

# 12<sup>th</sup> INTERNATIONAL MEETING

UMIST, MANCHESTER,

2-7 July 1995

## SCIENTIFIC PROGRAMME

The scientific sessions commence at 09.00 on Monday 3 July in the C16 Theatre in the Renold Building. Coffees and teas will be served in the **C Floor concourse**, of the Renold Building at the times stated in the programme.

The eight symposia which make up the meeting comprise both invited lectures and shorter contributed talks.

In addition, the main themes of the meeting are supported by an extensive poster session which will allow a wide coverage of related current activity and provide a forum for informal discussion. Timetabled sessions for formal viewing and discussion of posters are on **Tuesday 4 July (16.10-17.30) and Thursday 6 July (16.10-17.30)**, with **ODD** numbered posters officially manned on the Tuesday and **EVEN** numbered posters manned on the Thursday.

The poster display area is located in the **B Floor concourse** in the Renold Building.

**PARTICIPANTS ARE REMINDED THAT THE RECORDING OF LECTURES OR THE TAKING OF PHOTOGRAPHS DURING LECTURES IS NOT PERMITTED.**

The detailed programme of the Meeting is as follows:

*\* Denotes the presenter of the contributions.*

### Monday 3 July

09.00 Welcome and Opening Remarks

#### Symposium I - Experimental Techniques

**Chairman:** Dr J Keeler *University of Cambridge*

09.10 **I.1 <sup>13</sup>C-<sup>13</sup>C Magnetic Dipolar Couplings in Solids and Liquid Crystals.** M Levitt *University of Stockholm, Sweden*

10.00 **O.I Measurement and Use of In-phase and Antiphase Transverse Relaxation Times in Homonuclear Scalar Coupled Spin Systems.** T Norwood *University of Leicester*

10.30 COFFEE

11.00 **I.2 Recent Progress with NMR Methods.** G Wagner *Harvard Medical School. USA*

11.50 **I.3 New NMR Experiments using Excitation Sculpting.** A J Shaka *University of California, Irvine, USA*

12.30 LUNCH

**Symposium II - NMR of Biological Macromolecules**

**Chairman:** Dr M P Williamson *University of Sheffield*

\* Denotes the presenter of the contributions,

- 14.00 **I.4 Structures of Protein-Protein and Protein-DNA Complexes by MultiDimensional NMR.** G M Clore *National Institutes of Health, Bethesda, USA*
- 14.50 **O.2 Structure and Folding-Kinetics of Bovine  $\alpha$ -Lactalbumin, Determined with NMR Spectroscopy.** J Balbach\*, V Forge, C M Dobson *University of Oxford*
- 15.20 **O.3 An Investigation of NOE-Constrained Docking of Ligands to Proteins.** M J Gradwell *National Institute for Medical Research, London*
- 15.50 TEA
- 16.20 **O.4 Solution Structures of Complex Formation Between Analogues of a DMA Minor Groove Binding Molecule and the Duplex d(CGCGAATTCGCG)<sub>2</sub>.** J A Parkinson\*, I H Sadler, S E Ebrahimi, J H McKie and K T Douglas *University of Edinburgh*
- 16.50 **I.5 NMR Studies of RNA Recognition by Basic-Domain HIV Regulatory Proteins and by RNP Proteins.** G Varani *MRC Laboratory of Molecular Biology, Cambridge*
- 17.40 CLOSE

**Tuesday 4 July**

**Symposium III - Biomedical NMR Spectroscopy**

**Chairman:** Professor J K Nicholson *Birkbeck College, University of London*

- 09.00 **I.6 Molecular Diffusion in Cells.** P W Kuchel *University of Sydney, Australia*
- 09.50 **O.5 NMR Studies on Lipid Peroxidation in Human and Rat Plasma.** G E Hawkes\* and C Z Smith *Queen Mary & Westfield College, University of London*
- 10.25 COFFEE
- 11.00 **I.7 Metabolic Trafficking in Clonal and Primary Brain Cells.** D Leibfritz *University of Bremen, Germany*

11.50      **O.6 Metal- and Drug-Induced Structural Transitions of Albumin Detected in Human Blood Plasma by NMR Spectroscopy.** P J Sadler\*, J Christodoulou and A Tucker *Birkbeck College, University of London*

12.15      CLOSE

#### **Symposium IV - NMR in Inorganic Chemistry**

**Chairman:**     Dr K G Orrell *University of Exeter*

14.00      **I.8 Recent Applications of Chemical Shifts to Problems in Inorganic and Organometallic Chemistry.** B Wrackmeyer *University of Bayreuth, Germany*

14.45      **O.7 Detection of Hidden Intermediates in Polyoxometallate Chemistry.** O W Howarth\*, J J Hastings, I Andersson and L Pettersson *University of Warwick*

15.05      **O.8 The Immobilization of Transition Metal Catalysts - A Solid-State NMR Study.** J Blümel *Technical University of Munich, Germany*

15.25      **I.9 Two Dimensional Methods in Organometallic and Coordination Chemistry.** W McFarlane *University of Newcastle upon Tyne*

16.10      TEA AND POSTER SESSION

18.00      STUDENT RECEPTION

#### **Tuesday Evening - Postgraduate Session**

**Chairman:**     Professor L H Sutcliffe *University of Surrey*

20.00      **O.9 Magnetic Resonance Studies of Selected Model Traction Fluids.** M M Britton\*, D G Gillies and L H Sutcliffe *University of Surrey*

