

2023

Welcome to the second issue of the RSC Fluorine Chemistry Interest Group newsletter. We want to use this newsletter to inform you on what the Fluorine Chemistry Interest Group is doing and to highlight other events that are occurring within the fluorine community more broadly. We see fluorine chemistry as an area which spans disciplines, and we are always looking for new members and we especially welcome those who might have developed a recent interest in some aspects of fluorine. The Fluorine Chemistry interest group currently counts 220 members across 5 continents.

We hope you will enjoy this issue. Topics for the next issue can be discussed with the Group Secretary, Dr Will Brittain (<u>william.d.brittain@durham.ac.uk</u>). The Newsletter content is agreed by the Fluorine Chemistry Interest Group Committee.

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Editorial From the Chair

Dear RSC Fluorine Chemistry Interest Group members,

Welcome to the second edition of our interest group *Newsletter*. The RSC Fluorine Chemistry Interest Group was formed in 2001 in recognition of the importance of fluorine to all sectors of chemical enterprise. The group exists to promote activity in fluorine chemistry and to help develop the careers of RSC Members associated with the Interest Group. This is enabled through facilitating research discussions and interactions with a particular emphasis on bringing university researchers and industrialists together and at all career stages. This *Newsletter* is an initiative of the RSC Fluorine Interest Group committee aimed at improving communication with Members on an annual basis, as direct e-mailing is prohibited due to GDPR legislation.

With the departure of Prof Veronique Gouverneur, who came to the end of her term as committee member, we issued a call for new committee members last year, and we thank all applicants for their interest in serving on the committee. The ballot resulted in three new committee members joining us last April. A warm welcome to Anna, Ben and Matt, and many thanks to Veronique for her contributions! You will find information about the current committee membership below.

Our main activity is the organisation of the annual RSC Fluorine Symposium, which takes place over two days at a UK University each year. In this newsletter we report on the successful symposium held this year (April 12th&13th) at Merton College at the University of Oxford. It was delightful to see many new research groups attending, showcasing a very diverse range of research topics. You will also find the announcement of next year's symposium, which will be held in Newcastle.

Polyfluoroalkyl substances (PFAS) have been in the news a lot this year, and as fluorine chemists this is a topic that will concern us all. You will have been aware of the EU consulting exercise regarding a proposed ban of PFAS compounds, and we have sent you information about this back in September. Our main aim is to provide sound information to promote a healthy debate about this difficult issue, and hopefully to contribute to finding solutions big and small. We are maintaining a bank of interesting literature and policy documents on this topic which is available upon request. We will be grateful to receive additional interesting contributions.

We are of course very keen to include news from your side, and to highlight any events that you organise that would be of interest to Group members, awards/Prizes received etc. Please get in touch with the Group secretary if you wish to highlight such information in future issues.

Finally, I'd like to finish by asking you to encourage the new arrivals in your research group to apply for RSC membership and join the RSC Fluorine Chemistry group! I look forward to seeing you in Newcastle.

Best regards

Bruno Linclau (RSC Fluorine Committee Chair)

Fluorine Chemistry Interest Group Committee Members

Prof. Bruno Linclau (Chair)

Bruno Linclau is Professor of Organic Chemistry at Ghent University, Belgium, where he leads the Organic and Medicinal Chemistry Group. He also has a parttime appointment at Southampton University, where he was based until 2021. His research is focused on investigating the influence of fluorination on physical properties relevant in drug discovery, such as lipophilicity, hydrogen bonding, and conformation, working with small molecules, carbohydrates, steroids and amino acids. He has been the RSC Fluorine Group Chair since January 2022, having served



a stint as Secretary before that. After enjoying the hiking and mountainbiking in the Hampshire and Great Britain countryside, he now returned back to his roots, road cycling on the flat Flemish cycleways.

Dr Will Brittain (Secretary)



Will is currently a Leverhulme Early Career Fellow and Assistant Professor of Organic Chemistry at Durham University. His research group utilises fluorine chemistry to tackle a broad range of problems across organic synthesis and catalysis. Currently Will is working on using perfluorinated aromatic compounds in synthetic methodology development with an interest in the generation of highly reactive fluorinated species for example in his recent report on the use of pentafluoropyridine for the synthesis of acyl fluorides. Will was elected to the RSC

fluorine committee in 2020 and currently holds the role of secretary. Outside of chemistry Will enjoys walking and baking sourdough pizzas at the weekend.

