



Engineering and Physical Sciences  
Research Council

**PHYSICAL ORGANIC CHEMISTRY**

Report on the EPSRC workshop held on 27 April 2005  
The Institute of Physics, London.

Zoë Brown  
EPSRC  
Polaris House  
North Star Avenue  
Swindon  
SN2 1ET  
Zoe.Brown@epsrc.ac.uk

## Introduction

The aim of this workshop was to meet with members of the UK academic and industrial Chemistry community who had an interest in physical organic chemistry (POC) to discuss the issues and to establish a way forward to further develop the area.

Setting the scene for the day were presentations showing benefits and various perspectives on POC from an industrial viewpoint by Dr Brian Cox from AstraZeneca and from an academic viewpoint, by Professor Donna Blackmond of Imperial College.

A timetable for the day and a delegate list are shown in appendices 1 and 2. POC grants supported by EPSRC 2000 - 2005 are shown in appendix 3

## Definition and scope of physical organic chemistry

Delegates were asked for their opinions on the definition, adopted after previous consultation, of physical organic chemistry:

*"Studies of the dynamics, reactions and interactions of organic molecules and systems leading to quantitative understanding of the interplay between structure, function and reactivity"*

There was broad agreement, emphasising that quantitative analytical measurements are key to the fundamental understanding of chemical processes at a molecular level.

POC has evolved to address such diverse areas as:

- Interfacial/heterogeneous systems
- Mechanisms of catalysis and enzyme mediated reactions
- Kinetic and mechanistic studies of organic reactions
- Process development and design
- Supramolecular chemistry
- Self assembled systems
- Organic materials science
- Photochemistry
- Solvation
- Molecular recognition
- Modelling of relationships between structure and function
- Development of computational tools
- Understanding of the interactions between components in complex systems.

It was emphasised that quantitative approaches and understanding are key, and that no research themes should be excluded from future initiatives.

## Workshop outcomes

### Issues raised at the workshop

- In the UK, a number of physical organic chemists are nearing retirement or have already retired. If younger people are not encouraged to take up the subject, there is a danger of the field disappearing in the future.
- Synthetic chemistry PhD students are not always being taught the elements of POC.
- POC is not always taught as an element of undergraduate courses.
- POC is seen as "untrendy and unexciting"
- POC is no longer a core subject, as it was in the past.
- POC is perceived by potential students as difficult and mathematical.

- Some trained post-doctoral synthetic chemists are not always able to do kinetic measurements or relate mechanistic POC to their work.
- There is a relatively small, dispersed academic POC community in the UK.
- POC proposals can often be at the interface between EPSRC and BBSRC.
- There is a lack of lecturers/support at University level to teach POC.
- The area is not thriving because potential students don't think there are any jobs.
- Students are not aware of the industry need for POC. There is a need for industry to educate and raise awareness of the opportunities.
- Industry depends on POC and, in some cases, is having to teach it themselves.
- Industry is teaching chemical engineers POC as they have a good grounding in mathematics.
- Physical organic chemists in industry need to collaborate and use a common language with other disciplines as they are at the heart of process development.
- Lack of awareness between academia and industry.
- Scientific methodology is "dying". POC was a sound home for the methodology.
- Physical organic chemistry methodology has dispersed into many different areas and is no longer just kinetics and reaction mechanisms.
- Physical organic chemistry is declining in other countries across the world, although it was felt that expertise still resided in Canada, Eastern Europe, Italy and Spain.
- New industries e.g. Nanotechnology, will need POC generic skills.

## **What needs to be done – suggestions from the workshop**

Initiatives in priority order were:

### **Studentship Activities**

- Targeted studentships in POC, possibly 4 years long.
- Establish 2 or 3 Doctoral Training Centres in POC.
- CASE awards in POC – EPSRC/industry initiative to increase academic/industry collaboration.
- Allow support for overseas students.
- Funding to train physical organic chemists.
- POC students should be required to attend specific summer school activities.
- There should be an industrial input/context in training activities.
- A student initiative will raise the profile of UK POC.
- Cost effective way of increasing the skills base.
- There needs to be a sustained initiative with earmarked students (BBSRC style) - 15 students/annum for 3-5 years.
- Ring fenced studentships - > 1 per institution. Could lever lectureship appointments.
- 4 year PhD with the 3<sup>rd</sup> year spent in industry.
- More quantitative curriculum.
- Try to influence undergraduate teaching to include POC modules.
- Masters level courses.