20.20      **O.10 Measurement and Use of  $^{13}\text{C}$  and  $^1\text{H}$  Relaxation in Uniformly  $^{13}\text{C}$  Labelled Molecules.** A Chaudhry\*, L-Y Lian and T J Norwood *University of Leicester*

20.40      **O.11 A Robust NMR Technique for Isolating the Signal of Molecules Whose Diffusion has been Restricted.** S A Clark\*, M A Horsfield, S C R Williams and T J Norwood *University of Leicester*

21.00      **O.12 Temporal Development of Mesoporous Silica Studied using Deuterium NMR Spectroscopy.** M Edgar *University of Southampton*

21.20      **O.I 3 Spectral Editing Technique for the Detection of Ethanolamine *in vitro* and *in vivo*.** D L Hardy\*, R W Wilson, T Jessel, S C Smart, S C R Williams and T J Norwood *University of Leicester*

21.40      **O.I 4 Measurement of Long- Range Coupling Constants in Proteins.** J M C Ionides\*, J Keeler and D Neuhaus *Medical Research Council*

22.00      CLOSE

### Wednesday 5 July

#### Symposium V - Solid State NMR

**Chairman:**     Dr J Klinowski *University of Cambridge*

09.00      **I.10 Ultrasensitive NMR: Results and Prospects.** D Weitekamp  
*California Institute of Technology, USA*

09.45      **0.15 Elucidating the Structure of Inorganic Glasses: Progress by 2D NMR and Satellite Transition Spectroscopy.** C Jager\*, K Herzog, G Kunath, M Feike, B Thomas and H W Spiess *Max-Planck Institute, Germany*

10.05      **O.I6 Small Chemical Shielding Anisotropies and Quadrupole Couplings from  $^{133}\text{Cs}$  MAS NMR.** J Skibsted\*, T Vosegaard, H Bildsøe and H J Jakobsen *Aarhus University, Denmark*

10.25      COFFEE

10.55      **O.I7 Static, MAS and DOR Studies on Blends of Polyamide-6 and Polystyrene Ionomers.** T Nunes *ICTPOL, Portugal*

11.15      **O.I8 Scope and Limitations of Solid State  $^2\text{H}$  NMR Lineshape Analysis and Spin-Lattice Relaxation Time Measurements.** A E Aliev\* and K D M Harris *University College, London*

11.35      **I.11 The Structure and Dynamics of Inorganic Liquids and Glasses observed by Multi-Nuclear and Multi-Dimensional NMR.** I Farnan *CNRS, Centre de Recherches sur la Physique des Hautes Températures, Orléans, France*

12.20      CLOSE

### Thursday 6 July

#### Symposium VI - NMR in Physical Chemistry

**Chairman:**     Dr J W Emsley *University of Southampton*

09.00      **I.12 Molecular Dynamics Simulations and Spin Relaxation: Electronic and Nuclear Relaxation in Aqueous Ni(II).** J Kowalewski *University of Stockholm, Sweden*

09.50      **O.I9 Chemical Exchange in the Time Domain.** A D Bain\* and G J Duns *McMaster University, Ontario, Canada*

- 10.20 COFFEE
- 10.50 **I.13 Chemical Shift Tensors: Their Measurement and Utility in the Three Dimensional World of Chemistry.** D Grant *University of Utah, USA*
- 11.40 **I.14 Chemical Shifts in Proteins: Their Prediction and Use in Structure Refinement and Determination.** E Oldfield *University of Illinois at Urbana-Champaign, USA*
- 12.20 CLOSE

### Symposium VII - NMR Imaging

**Chairman:** Professor K J Packer *University of Nottingham*

- 14.00 **I.15 Rheological Characterisation of Complex Fluids by NMR Microscopy**  
P T Callaghan *Massey University, New Zealand*
- 14.50 **I.16 Chemical and Dynamic Information from Catalyst Systems Using In-situ NMR.** G Nesbitt *Koninklijke/Shell-Laboratorium, Amsterdam, The Netherlands*
- 15.40 **O.20 The Stray Field Imaging Technique: A Survey and Some New Results**  
E W Randall *Queen Mary & Westfield College, London*
- 16.10 TEA AND POSTER SESSION II

### Friday 7 July

### Symposium VIII - NMR in Organic Chemistry

**Chairman:** Dr A M Chippendale *Zeneca Specialities*

- 09.00 **I.17 The Conformation and Dynamics of Carbohydrates as Studied by NMR Spectroscopy.** H van Halbeek *University of Georgia, USA*
- 09.50 **O.21 Coupling Constant Criteria for Eclipsed Conformations.** J E Anderson\* and A I Ijeh *University College, London*
- 10.15 COFFEE
- 10.45 **O.22 High-Resolution Fluorine-19 Spectra of Organic Solids.** S Carss\* and R K Harris *University of Durham*
- 11.10 **O.23 Pattern Recognition Techniques Applied to <sup>1</sup>H and <sup>13</sup>C NMR Spectra of Edible Oils.** I J Colquhoun\*, E K Kemsley and R H Wilson *Institute of Food Research, Norwich*

11.35      **I.18 Damping, Deconvolution, Diffusion and Hofstadter's First Law.**  
G A Morris *University of Manchester*

12.25      CLOSE

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