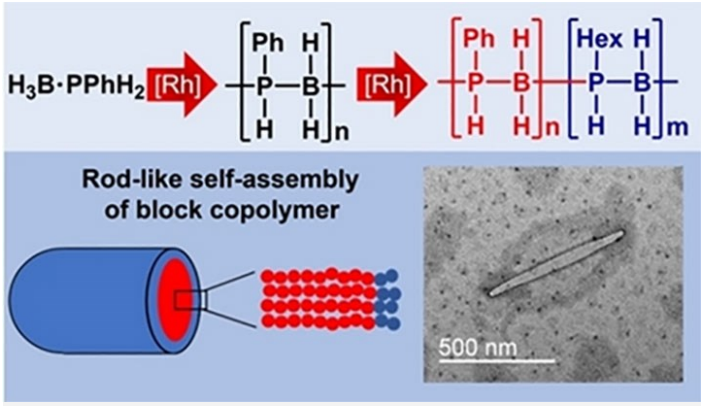
“This observation reconciled the very large discrepancies in the rates of renoxification found across multiple laboratory and field studies.

“It was also consistent with renoxification occurring on the surface of aerosols, rather than within their bulk, a new and exciting finding with implications for how this fundamental process is controlled and parameterised in models.”

Recycling of nitrogen oxides on nitrate aerosol could have important, increasing, and as yet unexplored implications for the trends and distributions of atmospheric oxidants such as tropospheric ozone, an important greenhouse gas.

New main-group polymers self-assemble into nanostructured materials

Novel catalytic methods developed in York have provided synthetic access to main-group based block co-polymers for the first time, which self-assemble into nanostructured materials.



Block-copolymer synthesised using rhodium catalyst, (Bottom) Scheme of the assembly of the block copolymer into a rod-like nanostructure

Polyphosphinoborane polymers with P–B bonds in their chains based on main-group elements, are chemically-related to technologically ubiquitous carbon-based polymers with C-C bonds (such as polyolefins). As well as being fundamentally interesting as a new class of polymer, polyphosphinoboranes could be used as flame retardants, precursors to high performance ceramics and etch resists in nanolithography.

An important class of polymer are block co-polymers – in which two different types of polymer chain are joined to give a new polymer, which has unique properties. Such polymers often self-assemble in solution to form nano-sized objects which may have many applications in energy research, catalysis, biology and separation science. However, until now, block co-polymers of polyphosphinoboranes could not be made.

Research led by PhD student James Race, who worked within the Weller Research Group in collaboration with Canadian researcher Ian Manners at the University of Victoria has found a solution to this problem. By developing a new rhodium-based catalyst system for the synthesis of polyphosphinoboranes, and performing detailed mechanistic studies into how the catalyst operates, the team were able to design the synthesis of a polyphosphinoborane block co-polymer, which has more hydrophilic phenyl groups at one end and more hydrophobic hexyl groups at the other. By dissolving these polymers in a solvent mixture of THF/hexane the polymers self-assembled to form nanoscale rods or spheres, where the hydrophobic hexyl groups sit on the outside, and the hydrophilic phenyl groups on the inside.

This work therefore opens up new routes to both the synthesis of main group block co-polymers and their application in assembling nanosized objects.

Reflecting on the next steps, Professor Weller said: “This work shows the possible, future, exciting applications for main-group polymers and nanomaterials made through atom efficient catalytic routes.

"Really pleasingly it was an idea that was initiated by James as a PhD student, and then brought to fruition by his research visit to Ian Manners’ labs in Canada. This shows how collaboration and PhD mobility in projects is so important. ”

James Race is now a PDRA with Martin Albrecht at the University of Bern.

The research was published as Hot Paper in *Angew. Chem. Int. Ed*.

Brian Sutcliffe (1936-2022) – From the picket line to Jupiter's aurora

An appreciation assembled by Robin Perutz (Jan 2023)

Brian and his second wife, Sylvia

Brian Sutcliffe, one of the great characters of the University, started as a lecturer in the Department of Chemistry at its outset in 1965 and stayed until his retirement in 1998. Knowledge poured off Brian like a waterfall, not just his own quantum chemistry, but political history, history of science, poetry and music. This wasn't show, it was just there. He was equally modest about his scientific achievements. He was totally committed to the students and to his colleagues. He stood up for the principles of high-quality teaching against the pressures to take more students. As rep for the Association of University Teachers, he was a thorn in the side of the University high-ups, but was nevertheless totally devoted to the success of the University. His views were expressed bluntly and to the point - Board of Studies meetings have never been the same since he retired. He educated and entertained us all - I recall a captivating double-act lecture with Brian and Jim Matthew (Physics) expounding about Schrödinger's Cat to a packed lecture theatre. I used to look forward to the days when Brian popped his head round the door – you could be sure that a fascinating conversation would ensue. If I challenged his political views, well to the left of my own more centrist ones, I knew I would be up against his encyclopaedic knowledge. Like others who have written to me about Brian, I miss him immensely.