Prof. David O'Hagan (Treasurer)

David O'Hagan is a Professor of Organic Chemistry at the University of St Andrews. He has explored the synthesis and properties of organofluorine compounds throughout his career and has had a long interest in fluorinated natural products. His lab identified a naturally occurring fluorination enzyme and the enzyme has been used to incorporate fluorine-18 into molecules for positron emission tomography (PET). Interests extend to the influence and properties of fluorination in organic compounds and extend to bioactives and fluorinated organic materials.



He was awarded the ACS Award for Fluorine Chemistry in 2012 and the Prix Moissan by the *Fondation de la Maison de la Chime* in 2018. He is a founding member and a past Chair of the RSC Fluorine Group and as well as keeping an eye on the finances of the Fluorine Group he has recently been elected President of the Organic Division of the RSC. Outside of chemistry he takes great pleasure in winding up his grandchildren and he likes climbing the Munroe mountains in Scotland.



Dr Matthew Hopkinson (member)

Matt Hopkinson is a Senior Lecturer in organic chemistry at Newcastle University. Before moving to the UK in 2021, he was based in Germany and started his independent career at the Freie Universität Berlin. A major part of his research programme concerns the development of new reaction methodologies for installing fluorine and larger fluorinated functional groups onto organic molecules. Current areas of interest include the exploration of novel nucleophilic reagents for preparing molecules featuring SR_F (R_F= poly- or perfluoroalkyl) and

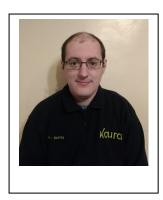
SeRF groups, radical trifluoromethoxylation methodologies and the development of selective C-F bond insertion reactions. Matt joined the RSC fluorine committee in 2023 and will host the next postgraduate meeting in Newcastle in April 2024. Outside of chemistry Matt enjoys getting out and about in the Northumberland countryside and can occasionally be found in the gym.

Dr Anna Vicini (member)

Anna Chiara Vicini is a senior scientist in Chemical Research and Development (CRD) at Pfizer, working on the development of APIs commercial routes and improvement of process sustainability. Her interest for "applied" and sustainable chemistry was apparent already during her PhD, conducted at the university of Oxford under the supervision of Prof. Veronique Gouverneur. Her research project focused on the activation of metal alkali fluorides with hydrogen bond



donor organocatalysts to obtain enantioenriched beta-fluoroamines and included scaling up this transformation to >100 g. Though not working every day on fluorination in her current role, she remains interested in the progress of the field and since 2023 she has joined the RSC fluorine group, bringing an industrial perspective to the committee.



Dr Ben Murray (member)

Ben Murray is a research chemist at, based at Thornton Science Park near Chester. Koura is the fluorinated solutions business of Orbia, a global business also operating in building & infrastructure, connectivity solutions, and precision agriculture. Koura operates a mine-to-market business model, converting CaF₂ from their fluorspar mines in Mexico to HF and AlF₃ then using that HF for the synthesis of more complex fluorinated products such as air-conditioning refrigerants, medical inhaler propellants, and energy storage materials. Ben

joined the company in late 2021 after completing a PhD in the group of Prof. Graham Sandford exploring transformations of fluoroalkene refrigerant gases to pharmaceutically relevant building blocks. His current research at Koura is focused on developing sustainable methods for the manufacture of fluorinated electrolyte salts and additives for lithium-ion batteries. Outside of chemistry, Ben is an avid collector of UNESCO world heritage sites and a keen quizzer, reaching the semifinals of University Challenge with Durham in 2019.

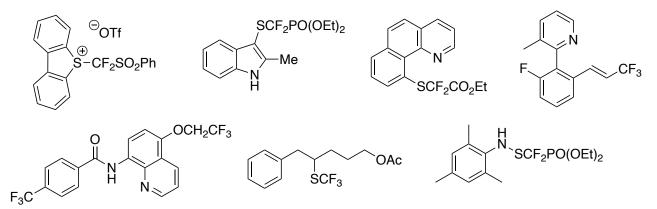


RSC Fluorine Prize 2021 – Dr Tatiana Besset

It is with great pleasure that we can announce that the winner of the 2023 RSC Fluorine Prize is <u>Dr Tatiana Besset</u> (UMR6014 COBRA, CNRS, INSA ROUEN Normandie, Université Rouen Normandie). The RSC Fluorine Prize is awarded to a young researcher who has made a significant contribution to the area of fluorine chemistry and is chosen by an international panel of fluorine chemists. Dr Besset's research focuses on the use of metal catalysed C-H activation and the development of new strategies for the synthesis of fluorinated building blocks. She has published >80 publications with recent highlights including the development of <u>palladium catalysed</u> (ethoxycarbonyl)difluoromethylthiolation reactions and the development of an electrophillic reagent for the direct

introduction of SCF₂PO(OEt)₂ groups into molecules. Dr Besset undertook doctoral studies with Dr Andrew E. Greene at the University of Grenoble followed by postdoctoral studies with Prof. Frank Glorius

(Westfälische Wilhelms Universität Münster) and Prof. Joost N. H. Reek (University of Amsterdam). In 2012 she became a CNRS Researcher in the "Fluorinated Biomolecules Synthesis" group of Prof. Xavier Pannecoucke (Université de Rouen) and in 2017 was awarded an ERC Starting Grant. Dr Besset has made a highly impactful contribution to fluorine chemistry and we are delighted to be able to award her the 2023 RSC Fluorine Prize. Just some of the types of fluorinated compounds Tatiana has prepared are shown below.



