Chemistry Update

Newsletter 325, 28 September 2020

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Calendar of Events

Chemistry Forum: Angewandte Chemie Editorial Policy and Gender Bias in Academic Publishing
Date: Thursday 1 October
Time: 2pm—3pm
Location: Virtual

KMS Winners' Seminar - Chair Dr Aneurin Kennerley
Winning speakers are Yr 3 PhD students:
Lucy Wheeler (KP), Ben Tickner (SBD), Natalie Wong (CED/MCRC), Anna Patterson (DKS)
Date: Wednesday 7 October
Time: 1pm—3pm
Location: Virtual

Complexity and Chemistry Content when Teaching in Interesting Times
Speaker: Prof Thomas Holme, Iowa State University
Date: Wednesday 14 October
Time: 2pm—3pm
Location: Virtual

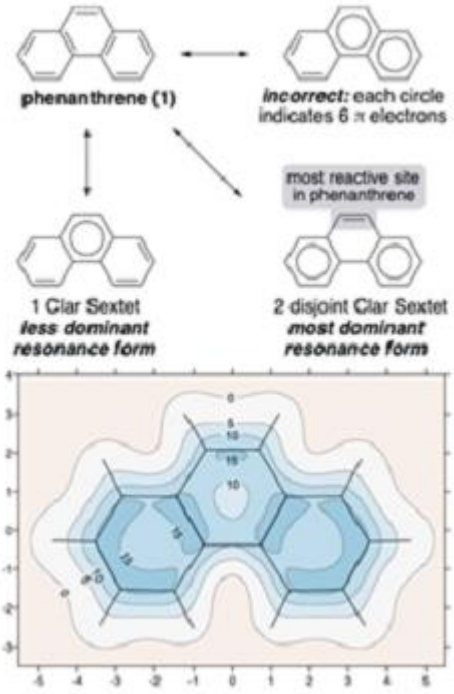
Organic Seminar
Speakers: Carmen Piras (University of York), James Firth (University of York), Ed Griffen (MedChemica)
Date: Wednesday 21 October
Time: 1pm—2.30pm
Location: Virtual

Physchem Seminar - Chair Dr Aneurin Kennerley
Speakers TBC
Date: Wednesday 28 October
Time: 12pm—3pm
Location: Virtual

Date of Next Issue:
30 October 2020

Enhancing the visualisation of aromatic molecules

A computational method developed in York provides an easy way of visualising the aromaticity of important polycyclic aromatic hydrocarbon molecules and gives new insights into their bonding.



(Top) Structure of phenanthrene drawn in the traditional way showing Clar sextets both correctly and incorrectly. (Bottom) The magnetic shielding map provides an intuitive way to understand aromaticity – in this case phenanthrene is shown and the darker blue indicates greater aromaticity, indicating that the terminal rings are more aromatic than the central one.

Dr Peter Karadakov from the Department of Chemistry here in York, working with Professor Brett VanVeller and Bryan Lampkin from Iowa State University in the USA have developed a method to create a better visualisation of aromaticity in polycyclic systems.

Aromaticity is a fuzzy concept, with the International Union of Pure and Applied Chemistry (IUPAC) defining an aromatic molecule as one that has '[a chemistry typified by benzene]' – a definition that's not particularly helpful when it comes to identifying aromaticity. Chemists often use simple qualitative rules such as Hückel's (4n + 2) electron-counting rule.

However, for polycyclic aromatic hydrocarbons (PAHs) such as phenanthrene which have multiple fused rings it's not sufficient to know whether the molecule is overall aromatic – the individual rings have varying degrees of aromatic character. Understanding the bonding and behaviour of PAHs is of great significance in part because they are environmental pollutants but also because they are abundant in the universe and it has been suggested they may have played a critical role in the origins of life.

Clar's sextet rule states that a molecule's dominant resonance structure is the one with the largest number of disjointed aromatic π-electron sextets. Clar sextets can be depicted by a circle drawn inside a benzene hexagon. Yet there's still a lot of confusion around Clar's rule, with many people simply incorrectly drawing a circle in all of the rings with any aromatic character.

In order to better visualise aromaticity in polycyclic systems the researchers created isotropic magnetic shielding (IMS) plots, which provide an intuitive picture of aromaticity – both overall and local. "Pictures are remarkably powerful - as soon as you see them, you can immediately start interpreting them" says Dr Karadakov. In phenanthrene for example the picture clearly shows that the terminal rings are darker in colour, therefore more aromatic, than the central ring – as is predicted by Clar's sextet rule.