Every chemist is familiar with the bent structure of the water molecule, but Brian's research showed that water becomes linear and quite floppy at high temperatures! It was discoveries like this that led Brian, in the last phase of his work, to seek the limits of conventional ideas of molecular structure and the chemical bond, an endeavour that took him into history and philosophy as well as chemistry. Another molecule that turned out to be floppy at high temperatures was H_3^+, the simplest 3-centre 2-electron molecule. The predictions of its vibration-rotation spectra by Brian and Jonathan Tennyson were picked up by scientists studying the aurora of Jupiter using images from the space and land-based telescopes. They were used to show that the aurora was far hotter than previously thought, as hot as 1000 K. Since then, these infrared emission spectra have become the thermometer for variations in the aurora in time and space. These were results from the 1980s and 1990s, when Brian developed methods of studying how the potential energy varied with structure under conditions varying from very cold to very hot. In earlier phases of his work, Brian concentrated on electronic structure of very simple molecules. Even a cursory reading of Brian's papers demonstrates the high level of the mathematics and the determination to predict and simulate spectra with high precision. His work saw him all the way from very primitive to modern supercomputers. To begin with, he would write the computer code and do the mathematics, but later he concentrated on the mathematics and left his collaborators to write the code. Brian continued publishing throughout his "retirement"; the last was a book chapter published in January

2022, entitled “Is chemistry really founded in quantum mechanics?”. As can be seen from the comments from his collaborators, he has left a band of people enthusiastic to push the limits of theoretical predictions.

Brian and his first wife, Eileen

As a child in WWII, Brian was evacuated from Croydon to Preston, but he returned to grammar school in Croydon. An undergraduate degree in physics and chemistry at the University of Keele was followed by a PhD and later a research fellowship, also at Keele. His PhD was supervised by Roy McWeeny, who he admired immensely. Between his PhD and returning to Keele as a researcher, he was a Fulbright Fellow at MIT under JC Slater (of Slater orbital fame) and JW Moskowitz at New York University. It was at Keele that he met his first wife, Eileen, who became a statistician in the Centre for Health Economics. The photo shows them both at MIT.

Brian at his 70th birthday party with his daughter Caroline and Richard Crossley (Maths)

David Waddington recalls meeting Brian in 1965 between his appointment and taking up his position in York. The meeting to discuss computer equipment for the infant department and University took place at a service station on the M6 near Keele. Brian came by bike entering the service station by a back entrance, David arrived in a dilapidated Mini. Later Brian championed computer facilities in the University and became one of the founders of the national Collaborative Computational Project (CCP1) that enabled high-level computing and sharing of programmes for quantum chemistry. In York, he somehow found time for science, popular lectures, the AUT, undergraduate teaching of maths and theory, Langwith Senior Common Room, as well as high-level university committees. His motto for teaching maths was unconventional: "You don't need to understand it. Just do it"! His influence on the development of quantum chemistry can be gauged from his visiting professorships in Denmark, the Netherlands, USA, Japan, Hungary, Germany, Mexico and Belgium. He became a foreign fellow of the Royal Danish Academy of Sciences and Letters in 1992. After Eileen’s premature death in 1992, Brian renewed his friendship with Sylvia Winstanley who had been the first Departmental Secretary (in old terminology) but then lived in Brussels. After his retirement in 1998, Brian married Sylvia, moved to be with her and continued his science from the Université Libre de Bruxelles.

From his research students and collaborators:

Hazel Cox (maths undergraduate, D Phil supervised by Brian, now Professor of Theoretical and Computational Quantum Chemistry, University of Sussex): Brian has been such a great mentor, friend and inspiration to me for over three decades, I can’t believe he’s gone. He agreed to “take me on” as his PhD student, after my maths PhD supervisor decided to retire, despite my non-chemical background. He taught me so much, not just about theoretical chemistry but also how to be an academic, University politics, and standing up for what you feel is right. He also tried to educate me regarding opera but on that account, he was less successful! Our work together formed the foundation of my passion for quantum chemistry. As a PhD student, if I had a question, he would get out a big sheet of

paper and write “The thoughts of Chairman Sutcliffe” and proceed to derive the answer. His deep understanding of the mathematics behind the chemistry, and his willingness to share his knowledge, has helped me enormously, and that support has been unwavering for the last three decades. His continuous interest in my academic career and his invaluable advice has defined my professional life. He was so clever and knowledgeable, and yet with his slightly eccentric, quirky ways and formidable breadth of knowledge on so many subjects, he was also captivating company. At tea breaks he would tell crazy tales of wild ventures, engaging us all. Brian was a charismatic, out-spoken, brilliant scientist and mentor, kind and generous with his expertise and time.

