

14th INTERNATIONAL MEETING ON NMR SPECTROSCOPY

UNIVERSITY OF EDINBURGH

27 June – 2 July 1999

Poster presentations form a significant part of the meeting and two formal poster sessions are included within the scientific programme. Tuesday 29 June at 16:20 Poster Session A Even *numbered posters* Thursday 1 July at 16:20 Poster Session B Odd *numbered posters*. Posters will be located on the Concourse and Balcony of Appleton Tower and will be on display from Monday through to the close of the Meeting. Posters can be mounted from 08:30 on Monday morning and should be removed at coffee time on Friday 2 July.

MONDAY 28 JUNE

09.00 WELCOME

SYMPOSIUM 1 - NEW EXPERIMENTAL TECHNIQUES

Chairman - Professor John Lindon, *Imperial College, London, UK*

* denotes the presenter of the paper; main author is underlined

- 09.05 I1 **"Lighting Up" NMR and MRI.** A Pines *University of California, Berkeley, USA*
- 09.55 O1 **Simulation of chemical exchange lineshapes.** A D Bain *McMaster University, Hamilton, Canada*
- 10.25 COFFEE
- 10.55 O2 **Application of a new high pressure NMR flow cell to the *in situ* study of homogeneous catalysis.** J A Iggo*. D Shirley, B T Heaton, N M Perex, R Mhyman and A Wright *University of Liverpool, UK*
- 11.25 I2 **Improving the performance of nanoliter-volume NMR using microcoils.** J Sweedler *University of Illinois, USA*
- 12.15 LUNCH

SYMPOSIUM 2 - PHYSICAL

Chairman - Dr Melinda Duer, *University of Cambridge, UK*

- 14.00 I3 **High resolution double quantum MAS NMR of solids: A new tool for structural investigations.** H W Spiess *Max-Planck Institute, Mainz, Germany*
- 14.50 O3 **The application of ¹H breadline, ¹³C MAS, Goldman-Shen and 2D-WISE methods to the morphology of nascent and moulded ultra-high molecular weight polyethylene.** P G Klein* and J T E Cook *University of Leeds, UK*

- 15.15 TEA
- 15.45 O4 **PFG NMR studies of diffusion in coked zeolite catalysts.** P J Barrie* and B Paweewan *University of Cambridge, UK*
- 16.10 O5 **Density functional theory study of the structural requirements for scalar-coupling and magnetic shielding associated with base pair hydrogen-bonding.** M Barfield*, A J Dingley and S Grzeziek *University of Arizona, USA*
- 16.35 I4 **Solid-state NMR: Structural and dynamical investigations.** B H Meier, *ETH Zentrum, Switzerland*
- 17.25 CLOSE OF SESSION

TUESDAY 29 JUNE

SYMPOSIUM 3 - MACROMOLECULAR

Chairman - Dr Jim Feeney, *National Institute for Medical Research, London, UK*

- 09.00 I5 **NMR and modular proteins.** I D Campbell *University of Oxford, UK*
- 09.50 O6 **Solution structure of an activity modulating domain from bovine inhibitor of F₁ ATPase (IFI).** D J Gordon-Smith, P J G Butler, J Walker and D Neuhaus* *MRC Laboratory of Molecular Biology, Oxford, UK*
- 10.15 COFFEE
- 10.45 I6 **Protein Folding Intermediates.** J Waltho *University of Sheffield, UK*
- 11.35 I7 **Advances in NMR Structure Refinements.** A Gronenborn *National Institutes of Health, Bethesda, USA*
- 12.25 LUNCH

SYMPOSIUM 4 - SOLID AND INORGANIC

Chairman - Dr Geoff Hawkes, *Queen Mary & Westfield College, London, UK*

- 14.00 I8 **From proteins to protozoa: NMR and quantum chemical studies in chemistry and biology.** E Oldfield *University of Illinois at Urbana-Champaign, USA*
- 14.50 O7 **¹H-¹¹⁹Sn J-HMBC spectroscopy in advanced structural organotin chemistry** R Willem*. M Biesemans, J C Martins, A Lycka, J Holecek and K Jurkschat *Vrije University Brussels, Belgium*
- 15.10 O8 **NMR characterisation of silicon clusters inside zeolite Y: ²⁹Si, ¹H spin counting and ²⁹Si-²⁷Al reapid** Y Ba, J He, CI Ratcliffe*, J A Ripmeester and J S Tse *Steacie Institute for Molecular Sciences, Canada*

15.30 **I9 MAS NMR - from isolated homonuclear spin pairs to large(r) (re)coupled spin systems** A Sebald *University of Bayreuth, Germany*

16.20 TEA and POSTER SESSION A

In recognition of the growing interest in robotic flow injection NMR, a discussion session will take place in Lecture Theatre 1 (Ground Floor Appleton Tower)

DISCUSSION SESSION-ROBOTIC FLOW INJECTION NMR

Chairman - Dr Mike Bernstein *Astra Charnwood, UK*

Start 15.10 in Lecture Theatre 1

Session closes 16.20 for TEA and POSTER SESSION A

TUESDAY EVENING - POSTGRADUATE SESSION

Chairman - Dr D B Davies, *Birkbeck College, University of London, UK*

17.00 **O9 MQMAS NMR for the study of alkali-metal distributions in alkali-metal silicate glasses.** A J Painter* and M J Duer *University of Cambridge, UK*