On their new visualisation technique, Professor VanVeller explains: "We can replicate Clar's rule when it is accurate, but importantly, we can go beyond it when it's inaccurate." For example the molecule coronene cannot be drawn with a single static representation that encompasses all of its resonance forms, but the new contour plots showed immediately that all of coronene's outer rings are equally aromatic.

Isotropic magnetic shielding - the method used by the researchers to create the plots - is essentially the same magnetic shielding that influences chemical shift in nuclear magnetic resonance spectroscopy. But

while NMR shifts are centred around an atom, IMS indicates what's happening between atoms, and hence provides insight into the bonding in such molecules. "The only drawback is that to obtain all this information, we need to do a lot of computational work" says Dr Karadakov.

Dr Karadakov and his co-workers are now developing a tutorial so other chemists can create their own aromaticity maps and hope that such plots may in the future enhance the intuitive understanding of these important molecules, find their way into textbooks and hopefully help avoid future aromaticity drawing disasters.

The research is published in *Angewandte Chemie*.

We're 6th in the UK

Chemistry at York in the top ten in the Times and Sunday Times Good University Guide.

THE TIMES
THE SUNDAY TIMES
Good University Guide 2021

The Department of Chemistry has once again been named one of the UK's most highly regarded departments for our subject. We are ranked 6th in the UK in the Times and Sunday Times Good University Guide 2021.

Published annually, the Times University Guide ranks 131 UK universities by undergraduate degree subjects according to teaching quality; student experience; research quality; entry standards; graduate prospects; Firsts and 2:1 degrees; completion rates; student-staff ratio; and spend on academic services and student facilities.

The rankings are based on official data collected by the Higher Education Statistics Agency (HESA), the National Student Survey and the Research Excellence Framework 2014.

The following departments at York also received top 10 rankings:

- Biological Sciences
- English
- Iberian Languages
- Nursing
- Psychology
- Social Work

The University of York was ranked 20th overall.

The Roger J Mawby Demonstrator Awards 2019/2020

Roger J Mawby was one of the founding academic staff members of the Department of Chemistry and was an inspirational teacher. Roger gave detailed and engaging lectures, frequently using chemical demonstrations to illustrate important concepts in transition metal chemistry and catalysis. In addition he gave stimulating and challenging tutorials that allowed students to develop and build their understanding of chemistry. **The Roger J Mawby Demonstrating Prize** is awarded to 5-6 students annually at a value of £150 per prize, to reflect Roger's passion for student learning. Winners also received a trophy made by glassblowing technician Abby Mortimer.

The Winners of the **The Roger J Mawby Demonstrating Prize for 2019/20 are**:

Conor Black	For incredibly diligent teaching, especially in Year 1. Conor puts great efforts into understanding the background behind the experiment, which is used to help students (and other GTAs where needed!) to a very high standard.
Paul Bond	For exceptional effort in writing a simulation software for the ICP course in a few weeks, allowing the key experimental design aspects of the course to be preserved. Student feedback for the course was exceptional.
Chris Goult	For efforts on the MChem Schlenk line experiment. Chris's calming influence makes for a very effective educator and is very supportive of students. Delivers information clearly and concisely, particularly important in avoiding risk and ensuring equipment is used correctly.
Nina Leeb	Nina is always bursting with enthusiasm across all her teaching and takes great pride in her work. She tries to get the best out of every student.
David Loades	Incredibly organised, efficient and always working hard to help students get the best out of themselves. Very patient and thorough in everything he does.
Anna Patterson	Always friendly and willing to help the students. Patiently helps students to overcome their own problems and develop their learning. Continuously seeks to identify improvements to experiments to improve the future running of the course.

Other GTAs nominated/shortlisted:

Giuseppina Barile	Alisa Doroshenko	David Husbands	Alastair Robinson
Sophie Berrell	Will Drysdale	Chris Maddocks	Freya Squires
Rosalind Booth	Giordaina Hartley	Alice McEllin	Nik Vagkidis
Michi Burrow	Peter Howe	Beth Nelson	Lucy Wheeler
Martina Conti	Chloe Howman	Tom Nicol	

As usual, we would like to thank all of our GTAs for their work during 2019/20, a year that was particularly challenging. Unfortunately we were not able to hold an event to celebrate this year, but still want to let all GTA know that their work and efforts are greatly appreciated.