### **Fellowships**

- Post –doctoral fellowships in POC (for three years, within 3 years of PhD)
- Fellowships with teaching elements
- Fellowships with industry experience/secondments
- Visiting fellowships from overseas

## **Sabbaticals**

- International exchange of trained people- dissemination of knowledge and skills
- Sabbaticals/secondments in industry for academics.
- Secondments to industry for lecturers for 2 years.
- Sabbaticals overseas and from overseas.
- Encourage overseas participation in teaching at summer schools.
- Encourage discipline hopping between organic chemistry, POC and chemical engineering.

## **Peer Review**

- Encourage POC applications through responsive mode.
- Improve appreciation and selection of who is appropriate to referee proposals.
- Encourage peer review to recognise value and importance of quantitative approaches and understanding.
- POC needs to be recognised as interdisciplinary.

## **Taught short courses and summer schools**

- Short courses in POC for PhD students and for others interested in POC
- Summer schools in POC for PhD students.
- RSC accredited training modules.
- Encourage expert overseas visitors to give summer school courses.
- RSC named lectures
- Advertise courses to POC community.

## **Network Activities**

- Create networks in POC.
- Improve communication between academics and industry.
- Better support and promotion to existing groups e.g. RSC Organic Reaction Mechanisms Group.

## **Chairs and lecturers**

- Focus effort on creating a few strong centres for POC.
- Create five chairs – one per region to create a “core” network.
- Create new lectureships and link to studentships.

## **Managed calls**

- Managed calls in POC – loose in its focus (actual research topic).
- Collaborative calls with industry.
- Targeted calls in interdisciplinary areas that must have a POC element.

## **Conclusions**

A clear message has emerged from the workshop that a people-focussed activity needs to be stimulated by EPSRC in this area, to increase the numbers of trained physical organic chemists and to strengthen the academic base.

The profile and benefits of POC needs to be raised to encourage people to become active in the area, and to demonstrate that their skills are valued, particularly in industry.

Industry participation would be particularly welcomed, as it is clear that industry is reliant on the skills physical organic chemists bring to activities which are at the heart of process development.

Communication between academia and industry also needs to be improved, with mechanisms to encourage collaboration.

### **What has been done so far**

The recent "Science and Innovation" pilot exercise by EPSRC - for increasing research activity and leadership capacity in areas where there is lack of critical mass in the UK - resulted in five awards being made in mid 2005.

One of the awards, to Cardiff University, was to set up a centre in POC, with the future recruitment of a Chair and lecturers. Another award went to Nottingham University at the chemistry/chemical engineering interface, and also included a large integral POC content.

### **Possible mechanisms for further targeted activities**

A specific EPSRC activity to support the area will take place in the financial year 2006/2007, and funding has already been earmarked in the business planning for that year.

This activity will consist of CASE style four year collaborative project studentships in POC, with the inclusion of a minimum 3 month period in industry. Elements of taught course modules should be included, that would be available to all the studentships and to other researchers in POC. Issues regarding Undergraduate and Postgraduate teaching will be discussed with the RSC.

Networking would be encouraged, for example via the modules that could be held at summer schools, and participation encouraged in the RSC Organic Reaction Mechanism network.

### **Acknowledgements**

Before arranging this workshop, consultations were held with members of the POC academic community, the RSC, industry and members of the Innovation Task Force of the Chemistry Leadership Council.

Thanks also to those who made the time to take part in the workshop.

## Appendix 1

### Physical Organic Chemistry Workshop Institute of Physics

09.30 - 10.00	Registration	
10.00	Introduction and objectives (Franklin Theatre)	John Baird and Zoë Brown
10.15	Presentation: Physical Organic Chemistry from an academic viewpoint.	Professor Donna Blackmond Imperial College
10.45	Presentation: Physical Organic Chemistry from an industrial viewpoint	Dr Brian Cox AstraZeneca
11.15	Questions and Answers	Professor Donna Blackmond Dr Brian Cox
11.30 – 12.45	Breakout Session 1  a) Defining and the Scope of Physical Organic Chemistry  b) What are the issues and opportunities	
12.45 – 13.15	Feedback from Breakouts	
13.15 - 14.00	Lunch	
14.00 – 14.15	Setting the scene for breakouts	John Baird and Zoë Brown
14.15 – 15.45	Breakout Session 2  What do we need to do in terms of: <ul style="list-style-type: none"><li>• Research (Themes)</li><li>• Training (People and Skills)</li></ul>	
15.45 – 16.15	Feedback from Breakouts	
16.30	Meeting will close	