Tatiana will be giving a lecture on her awarding winning chemistry at the 22nd RSC Fluorine Postgraduate Meeting (details below).

21st RSC Fluorine Postgraduate Meeting

This year the RSC Fluorine Postgraduate Meeting was held for the first time in person following the COVID pandemic. The meeting was held over the course of 2 days at the beautiful Merton College Oxford and gave



the opportunity for the fluorine community to come together and reestablish links that had been hindered by the pandemic. The meeting kicked off with Dr Pavel Mykhailiuk from Enamine who was giving his delayed 2021 RSC Fluorine Prize lecture. Giving his talk remotely from Kyiv Pavel gave us a tour-de-force in organic methodology

Merton College Oxford, the location of the 21st RSC Fluorine Postgraduate Meeting

development and medicinal chemistry. He discussed the work that he and Enamine have be doing to access small, fluorinated ring systems which have now been incorporated into Enamine's catalogue. The first session was then complemented by a trio of early career talks from Alexander Atkins on electrochemical benzylic fluorination, Dr Helen Allan on utilising reductase enzymes to access enantioenriched sp3 fluorides and finally a talk from Valeria Burianova on the asymmetric synthesis of a PET imaging agent for the SV2A receptor.

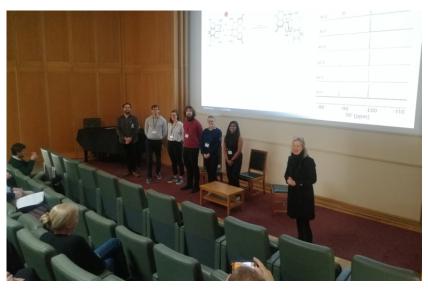
Our next plenary speaker was Prof. Mark Crimmin from Imperial College London who gave an overview of his recent efforts in the area of utilising main group elements both create and break bonds to fluorine. This was a fascinating talk that showcased some cutting-edge developments on how mixed metal containing systems can selectively remove fluorine from compounds. Following the plenary Sam Dearman gave a presentation on his efforts in the preparation of hypervalent iodine (V) fluorides. The day was then wrapped

up with Stephen Sweeting's talk on his investigations into how HF reagents mixtures are not all created equal in terms of their reactivity.

After a day of enlightening talks a poster session was held with a chance to network and chat with poster presenters on their research. The conference dinner was then held in the dining hall of Merton College and many friends were made over the course of dinner. The festivities continued into the evening with a trip to a local inn for some refreshments and good chat.

The second day of the meeting began with a series of fantastic ECR talks on a variety applications of fluorine of across chemistry and biology. To begin Isabeau Lüddecke gave a great talk on the design of artificial fluorinases which followed by Gabija Poskaite describing their work on asymmetric nucleophilic fluorination using hydrogen bonding phase transfer catalysts. The session was concluded with Sam Hanson presenting his work on the use of fluoroaromatics as versatile tools for chemical biology application.

The final session of the meeting began with Arushi Garg discussing the development of a new reaction which inserts alkenes into C(sp³)-F bonds. This



After much deliberation prize winners receive the news at the close of the meeting.

was followed by Luca Dobson presenting new developments on the synthesis and application of the tri-fluoro t-butyl group. The session was concluded with our third and final plenary speaker Prof Simon Aldridge from the University of Oxford who showcased his work on the harvesting and delivery of fluoride utilising molecular complexes of the group 2 metals.

Finally, after much deliberation prizes were presented for the best talks and posters from the ECRs. The 1st place talk prize was awarded to Arushi Garg from Newcastle University for their talk entitled "Insertion of Alkenes Into C(sp3)–F Bonds Mediated by Fluorine-Hydrogen Bonding".

The 2nd place talk was awarded to Valeria Burianova from the University of Glasgow for their talk entitled *"Organocatalytic Asymmetric Synthesis of SynVesT-1, a PET Imaging Agent of the SV2A Receptor".*

The 1st place poster prize was awarded to Andrew Lacey from the University of Bristol for their poster on *"Mechanistic Investigation into Diastereodivergent Alkene Chlorofluorination"*.