Board of Studies—Calendar of Meetings 2020-2021

Term	Week	Date	Day/Time	Room
2020				
Autumn	SV14	23 September	Wednesday 14:00	Via Zoom
	7	11 November	Wednesday 14:00	Via Zoom
2021				
Spring	5	10 February	Wednesday 14:00	TBC
Summer	4	12 May	Wednesday 14:00	TBC
	9	16 June +	Wednesday 11:00	TBC
	10	23 June *	Wednesday 13:30	TBC
	10	24 June *	Thursday 13:30	TBC
	SV2	7 July	Wednesday 14:00	TBC

+ Internal Examiners Meeting – Wed 16 June 2021

* Provisional dates for Board of Examiners meetings for Examinations results

Graduation Ceremony Dates (provisional):

Wednesday 20—Friday 22 January 2021

Wednesday 21—Saturday 24 July 2021

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 on the intranet homepage or at this link.

Guardian University Guide 2021

Chemistry at York is ranked sixth, confirming its place as one of the top Chemistry departments in the UK.

This week the Department maintained its place among the UK's most highly regarded departments for the subject of Chemistry. The Department is ranked 6th in the UK in the Guardian University Guide.

The league table, which ranks fifty-three UK Chemistry departments, highlighted the consistently excellent performance of Chemistry at York in various areas including *satisfied with course*, *satisfied with teaching*, and *continuation*.

Published annually, the Guardian University Guide is aimed specifically at students choosing a university course. It ranks UK universities by undergraduate degree subjects in a variety of metrics. The rankings are based on official data collected by the Higher Education Statistics Agency (HESA) and the National Student Survey.

Head of Department, Professor Duncan Bruce, said: "It is extremely pleasing once more to be recognised among the top Chemistry departments in the country. We are fortunate in having a wonderful community of talented and committed students for whom our staff work tirelessly to deliver a unique teaching and learning experience."

In total, eight subjects at the University were ranked in the UK top 10: Archaeology and Forensic Science (9th), Biosciences (6th), Chemistry (6th), Film Production and Photography (5th), History of Art (4th), Nursing and Midwifery (6th), Physics (9th) and Psychology (9th).

Air Quality & COVID-19 event report published

The report from the event 'Co-ordinating Research Action: Air Quality & COVID-19' was published in September 2020. The report was jointly authored by STFC Air Quality Network (SAQN), UKIEG and AQNUK as convenors of the workshop. In addition to the Executive Summary and Calls to Action, the report contains summaries of the speaker presentations, the workshop methodology, and information on ways to connect with STFC.

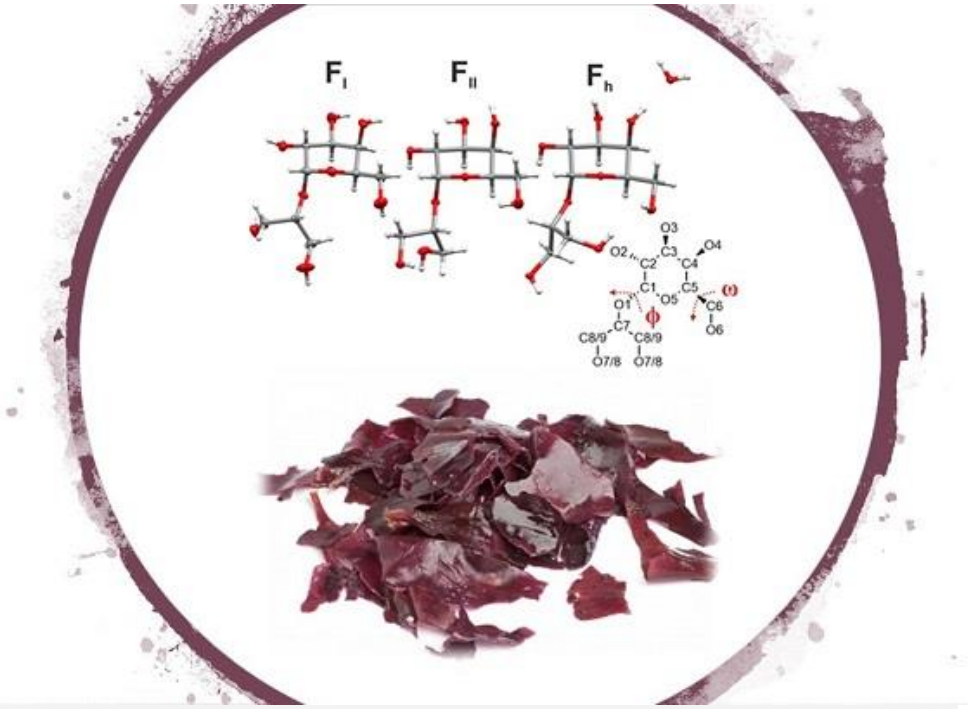
SAQN are keen to encourage further interdisciplinary work with others interested in air quality challenges, and have invited the community to get in touch with their responses to the Calls to Action. SAQN will be doing further work to identify what work is happening in the different research areas, and finding areas where STFC capabilities can contribute to the research.