## Attendees

Title	Name	Surname	Institution
Professor	Michael	Abraham	Chemistry - University College London
Professor	Roger	Alder	Chemistry - University of Bristol
Dr	David	Alker	Pfizer Global Research & Development
Professor	Rudolf	Allemann	Chemistry - University of Cardiff
Prof	Harry	Anderson	Chemistry Research Lab - University of Oxford
Dr	John	Atherton	BRITEST
Dr	Bill	Bentley	Chemistry - University of Swansea
Professor	Donna	Blackmond	Imperial College London
Dr	Colin	Brennan	Syngenta
Dr	Victor	Chechik	Chemistry - University of York
Dr	Nicola	Colclough	Astra Zeneca Pharmaceuticals
Dr	Brian	Cox	Astra Zeneca
Dr	Anna	Croft	Chemistry - University of Wales, Bangor
Dr	Ian	Cunningham	Chemistry - University of Surrey
Professor	Anthony	Davis	Chemistry - University of Bristol
Professor Sir	Alan	Fersht	MRC Centre for Protein Engineering
Dr	John	Gilday	Astra Zeneca
Professor	Bernard	Golding	Natural Science - University of Newcastle Upon Tyne
Mr	Brain	Gourlay	Avecia Pharmaceuticals
Ms	Debbie	Harding	BBSRC
Dr	Jeremy	Harvey	Chemistry - University of Bristol
Dr	George	Hodges	Avecia
Dr	David	Hodgson	Science Labs - University of Durham
Dr	Wilfred	Hoffman	Pfizer Global Research & Development
Dr	Florian	Hollfelder	University of Cambridge
Professor	David	Knight	Chemistry - University of Cardiff
Dr	Jerry	Lewis	ICI - Uniqema
Dr	Hamish	McNab	Chemistry - University of Edinburgh
Dr	Ian	McRobbie	Octel Corporation
Dr	Mario	Moustras	Royal Society of Chemistry
Dr	Sijbren	Otto	Chemistry - University of Cambridge

<b>Title</b>	<b>Name</b>	<b>Surname</b>	<b>Institution</b>
Professor	Mike	Page	Pro-Vice Chancellor - University of Huddersfield
Dr	Alejandra	Palermo	Royal Society of Chemistry
Professor	Jonathan	Percy	Chemistry - University of Leicester
Dr	Douglas	Philp	Centre for Biomolecular Sciences - University of St Andrews
Dr	Ian	Watt	Chemistry - University of Manchester
Professor	Tom	Welton	Chemistry- Imperial College, London
Professor	Chris	Wharton	Biosciences - University of Birmingham
Dr	Paul	Wight	Avecia
Mr	Malcolm	Wilkinson	IChemE
Professor	Ian	Williams	Chemistry - University of Bath
Dr	Nick	Williams	Chemistry - University of Sheffield

### **Staff**

Dr	John	Baird	Programme Manager - Chemistry
Mrs	Zoë	Brown	Associate Programme Manager Chemistry
Mrs	Sue	Carter	EPSRC Project Management Group
Dr	Paula	Duxbury	Associate Programme Manager Chemistry
Dr	Emma	Feltham	Associate Programme Manager Engineering
Dr	Jason	Green	Associate Programme Manager Chemistry
Dr	Christina	Guindy	Associate Programme Manager - High End Computing
Dr	Emma	Jones	Associate Programme Manager Chemistry
Dr	Carmine	Ruggerio	Associate Programme Manager Chemistry
Mr	Paul	Tomsen	Associate Programme Manager - Life Science Interface
Dr	Nicolas	Guernion	Associate Programme Manager -Technology



