

The **EPSRC National EPR/ENDOR Service** is based across the Universities of Manchester, St Andrews and Cardiff. Manchester (Chemistry Department) provides facilities for CW EPR at L (ca. 1), S (4), X (9), K (24) and Q-bands (34 GHz) at temperatures between 4 and 300 K at all frequencies, and up to 700 K at X-band. X- and Q-band CW ENDOR facilities are available at Cardiff. St Andrews (Physics and Astronomy Department) offer CW EPR at 90, 180 and 270 GHz. The Service is available to all academic researchers eligible for EPSRC funding, and is free at "point of sale". Workers in the areas of biological, pharmaceutical or materials science are welcomed. Research collaborations with international, industrial or institutional organisations are possible. Anyone interested in using the Service should contact: Dr David Collison (david.collison@man.ac.uk) or Dr Eric McInnes (eric.mcinnnes@man.ac.uk), Dr Graham Smith (St Andrews, gms@st-andrews.ac.uk), or Dr Damien Murphy (Cardiff, MurphyDM@cardiff.ac.uk) in the first instance. *Eric McInnes*

## ESR GROUP COMMITTEE.

The ESR Group committee was elected at the AGM held in Aberdeen on 10th April 2002 and has the following members:

### Chair

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

### Secretary/Treasurer

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

### Conference Organisers

Drs Eric McInnes and David Collinson, Department of Chemistry, University of Manchester

### Ordinary Members

Dr Shirley A. Fairhurst, John Innes Centre, Norwich

Dr Simon K. Jackson, Dept. Medical Microbiology, University of Wales College of Medicine, Cardiff

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

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

Dr David J. Lowe, John Innes Centre, Norwich

Dr Mark E. Newton, Department of Chemistry, University of Warwick  
Dr Graham Smith, School of Physics, University of St. Andrews  
Dr Lesley Yellowlees, Department of Chemistry, Edinburgh University

**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 £2 per annum! Membership carries entitlement to reduced registration fees at ESR Group annual conferences.

### Website

<http://www.cardiff.ac.uk/esr/Group/homepage.html>



**Newsletter**  
edited by  
**John**  
**Walton**

Hypotheses are nets: only he who casts will catch" *Novalis*

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# ELECTRON SPIN RESONANCE GROUP

## Newsletter March 2003

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**RS•C**  
ROYAL SOCIETY OF CHEMISTRY

### SpinDrift *from John Walton*

In its early years ESR spectroscopy was one of the key reference points for testing QM theory. The classic INDO semi-empirical MO method related experimental data to predictions from quantum mechanics. Modern ab initio DFT theory, with sophisticated basis sets, enables isotropic and anisotropic hyperfine interactions to be computed with an accuracy undreamed of a few years ago. However, a major trend in the last few years has been away from theory and towards the application of ESR techniques to probing natural phenomena and solving problems in biology, chemistry, catalysis and related branches of science. ESR and its sibling techniques are becoming integrated with large projects bringing a whole armoury of analytical instrumentation to the most challenging projects in a holistic fashion.

More than 1500 papers on ESR appeared in 2002-03. Many of these were orthodox studies in well trodden areas such as polymerisation, oxidative stress, spin trapping or TM complex characterisation. Notable growth was registered in the area of spin labelling

(83 papers) with applications to protein dynamics, membrane-peptide interactions, muscle fibers and carbohydrates. ESR has penetrated into areas as diverse as spin mapping in organic conductors, analysis of spectra with large quadrupole couplings, gut fluids of caterpillars, dating of hominid sites in Southern China and dose rates in tooth enamels. This is rather vivid evidence of the robust adaptability of the technique to 21st. century demands.

**The 35<sup>th</sup> ESR Group Meeting** took place last April amidst the baronial splendour of **Aberdeen University's King's College Conference Centre**. ESR depends critically on a combination of electric and magnetic fields. It was most appropriate therefore that ESR should "come home" to the place where James Clerk Maxwell, the father of modern electro-magnetic theory, worked for many years. The global importance of ESR was illustrated by the large range of nationalities and disciplines represented amongst the 110 participants. The quality of the scientific programme matched the senatorial character of the conference lecture facilities. The programme commenced with a fine lecture on Imaging of Free Radicals In Vivo Using Overhauser Techniques by [cont. over]

"Optimism is the oxygen of innovation and the ozone of discovery" – *Anon*

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

Aberdeen's David Lurie. Plenary lectures by Jay Sweier (John Hopkins), Karsten Mäder (Hoffmann-LaRoche, Basel), Bernard Goodman (Scottish Crop Research Institute), Ronald Mason (NIEH), David Collison (Manchester), Angelo Alberti (Bologna), Thomas Prisner (JW Goethe University) were balanced by shorter talks covering many new applications and techniques. The keynote Bruker Lecture was given jointly by **Gareth** and **Sandra Eaton** (Denver) on the general theme of interaction of electron spins. The Jeol session, where three PG students gave showcase lectures in competition for the Jeol student prize, was another highlight. Congratulations to **Anna Ferretti** (Milano) the eventual winner. Bernard Goodman's dictum that "*the only place for 'spin' in science should be in the context of magnetic resonance*" received vigorous endorsement throughout this outstanding conference.