The upcoming Collaboration Building Workshop offers an opportunity to connect with researchers in different disciplines and apply for Scoping Study funding for new work using STFC capabilities. The starting points for discussion will be the themes identified at the launch event and the calls to action from this report, as the most pressing challenges in air quality at the moment. Applications are welcomed from a wide range of disciplines.

New crystal forms from red algae

Applying circular economy principles to resource recovery from red algae has revealed two unforeseen crystal forms of floridoside – an intriguing natural product.

Floridoside (2-α-O-D-galactopyranosyl glycerol) is an important, naturally-occurring glycerol glycoside biosynthesised by most species of red algae. Within these organisms, floridoside has been implicated as an intracellular regulator of various fundamental functions. Most notably, floridoside helps control osmotic pressure – it's accumulation in cells can effectively counteract high external solute levels that would otherwise cause loss of water from the cells. This is important for algae which live in high salt environments.



The new crystal structures of floridoside (FII and Fh), as extracted from red algae, are displayed alongside the known structure (FI)

Floridoside is often considered a so-called 'compatible solute' and represents a less-detrimental method of adapting osmotic pressure compared with alternative approaches such as accumulation of inorganic salts, metabolically disruptive solutes, or abrupt changes in cell volume. This, and its other properties, make it of interest for a range of applications.

In their new work, Dr Avtar Matharu and co-workers report previously unforeseen crystal forms of floridoside: an anhydrous polymorph (F_{II}) and a crystalline stoichiometric monohydrate (F_h). This work advances the characterisation of this important natural biomolecule, could help facilitate its use in a variety of applications and help understanding of its role in vivo as a 'compatible solute'. Importantly, the researchers noted that the physicochemical properties of the new crystal polymorphs were significantly different to those of the known polymorph.

Dr Matharu said: "My final year PhD student, Andrew Maneffa, was pivotal in isolating floridoside from algae. His thoroughness and attention to detail meant he was able to identify two new forms of floridoside – one of them completely unheralded.

The development of circular economies based on renewable resources is a key strategy for sustainable development. Fully understanding what Nature already provides us with is very important for many industrial applications".

The research is published open access in *Communications Chemistry.*

Prize for Chemistry graduate student

Rob Ives to receive Chancellor's Leadership Award at this year's Graduation ceremony

Chemistry students graduated as part of an online ceremony on Friday 28 August. As part of this summer's graduation, Rob Ives received a prestigious Chancellor's Leadership Award, which is awarded to University of York students who have demonstrated a commitment to academic study, work experience and track record that has benefited others and made a significant and lasting contribution to both the University community and the city of York. Only three students are selected for the award after excelling on the York Award and York Leaders programme.

Rob has just successfully completed a masters research project in Organic Molecular Materials Chemistry in the group of Dr Alyssa-Jennifer Avestro. During his time at York, he was elected as Chair of the Chemistry Society and was also a member of the executive board of the York Science Conference. In the Summer of 2019, Rob was also a visiting research scholar gaining international research experience at the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences in Prague.

On receiving the news of the award, Rob said: "I feel truly humbled. Over my time at York, I've pushed myself as much as possible – dedicating countless hours to develop personally & professionally. It is really pleasing to be recognised for my efforts with such a prestigious award presented to a select few. Above all else, I believe University is more than studying solely for a degree. For myself, it has been about developing a willingness to take a chance, no matter how daunting or difficult. I've aimed to develop a confident, resolute and diligent mindset to overcome fear and risk: insecurities that I strongly believe to be prerequisites to the journey of adventure and success."

Looking ahead, Rob will progress to postgraduate study doing a PhD in Organic Chemistry at Durham University with the long term intention of following a career in academia or industry.

New starters

Ben Reader, Green Chemistry Research Technician - THYME project
Room: C/F120 and lab C/F119; Ext: 4549; Email: benjamin.reader@york.ac.uk

Dr Fergal Byrne (new role), Green Chemistry PDRA, Furafact Project
Room: C/F111; Ext: 4547; Email: fergal.byrne@york.ac.uk

Mackayla Millar (new role), CIEC Primary Science Advisory Teacher for the Humber Region
Room: C/B013; Ext: 2523; Email: mackayla.millar@york.ac.uk

Nick Heywood, Teaching Laboratory Demonstrator
Room: C/B103; Ext: 5872; Email: nick.heywood@york.ac.uk