EPSRC POC Grants supported in 2000 – 2005

Appendix 3

Status Description	Grant Ref Number	Name	Programme Area Name	GrantTitle	Total Grant Value	StartDate	EndDate	Organisation	Department
Reconciled/Finished	GR/M16962/01	Dr N Williams	Chemistry	DISSECTING METAL ION CATALYSED PHOSPHATE HYDROLYSIS	£48,874.00	01-Oct-99	30-Sep-02	University of Sheffield	Chemistry
Not Accepted	GR/R76738/01	Dr CR Timmel	Chemistry	A study of magnetic field effects: From radical recombination reactions to paramagnetic convention.	£221,196.49	01-Oct-02	30-Sep-07	University of Oxford	Oxford Physics
Reconciled/Finished	GR/L39889/01	Professor J Connor	Chemistry	NEW THEORIES OF CHEMICAL REACTIONS AND MOLECULAR COLLISIONS	£156,993.00	27-Oct-97	26-Apr-01	The Victoria University of Manchester	Chemistry
Reconciled	GR/R13913/01	Professor J Connor	Chemistry	New Theories of Chemical Reactions	£189,830.15	01-Oct-01	31-May-05	The University of Manchester	Chemistry
Started (Payments being Made)	EP/C510267/1	Professor DG Blackmond	Chemistry	Exploring and Exploiting an Unprecedented Observation of Asymmetric Amplification and Autoinduction in Amino Acid Catalysts	£292,422.27	01-Jan-05	31-Dec-07	Imperial College London	Department of Chemistry
Started (Payments being Made)	GR/S62659/01	Professor CL Willis	Chemistry	Mechanistic Studies on Prins-Type Cyclisations for the Stereocontrolled Synthesis of Heterocycles	£96,896.08	02-Feb-04	01-Feb-07	University of Bristol	Chemistry
Announced	EP/C545834/1	Professor CA Hunter	Chemistry	Understanding Solvation Using High Throughput Physical Organic Chemistry	£362,159.59	01-Oct-05	30-Sep-10	University of Sheffield	Chemistry
Announced	EP/C545842/1	Professor CA Hunter	Chemistry	Understanding Solvation Using High Throughput Physical Organic Chemistry	£488,678.51	01-Oct-05	30-Sep-08	University of Sheffield	Chemistry
Started (Payments being Made)	GR/S79060/01	Dr D Philp	Life Sciences Interface	JEFI: Probing the relative efficiencies of direct and reciprocal replication strategies	£94,268.00	01-Oct-03	30-Sep-06	University of St Andrews	Chemistry
Reconciled/Finished	GR/R66111/01	Dr JR Woodward	Chemistry	The study of magnetic field effects on radical reactions in solution using nanosecond time resolved infrared spectroscopy	£60,311.11	04-Oct-01	03-Oct-04	University of Leicester	Chemistry
Announced	EP/D000866/1	Professor R Lambert	Chemistry	New Directions in Physical Organic Chemistry: The Heterogeneously Catalysed Asymmetric Hydrogenation of C=C Bonds	£422,647.64	01-Oct-05	30-Sep-08	University of Cambridge	Chemistry
Reconciled/Finished	GR/K82956/01	Professor M Page	Chemistry	REACTIVITY AND MECHANISMS OF REACTIONS OF FOUR MEMBERED AZAPHOSPHETIDINE RINGS	£51,242.00	01-Oct-96	30-Sep-99	University of Huddersfield	Chemical and Biological Sciences
Reconciled/Finished	GR/N06854/01	Professor J Sanders	Chemistry	MICRO ENVIRONMENT AND REACTIVITY WITHIN PORPHYRIN CAVITIES	£63,182.00	14-Apr-00	13-Apr-01	University of Cambridge	Chemistry
Reconciled/Finished	GR/M40851/01	Professor I Williams	Chemistry	COMPUTATIONAL EXPLORATION OF MECHANISTIC BORDERLINES FOR REACTIONS IN SOLUTION	£96,485.00	01-Mar-99	28-Feb-01	University of Bath	Chemistry
Announced	EP/D001641/1	Professor GJ Hutchings	Engineering & Phy Sciences Council	Cardiff Centre for Physical Organic Chemistry	£2,956,344.25	01-Oct-05	30-Sep-10	Cardiff University	Chemistry
Reconciled/Finished	GR/L58842/01	Professor GJ Hutchings	Infrastructure and Environment	NOVEL FRIEDL CRAFTS CATALYSTS USING CATION EXCHANGED ZEOLITES FOR THE CLEAN SYNTHESIS OF FINE CHEMICALS	£184,999.00	01-Oct-97	30-Sep-00	University of Liverpool	Chemistry