Jonathan Tennyson (collaborator in the 1980s and 90s, Professor of Physics, UCL): Brian was very much my mentor as a young scientist. I met him as a postdoc in Nijmegen where he held a visiting Professorship for the first part of my stay. Brian gave a lecture there entitled “Sex and the single electron” - he attracted a huge audience and had everyone in stitches, but his host disapproved of such a flippant title. He taught me a vast amount, much more than my PhD advisor. He inducted me into a whole new area of science upon which I have built my career. His deep understanding of the problems we worked on was fundamental to our work together and widely underappreciated. My work with Brian, which was intense for a decade and lasted until his retirement, has completely underpinned my career. For example, I run a major ERC-funded project which is built entirely on codes I developed in collaboration with Brian. At the same time, he was good friend. Happy and selfless in his advice and encouragement. Endlessly amusing: you would tell him a story and hear it from his lips sometime later altogether better told and wittier. I will never meet his like again.

Michael Chiu (Chemistry undergraduate 1965-68, DPhil 1968-1971 supervised by Brian and Bruce Gilbert, later worked at Atlas Lab): I was very taken with the idea that one could predict the properties of atoms and molecules from pure mathematics, so Brian's lectures held a fascination for me. Also appealing to me was the fact that he spiced his lectures with Latin epithets and quotes from English literature. If challenged, he was always able to name his sources precisely. As Brian's first graduate supervisee from York, I shared a large office with another graduate and a £1000 Hewlett Packard programmable calculator. When I asked Brian about his own research as a doctoral student, he told me that he had carried out his calculations on a Whirlwind computer with 24-bits of memory.

Attila Császár (Professor of theoretical chemistry, Eötvös University, Budapest, Hungary): In the second half of the 2000s, Brian and Sylvia spent time in Budapest supported by the Szent-Györgyi Professorial Fellowship. Later they came "just" to enjoy science as well as life and the music scene. Having Brian around was a blessing for our research group. While this was a scientifically rewarding time, for Brian and Sylvia these trips also meant regular visits to the local markets, museums, attending concerts almost daily, and even a dancing school. Brian also learned a little bit of Hungarian and could even recite poems by a famous Hungarian poet, Sándor Petőfi.

From Colleagues in the University:

Rod Hubbard: We had one tutorial with Brian in the third year because our tutor was absent, when the topic was supposed to be Statistical Thermodynamics. He asked us instead to research and write an essay titled "What is chemistry?", which he initiated with a wide-ranging discussion on the history of science a couple of weeks ahead, challenging us then to read and think for ourselves. It was the most memorable educational experience of my undergraduate days, the closest to what my younger, idealistic self had imagined for university experience.

Caroline Myers: His occasional visits to our office were always a joy. He was a fine example of how to make the most of life. I once asked him how he found the energy to be up and doing all the time… his reply was, "Well, you're a long time dead!"

James Clark: Brian was an intellectual giant. As a new academic, I lived close to Brian and Eileen in Acomb and they sometimes gave me a lift to the university. I remember sitting in the back of their car often overwhelmed by whatever the day's discussion topic was - politics, current affairs, academia… though not sport! After he retired from York, he often came to see me on his visits from Brussels and wanted to know about and encourage my research.

Martin Cockett: Brian was a huge character and played a large part in my own integration into the department as a young lecturer. He always went out of his way to pop his head into my office to say hello on his visits from Brussels and shoot the breeze.

Paul Walton: As a new academic staff member, I sat-in and managed to survive his graduate group theory course despite being the only person in the class. He delivered this course with such gusto that it was as if there were several hundred people in the room. Dan and I once bumped into him at York Theatre Royal. Before the play, we had coffee together where he proceeded to tell Dan (eight or so I think) that "his father had written a very good book on group theory". Dan was nonplussed; I was as pleased as punch.

Tony Sudbery: (Mathematics) When I came to York, theoretical research in quantum mechanics was spread across the departments of Chemistry, Physics and Maths, with one practitioner in each: Brian Sutcliffe, Jim Matthew and Richard Crossley, forming a coherent cross-departmental research group. It is sad to see the departure of the last of that group. Brian and Jim formed a classic double act, delivering wonderfully entertaining and informative public lectures. Brian's interests went well beyond the confines of quantum chemistry; he had a wide knowledge of philosophy, and I remember deep and extensive discussions on the philosophy of quantum theory.

