

## Development of the UK EPR National Service at Manchester

The EPR National Service provides high quality EPR facilities and expertise for members of the UK academic community. Funded through the EPSRC Chemistry Programme, the service has a unique range of EPR instrumentation and will now be developed to include a commercial high field W-band instrument. The service is also being restructured to locate all the instrumentation at a single centre at Manchester having an equipment base allowing 6 microwave frequencies (L, S, X, K, Q and W-bands), with options for variable temperature, single crystal, electrochemical studies, and spectrum simulation. During the one-year transitional phase there will also be a continuation of the high field service element at St-Andrews (90/180/270 GHz). Access to ENDOR measurements can be made via collaborative arrangements at Cardiff.

Training and extending the user base are important elements of the service and the centre encourages suppliers of samples to visit the centre in order to gain hands on experience in EPR.

General information on the EPR Service can be found at the service web site: <http://mch3w.ch.man.ac.uk/services/epresr/EPRmain.htm>. Contact Carmine Ruggiero at [carmine.ruggiero@epsrc.ac.uk](mailto:carmine.ruggiero@epsrc.ac.uk) for information about other EPSRC services.

*David Collison*

## ESR GROUP COMMITTEE.

The ESR Group committee was elected at the AGM held in Manchester on the 9 th. April 2003 and has the following members:

### Chair

Professor John C. Walton, *School of Chemistry, University of St. Andrews*

### Secretary

Dr John Maher, *Shanboe, Clarendon Avenue, Bishopston, Bristol, BS7 8JD*

### Treasurer

Dr Damien M. Murphy, *Department of Chemistry, Cardiff University*

### Ordinary Members

Dr Victor Chechik, *Dept. of Chemistry, York University*

Dr David Collison, *University of Manchester, Department of Chemistry*

Dr Shirley A. Fairhurst, *John Innes Centre, Norwich*

Dr Chris W. M. Kay, *Institut für Experimentalphysik, Free University of Berlin, Germany*

Dr Paul J. Krusic, *DuPont, Wilmington, Delaware, USA*

Dr Fraser Macmillan, *Universität Frankfurt, Department of Chemistry*

Dr Mark E. Newton, *Department of Chemistry, University of Warwick*

Dr Lesley Yellowlees, *Department of Chemistry, Edinburgh University*

Mr Richard Arnott, *Jeol UK.*

**Membership** of the ESR Group currently stands at about 100. All scientists who are members of the Royal Society of Chemistry, and have an interest in ESR/EPR spectroscopy, are invited and urged to tick the ESR Group box on their membership renewal forms. The cost is only £5 per annum! Membership carries entitlement to reduced registration fees at ESR Group annual conferences.

**Bursaries** are awarded for most of our annual meetings, and student attendance is subsidised. In 2004 there were 3 bursaries. Applicants should write to the Secretary to register their interest: give a brief CV. Preference is given to students presenting talks and posters.

### Website:

<http://www.esr-group.org.uk>



**Newsletter**

**edited by**

**John Walton**

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# ELECTRON SPIN RESONANCE GROUP

**RS•C**

ROYAL SOCIETY OF CHEMISTRY

## Newsletter March 2004

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### SpinDrift *from John Walton*

More than 4000 papers on ESR and its sibling techniques appeared in the last 15 months. The huge range of applications is remarkable. Growth areas include transition metal complexes, applications in medicine and dentistry, geochronological studies and multifrequency studies of spins in many types of materials and biological structures. Most regions of the Periodic Table are regularly visited by ESR spectroscopists although the most trodden areas contain the first row p- and d-elements. The phenomenal popularity of nitroxides (aminoxyls) continues unabated. This functional group attracts little attention from conventional organic chemists and hardly figures at all in undergraduate study programs. However, nitroxides exhibit just the right blend of chemical stability coupled with magnetic parameters that lead to information rich ESR spectra. Spin trapping with nitrones and nitroso-compounds is as popular as ever, particularly for "reactive oxygen species". Study of protein dynamics by spin labelling with nitroxides has been underway for some time. Then came the development of site directed mutagenesis.

These two techniques were then elegantly combined to produce site directed spin labelling. Extending this to double labelling of proteins has given impetus to quantitative structural studies. This is not the end of the nitroxide story, however. The same functional group is important in ESR imaging. Furthermore, the discovery of living radical polymerisation guarantees that the 3-line nitroxide triplet will be an ESR trademark for many years to come.

**The 36<sup>th</sup> ESR Group Meeting** took place last April at **Chancellor's Hotel & Conference Centre, University of Manchester**. Modern ESR relies heavily on computer control and computer analysis, so it was most appropriate that the conference was hosted at the centre where the first modern computer with a stored memory, the "Baby", was designed and built. The international appeal of ESR was emphasised by the wide mix of countries and cultures represented. The programme began with a lecture from Dr Eric McInnes of Manchester University who is manager of the EPSRC multifrequency EPR service. He described some rather nice examples of theory in action teasing out meaning from multifrequency experimental studies of large spin molecules. [cont. over]

*"Not the possession of truth but the effort in struggling to attain it brings joy to the researcher"– G. E. Lessing*

### 36<sup>th</sup> ESR Group Meeting (cont.)

Understanding photosynthesis remains a major driver of ESR innovation and this topic provided a cardinal theme running through the entire conference. Important contributions to understanding photosystem I, photosystem II and associated structures were made by David Britt, Mike Evans, Peter Heathcote, Ping Huang-Kenéz, William Rutherford, Oleg Poluektov and Chris Kay. The entire photosynthesis scenario was nicely integrated by Wolfgang Lubitz in his Bruker Prize lecture entitled "Signals from the Reaction Centre". Other themes included metalloenzymes, macromolecules (including dendrimers), molecular magnets, organic reactions and novel techniques. The Jeol student session, showcasing research from younger scientists, was notable for three high quality presentations and culminated in the award of the prize to Stephan Stoll. A bright display of posters on a diverse range of topics added colour and cachet to an outstanding conference.