The 2nd place poster prize was awarded to Kler Huonnic from the University of Southampton for their poster on *"Glycosylation of Polyfluorinated Carbohydrates"*.

This bought what had been a fantastic event to a close. The meeting at Oxford was a thoroughly enjoyable event and really bought the fluorine chemistry community from around the UK and further afield back together following the hiatus created by COVID.

Following the success of the 2023 meeting It is our pleasure to announce that the 22nd RSC Fluorine Postgraduate meeting will take place at Newcastle University on the 4th and 5th of April.

22nd RSC Fluorine Postgraduate Meeting

The 22nd RSC Fluorine Postgraduate meeting will take place at Newcastle University on the 4th and 5th of April.

The programme of the meeting consists of invited lectures from established researchers, but there is a particular emphasis on enabling early career researchers (ECRs) including postgraduate students and postdoctoral researchers to present their recent work, both as oral presentations and in posters. Many companies attend and the meeting is an excellent opportunity for networking, exploring career opportunities and to discuss the exciting and varied science that is being carried out within our community. In this regard we value contributions from organofluorine groups and researchers who are developing new methodologies for preparing or analysing fluorine containing compounds or from those who are predicting the behaviour assessing the performance of fluorinated compound for different applications. It is recognised that cross-fertilisation between different disciplines and across the academia-industry interface is a major driver of innovation, and the Fluorine Group aims to facilitate that.

We will be in touch with information regarding registration and abstract submission for the meeting in the new year.

EU PFAS Consultation

The RSC Fluorine Interest Group committee emailed the membership on the 3rd September about the then ongoing EU consultation exercise regarding a proposed ban on polyfluoroalkyl (PFAS) compounds. The consultation exercise yielded more than 5,600 comments from more than 4,400 organisations, companies, and individuals. See the news update on the ECHA (European Chemicals agency) website:

https://echa.europa.eu/-/echa-receives-5-600-comments-on-pfas-restriction-proposal

The RSC has also submitted a response to the consultation, which is reproduced below with permission from the RSC. In our earlier email we provided information, such as the RSC policy document on PFAS regulation, an academic paper proposing the principle of 'essential use', and a publication outlining the potential impact of a ban in many industries. The links to this information is provided again, together with a new review article about the abundance of PFAS.

We are keeping a bank of policy documents, papers and news articles that are immediately relevant to the PFAS issue. You are welcome to send any relevant papers/contributions that you come across and conversely, you are welcome to contact me or the Group's secretary if you would like to consult this information.

- RSC policy on PFAS regulation (<u>link</u>), with the RSC policy on *Risk based regulation for per- and polyfluoroalkyl substances* (<u>link</u>) and policy position on *PFAS in UK drinking water* (<u>link</u>)
- The principle of essential use (link)
- Abundance of fluorochemicals in the environment (<u>link</u>)
- Impact of a PFAS ban in industry (link)

(Note: some links are to the primary literature, not all are open access).

We hope that this will be useful.

RSC response to the consultation, as submitted on the web form:

"Text submitted to web form:

In response to the consultation on the Restriction on the manufacture, placing on the market and use of PFASs in the EU, the Royal Society of Chemistry (RSC) is submitting three documents for reference: our policy position on *Risk based regulation for per- and poly-fluoroalkyl substances*, our policy position on *PFAS in UK drinking water*, and our report *When the science is uncertain, what is the role of risk-based approaches and precautionary control in chemicals policy*?

A summary of our approach to chemicals regulation and PFAS follows:

To direct risk assessment in the most useful, efficient, timely and relevant way there needs to be (i) criteria for prioritising those substances that require a full scientific safety evaluation and (ii) a pragmatic way of performing a risk assessment for a single PFAS or ideally for a PFAS that is defined as representative of a group/category of PFAS. Banning all PFAS on persistence alone would take little scientific resource but could have massive unintended consequences for society with loss of important products and disruption of vital processes. Similarly doing nothing, when we have good evidence of the toxicity of some PFAS, is not an option as we must protect public health and the environment.

A framework based on a multi-step 'traffic-light' decision-tree approach around PFAS use in society and on the basis of safety risk and impact assessments may be useful for regulatory action. We put forward a green, amber, and red list approach (further explained in the policy position) to take appropriate regulatory action based on a defined level of acceptable risk according to an agreed set of criteria, as defined by the regulator working with science advisory mechanisms within government. This approach is designed to be proportionate, iterative, and agile, to ensure it accounts for evolving scientific evidence on PFAS.