**David H Whiffen**, pioneer ESR spectroscopist died in December 2002.

His research career began at Oxford in 1943 where he worked on IR and microwave radiation with Sir Harold W. Thompson. Moving to Birmingham in 1949 he continued work with IR but became interested in free radicals. He constructed an early ESR spectrometer and carried out world-leading experimental and theoretical work on glycine and other radicals trapped in crystals. At John Pople's invitation he moved to the National Physical Laboratory in 1958 and over the next few years published many seminal papers on EPR and ENDOR spectra of inorganic ions and organic free radicals at 9 and 35 GHz. He was elected FRS in 1966. Whiffen became Professor of Physical Chemistry at Newcastle in 1968 eventually rising to Pro-Vice-Chancellor. He will be remembered for, among other attributes, his brilliant and insightful mind.

**THANKS** The RSC ESR Group thanks **Dr David Lurie**, head of the Free Radicals Imaging Group at Aberdeen University, for his admirable work as local organiser of the 35<sup>th</sup> Group Meeting at Aberdeen.

### CONGRATULATIONS

To Professor **Wolfgang Lubitz** of the Max Plank Institute for Radiation Chemistry at Mülheim an der Ruhr on the award of the **Bruker Prize 2003** by the Royal Society of Chemistry ESR Group. Recent articles include: *Single Crystal EPR Studies of the Reduced Active Site of [NiFe]-Hydrogenase from Desulfovibrio vulgaris Miyazaki FS*. Foerster, M.; Stein, M.; Brecht, H.; Ogata, Y.; Higuchi, H. Lubitz, W., *J. Am. Chem. Soc.* **2003**, *125*, 83 and *Radicals, Radical Pairs and Triplet States in Photosynthesis*. Lubitz, W.; Lenzian, F.; Bittl, R. *Acc. Chem. Res.* **2002**, *35*, 313.

To Stefan Stoll (Swiss Federal Institute of Technology), Franco Bella (St. Andrews) and Antonio Catalan (Cambridge) on their selection as candidates for the **JEOL** Young Investigator Prizes 2003.

### FORTHCOMING EVENTS

37<sup>th</sup> International Meeting of the RSC ESR Group will take place in April 2004: venue to be announced.

5<sup>th</sup> Meeting of the European Federation of EPR Groups will be held in Lisbon, Portugal, from Sunday 7<sup>th</sup> to Thursday 11<sup>th</sup> September 2003. Details at: [\*http://dequim.ist.utl.pt/EFEP/\*](http://dequim.ist.utl.pt/EFEP/)

26<sup>th</sup> International EPR Symposium at 45<sup>th</sup> Rocky Mountain Conference on Analytical Chemistry, July 27-August 31, 2003, Denver, Colorado, USA.

8th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena (SCM2003), will take place in Chapel Hill, North Carolina, September 21-26, 2003. Details at: [\*www.chem.unc.edu/conferences/SCM2003\*](http://www.chem.unc.edu/conferences/SCM2003).

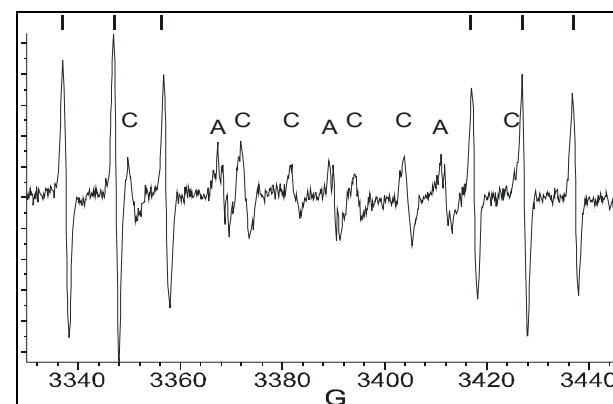
The Asia-Pacific EPR/ESR Symposium 2003 (APES03), November 17-20 at the Indian Institute of Science, Bangalore, India. Contact Prof. S.V. Bhat, Department of Physics, Indian Institute of Science, Bangalore 560012, India. Details at: [\*http://physics.iisc.ernet.in/~apes03\*](http://physics.iisc.ernet.in/~apes03)

9th International Symposium on Organic Free Radicals to be held June 11th to 16th, 2004, in Porto Vecchio, Corsica (France). [\*http://www.isofr9.com\*](http://www.isofr9.com)

### LAUNCH OF ORGANIC & BIOMOLECULAR CHEMISTRY

For many decades Perkin Transactions 2 served the world community of physical organic chemists as the premier journal for dissemination of their major advances. Irresistible winds of change blew through the RSC in 2002 and snuffed out publication. May this treasury of top quality science rest in peace!! *Organic & Biomolecular Chemistry* was launched in January 2003 as the successor to *Perkin 1 & 2*. The new journal is edited by Ben Feringa, of Groningen University, whose main research interests centre in organic synthesis and stereochemistry. *OBC* will have broad scope including established areas, outstanding achievements in Organic Chemistry as well as the interface with Biology, Medicine and Materials Science. *OBC* is lavish in its use of colour. We wish *OBC* every success in its quest for comprehensive excellence.

### QUIZ



The 9 GHz EPR spectrum shown to the left was obtained on photolysis of a solution of  $\text{PhCH=NOC(O)C(O)N(Bn)-(CH}_2\text{)}_3\text{CH=CH}_2$  and *p*-methoxybenzophenone in *t*-butylbenzene at 220 K. Identify the 3 radicals I, A and C. (For the answer see: *Chem. Commun.* **2002**, 2086.)

"Everything has been thought of before, but the problem is to think of it again" *J. W. von Goethe*