**THANKS** The whole ESR community owes a huge debt of gratitude to **Dr Damien Murphy** University of Cardiff, Department of Chemistry for the many years he has worked tirelessly and efficiently as secretary of the ESR Group. It is largely due to his organisational skills that Group conferences and Group business have continued to flourish during the last few years. All Damien's endeavours have been marked by his characteristic charm and good taste that have endowed Group activities with style and polish. Sincere thanks are extended to Damien on behalf of the entire ESR constituency.

The RSC ESR Group thanks **Drs David Collison** and **Eric McInnes**, University of Manchester, Department of Chemistry, for their admirable work as local organisers of the 36th Group Meeting at Manchester.

### CONGRATULATIONS

To Professor **Wayne L. Hubbell**, Department of Chemistry and Biochemistry, UCLA on the award of the **Bruker Prize 2004** by the Royal Society of Chemistry ESR Group.

To **Dariusz Hinderberger**, Max-Planck-Institut Mainz, **Robert Hodgkins**, University of St. Andrews and **Maria Fittipaldi**, Leiden University on their selection as candidates for the **JEOL** Young Investigator Prize 2003.

### CALL FOR NOMINATIONS

The RSC ESR Group invites nominations for the Bruker Lecturer 2005. All nominations must be accompanied by a one page citation and should be sent to Dr John Maher c/o **Secretary@esr-group.org.uk**

### New Basic Technology Grant in Nanosecond Pulse ESR announced.

The UK Basic Technology Program is a major government initiative run by EPSRC "to develop UK capability in technology research to underpin the next generation of tools, techniques and processes that will form the basis of the industries of the future." This year the top rated proposal was a program to develop the mm-wave technologies required to build a next generation pulse ESR spectrometer capable of sub-nanosecond  $\pi/2$  pulses combined with sub-nanosecond deadtimes. Such a spectrometer would open powerful pulse ESR methodologies to perhaps the majority of paramagnetic systems studied today and provide the ability to take molecular snapshots at the earliest stages of many important chemical reactions. Collaborating universities on the program include St. Andrews, Dundee, Cardiff, Manchester, Warwick, UEA and QMC. For further information contact *Dr Graham Smith* (gms@st-andrews.ac.uk).

The IES invites nominations for: Gold Medal, Silver Medal (Instrumentation) and Young Investigator Awards and for Fellowship of the Society (visit <http://ieprs.org>). All nominations must be accompanied by a 100-150 word citation and should be made to Prof Yu. D. Tsvetkov; [tsvetkov@kinetics.nsc.ru](mailto:tsvetkov@kinetics.nsc.ru). The closing date is 15 November 2004.

### FORTHCOMING EVENTS

**June 11-16**, 2004; 9<sup>th</sup> International Symposium on Organic Free Radicals, Porto Vecchio, Corsica (France); Web: <http://www.iso9.com>.

**August 1-4**, 2004; International EPR Symposium of the Rocky Mountain Conference Denver, Colorado, USA; Web: <http://www.epr-symposium.du.edu/>.

**August 15-20**, 2004; EPR<sub>60</sub> Modern Development of Magnetic Resonance, Kazan, Russia; Web: <http://www.kfti.knc.ru/EPR60/eng/>

**October 24-29** 2004; 15<sup>th</sup> ISMAR Meeting, Jacksonville, Florida, USA; Web: <http://www.ismar.org/>

**April** 2005; 38<sup>th</sup> International Meeting of the RSC ESR Group in Bath and **April 2006** in Edinburgh.

### THE ESR GROUP WEB SITE – <http://www.esr-group.org.uk>

Apart from discovering a willing horse to act as the ESR Group Secretary, the other reason that I was elected was to start a new Web site! The previous site was ably run by Chris Rowlands and was hosted on a server in the Chemistry Department at Cardiff University. Chris retired so that we needed a new Web maestro. It is now important for Groups such as ours to have as high a profile Web site as possible. In the dozen years since the World Wide Web first started, it has changed from a physicist's communication tool to a new medium altogether, and 'wwws' appear as commonly as telephone numbers.

We are registered with Nominet, the UK internet naming organisation, as **esr-group.org.uk**, you can see our details at <http://www.nominet.org.uk> by doing a 'whois' search. Note that we have an alternative name appearing on the web as <http://www.epr-group.org.uk>, the reason for this was that we felt that it would be sensible to have the 'EPR' name as well. We are the first RSC special interest group to register a name, all of the others, if they have a web site, then you find it buried in a long URL. Our profile must have increased; during January we were 'hacked' and our top index page replaced with a nasty, but juvenile, announcement from the 'clever' perpetrators of the hack. Did anyone notice?

The design of web sites is somewhat of an art form nowadays, but apart from looking attractive, the most important aspects are that it is up to date, that the information is accurate, that it is easy to navigate, and that it 'works' with whomsoever is looking at the information. I have tried to make the site conformant with present web standards, this should help to make it readable 'out there', there are still problems, and I'm indebted to the Committee for their comments. The main purpose of the site is to act as a flagship for our annual international meetings and to provide an advertisement for our ESR Group. I have put some historical information onto it – both about the ESR Group's previous conferences, and about our subject. We need some more general information for the lay public since the public understanding of our science is very important. In future I hope that much of the annual conference proceedings can be published, so for the 2004 Warwick meeting you should be able to see abstracts of the plenary lectures, general lectures and poster information. This is only a start and other ideas will no doubt develop, so over to you the members: ideas please?

*John Maher, ESR Group Secretary*