We do acknowledge and agree with the need to take a precautionary approach where the science is uncertain, and the lack of toxicity and exposure data for many PFAS makes this concept applicable. The idea of essential use may be useful here, and it is included as a step in our risk assessment framework. The following could be considered when applying the essential use concept:

- An authorisation system could be used for essential uses.
- Uncertainty should not prevent action if there is some evidence of harm.
- Regulate chemicals in groups to increase efficiency.
- Transparency from industry will make regulation using the essential use concept more efficient.

However, care should be taken in banning PFAS without understanding the alternatives (which also may be manufactured at <1tpa and thus be missed by REACH regulation) to avoid unintended and potentially worse consequences from the use of other more harmful or equally persistent substances. There should be a continuous review of the alternatives used to quickly identify new evidence on safety.

We have also attached our policy position on PFAS in drinking water. Although partly covering the case for tighter drinking water standards in the UK, it is relevant to the regulation of PFAS because it recommends that companies that manufacture or use PFAS should be required to submit data to a central and public database. Compiling such data in a central and accessible database will allow regulators to make decisions based on complete information about the sources of PFAS. It is also important for companies to have better knowledge of their own PFAS use to fully control emissions. Requiring annual reporting will increase awareness in company management of the potential benefits and harms of PFAS use, transparency with regulators and the public, and opportunities to phase out PFAS and/or substitute to other substances. Regardless of the outcome of the proposal to ban PFAS, this action could be implemented in support of other PFAS control policies.

The RSC works with a broad network of scientists in industry, academia, and government with expertise in this area, across Europe and globally. We would welcome any questions on our position or requests for more information.

About us

With about 50,000 members in over 100 countries and a knowledge business that spans the globe, the Royal Society of Chemistry is the UK's professional body for chemical scientists, supporting and representing our members and bringing together chemical scientists from all over the world. Our members include those working in large multinational companies and small to medium enterprises, researchers and students in universities, teachers, and regulators. "

Celebrating Recent Successes

In this section we would like to highlight some recent advances in fluorine chemistry and the industries that rely on it.

New fluorination reactions directly from Fluorspar

Recently a team of researchers headed by Prof. Véronique Gouverneur from the University of Oxford have reported on a mechanochemical method for the generation of C-F bonds directly from Fluorspar. This breakthrough technology is the first example of a fluorination reagent that does not require the creation of highly dangerous hydrogen fluoride (HF). The new methodology utilises mechanochemical force to generate a fluorinating reagent (Fluoromix) from Fluorspar and a potassium phosphate salt. This solid powder can then be directly employed into fluorination reactions to generate a range of small fluorine containing molecules. This methodology is the first example of a completely HF free process and could be a highly safe and sustainable manner to access fluorinated molecules. If you would like to read more about this technology the full paper can be found <u>here</u>.

Perfluorocubane wins C&EN's Molecule of the Year 2022

Prepared by Okazoe and co-workers, perfluorocubane was voted by the readers of ACS Chemical and Engineering News to be the Molecule of the Year for 2022. The compound with a molecular formula of C_8F_8 incorporates fluorine atoms at each of its vertices. The synthesis of the molecule was a tour de force in organofluorine chemistry with the use of direct electrophilic fluorination utilising elemental F_2 gas. This molecule is highly unusual as the C-F antibonding orbitals geometry can trap a single electron within the cube to generate a short-lived radical anion. If you want to read more about the very unique properties of perfluorocubane you can find the full paper <u>here</u>.

Orbita and Solvay agree to build PVDF facilities for lithium ion batteries

In industrial successes this year it was announced that Orbita and Solvay will come together to build the largest polyvinylidene fluoride (PVDF) production facility in North America. This new facility will rise to meet the growing demand for lithium-ion batteries in the worlds EV and stationary energy storage markets. The new technologies that will be developed in PVDF will allow for electric vehicles that go further on each charge, extended battery lives and in turn improved battery safety. If you would like to read more about this news the full press release can be found <u>here</u>.

Next Committee Meeting

The next committee meeting will take place around the end of January 2024. If you have matters you would like to see discussed, please get in touch with a committee member.

Dates for the Diary

Below are some dates that might be of interest if you are into fluorine chemistry

22nd RSC Fluorine Postgraduate Meeting – Newcastle University - 4th & 5th April, 2024

24th International Symposium on Fluorine Chemistry - Shanghai, Peoples Republic of China - 28th July – 2nd August, 2024.

21st European Symposium on Fluorine Chemistry – Lisbon, Portugal - 3rd–9th August, 2025

South African Fluorine Symposium 2024 – Sun City, South Africa - 11th-15th February, 2024

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