Bill Trythall: (History and AUT) Through the 1970s and 1990s, Brian Sutcliffe was the heart, soul and conscience of the York Association of University Teachers. He participated fully in local collective bargaining, but his greater contribution was his practical commitment to make AUT work in detail. For example, he patiently listened to and skilfully advocated for members in trouble, reassuring them but curbing their self-destructive inclinations; also vitally in the pre-email world, he filled and labelled envelopes with newsletters etc. All this with warmth and humour – and with no thought of self-promotion but because he saw it as the right thing to make space for in his professional career.

Nigel Lowe: Back in the time when the University Library had a little room dedicated to the various daily papers, Brian was in there reading one of them, with his arm hovering over a copy of *The Times*. A student enquired rather politely whether Brian had finished with it, only to be informed, albeit cheerily, that he had never had any intention of consulting 'that disgusting rag'!

Bruce Gilbert: My first and lasting impression of Brian was formed on meeting him with the very small group of academics early in 1965 to design the Chemistry course. Then, as ever, he showed a brilliant mind, incredibly wide knowledge, deep interest in teaching and learning, and an awesome background in Maths and Quantum chemistry. I'd never met a polymath before, let alone worked with one, and here there were two (with John Garratt). He was a particularly enthusiastic collaborator in his teaching and research, rapidly raising the breadth and depth of my knowledge. Research students, as well as staff, soon learned from Brian how to use computers to perform the Hückel molecular orbital calculations and

even simulate spectra. More than 30 years later, I spoke at his retirement party and finished my speech with the following quote from Oliver Goldsmith's The Deserted Village. To my delight Brian soon joined in:

In arguing too, the parson owned his skill,
For even tho' vanquished, he could argue still;
While words of learned length and thundering sound,
Amazed the gazing rustics ranged around;
And still they gazed, and still the wonder grew,
That one small head could carry all he knew.

I would like to thank all the contributors, Brian's son and daughter Edmund and Caroline for the photos, and especially Hazel Cox, Jonathan Tennyson and Edit Matyus for their help with the science.

Save the Date: LGBTQ+ History Month event

Friday 10 February, 12:30-14:00, C/B/102

To mark LGBTQ+ History Month, the Chemistry Equality and Diversity Group will be screening an archive recording of the amazing Equality Diversity and Inclusion lecture given by Nobel laureate Prof Carolyn Bertozzi of Stanford University.

Prof. Carolyn Bertozzi is the Anne T and Robert M Bass Professor of Chemistry at Stanford University, an Investigator at the Howard Hughes Medical Institute, and Co-Director of Stanford ChEM-H. She was jointly awarded the Nobel Prize for Chemistry in 2022 for the development of Click chemistry and bioorthogonal chemistry. She has strong ties with the department - in 2020 she was made an Honorary Graduate of the Faculty of Sciences and visited the department in 2018 to give a keynote and public lecture at a celebration to mark 10 years of Chemistry Athena SWAN Gold.

In her fantastic Beacon public lecture "The long game of STEM diversification", Professor Bertozzi talks powerfully about her own life and career experiences including what it means to be a gay woman in Chemistry in the US. It is just as moving and relevant today (if not more so). There will be an opportunity to talk about some of the issues raised and some refreshments - feel free to bring your lunch and a mug.

Free hybrid event: Integrating green chemistry into higher education day

Friday 7 July 2023, 10am—4pm, GCCE, Department of Chemistry

This FREE event will explore strategies for integrating green chemistry into higher education curricula so that we may prepare the next generation of scientists, engineers, and policymakers to tackle grand challenges of sustainability through chemistry. This event is aimed at chemistry educators that are new to green chemistry through to those that are leaders in the field. Register for the event via this link.

Returning equipment for repair outside the UK

Advice from Stores/Procurement:

If you are sending goods abroad **for repair** then the shipping agent/courier handling the goods should be made aware of this so when the goods are being returned to the UK they know to declare them under Outward Processing Relief (OPR).

This relief allows goods to return to the UK after processing or repair without duty/VAT being paid on them. The shipping agent is responsible for making this declaration on your behalf so you should communicate with them to see what information they require of you, as each agent may ask for different pieces of information for their own records.

In the first instance, please contact the University Mailroom for more information.

Introduction to Intellectual Property & Commercialisation Support Available

There is a very well received short 30-minute training course being provided by the University's commercialisation department called "Introduction to Intellectual Property & Commercialisation Support Available" that may be of interest to you.

The next sessions are on:

- Wed 15 Feb 13:00 till 13:30
- Wed 22 Mar 13:00 till 13:30

The session blurb: A brief overview of what intellectual property (IP) is and how it can support research impact. You will learn how to identify potentially valuable IP and how the commercialisation team can support you.

Book your place onto this quick 30-minute course and see how the commercialisation team can help support you.

It runs monthly with the next session running on Wed 15 Feb; the link can be found here to sign up.

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 Google form at this link.