17.20 **O10 Heteronuclear chemical shift correlation in solid-state NMR by through-bond multiple-quantum spectroscopy.** D Sakellariou *Ecole Normal Supérieure de Lyon, France*

17.40 **O11 Enhancing NMR signals with laser-polarized xenon.** B M Goodson *University of California Berkeley, USA*

18.00 **O12 Resolution of overlapping peaks in ^1H - ^{15}N relaxation experiments.** C Webb *University of Leicester, UK*

18.20 SESSION ENDS

WEDNESDAY 30 JUNE

SYMPOSIUM 5 - BIOMEDICAL I (emphasis on Cellular Aspects)

Chairman - Professor Jeremy Everett, *Pfizer Central Research, UK*

09.00 **I10 Subcellular metabolism of water and heavy water as detected by ^{13}C NMR.** S Cerdan *Institute Investigadones Biomedicas CSIC, Spain*

09.45 **I11 Diffusion coherence in erythrocytes.** P Kuchel *University of Sydney, Australia*

10.30 COFFEE

11.00 **O13 ^1H NMR spectroscopy as a tool for assessing the effect of moderate hypothermia on primary porcine hepatocyte metabolism.** K J Dabos*. J A Parkinson, L J Nelson, C Hewage, J N Plevris, P C Hayes and I H Sadler *University of Edinburgh, UK*

- 11.20 O14 **New methods in ^1H *in vivo* spectral editing.** D L Hardy *University of Leicester, UK*
- 11.40 I12 **Studies of tumour cell metabolism by ^{31}P NMR spectroscopy.** W Hull *German Cancer Research Centre, Heidelberg, Germany*
- 12.25 LUNCH - Excursions

EXCURSIONS

PLEASE NOTE that due to the full programmes for Excursion 2 (Glenturret Distillery) and Excursion 3 (Loch Lomond Cruise), coaches will depart at 13.00 from Appleton Tower. This allows just over 30 minutes for lunch in Teviot Row - excursion ticket holders are asked to go to the dining hall as quickly as possible. The organisers apologise for the inconvenience, but feel sure that the excursions will be worth the slight rush!

THURSDAY 1 JULY

SYMPOSIUM 6 - ORGANIC

Chairman - Dr David Rycroft, *University of Glasgow, Scotland, UK*

- 09.00 I13 **Use of primary and secondary deuterium isotope effects on chemical shifts and theoretical calculations of these in structural and conformational studies of hydrogen-bonded and/or tautomeric systems .** P-E Hansen *Roskilde University, Denmark*
- 09.50 O15 **Intramolecular hydrogen-bonding in nipecotic acid derivatives. Conformational analysis by NMR spectroscopy.** N Aboitiz *, R J Abraham, B S Sherborne and I Whitcombe *University of Liverpool, UK*
- 10.15 COFFEE
- 10.45 I14 **Automated structure elucidation of organic molecules based on NMR correlation spectroscopy.** J-M Nuzillard *University of Reims, France*
- 11.35 I15 **Spectrum estimation of ^{13}C -NMR spectra using stereochemical information: A decisive tool during the structure elucidation process.** W Robien *University of Vienna, Austria*
- 12.25 LUNCH

SYMPOSIUM 7 - HYPHENATED NMR TECHNIQUES

Chairman - Dr Alistair Swanson, *Pfizer Central Research, Kent, UK*

- 14.00 I16 **Application of hyphenated NMR techniques for the rapid characterisation of drug metabolites and process impurities.** J P Shockcor *DuPont Pharmaceutical, USA*

- 14.50 O16 **Determination of sites of glucuronidation using LC-NMR.** R J Lewis*. M A Bernstein and IJ Martin *Astra CHarnwood, UK*
- 15.10 O17 **HPLC-NMR coupling: A tool for rapid assignment and quantification of complex mixtures.** Maier *BASF, Ludwigshafen, Germany*
- 15.30 I17 **Hyphenation of capillary separation techniques with NMR spectroscopy**
K Albert *University of Tübingen, Germany*
- 16.20 **TEA and POSTER SESSION B**

THURSDAY EVENING - POSTGRADUATE SESSION

Chairman - Dr H Parkes *Institute of Child Health, London, UK*

- 17.00 O18 **Quantitative measurement of long range NOEs.** G J Harris
University of Leicester, UK
- 17.20 O19 **Solid-state NMR studies of PrP89-143.** D D Laws *University of California Berkeley, USA*
- 17.40 O20 **Chain diffusion in long n-alkane crystals studied by ¹³C NMR.** M A Driver *University of Leeds, UK*
- 18.00 O21 **High resolution magic angle spinning NMR spectroscopy of living tissues and its application in toxicology.** S Garrod *Imperial College, London, UK*
- 18.20 SESSION ENDS

FRIDAY 2 JULY

SYMPOSIUM 8 - BIOMEDICAL II

Chairman - Professor Peter Sadler, *University of Edinburgh, Scotland, UK*

- 09.00 I18 **Exploiting Paramagnetism in Biological NMR.** C Luchinat *University of Florence, Italy*
- 09.50 I19 **Unusual proteins and uncommon NMR nuclei.** H Vogel *University of Calgary, Canada*
- 10.40 COFFEE
- 11.10 I20 **TROSY in Structural Biology.** K Wüthrich *ETH, Zürich, Switzerland*
- 12.00 CLOSE OF MEETING
