

10th INTERNATIONAL MEETING, UNIVERSITY OF ST ANDREWS,

8-12 July 1991

SCIENTIFIC PROGRAMME

The scientific sessions take place in Theatre 300 in the Department of Chemistry, Purdie Building. Coffees and teas will be served in the Student Common Room, Department of Chemistry at the times stated in the programme.

All eight symposia, which make up the meeting, have Plenary Lectures and shorter talks associated with them, and each is in charge of its chairman.

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. Time tabled sessions for formal viewing and discussion of posters are on Tuesday 9 July (16.10 to 17.00) and Thursday 11 July (16.10 to 17.00), with EVEN numbered posters being formally manned on the Tuesday and ODD numbered posters - being manned on the Thursday.

The poster display area is in the Heddle and Connell Laboratories (Rooms 109 and 110).

The underlining of the name denotes the presenter of the contributions (where known).

The detailed programme of the Meeting is as follows:

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

MONDAY 8 JULY

09.00 WELCOME by the Principal of the University of St Andrews, Professor S Arnott, FRS

SYMPOSIUM A - New Experimental Techniques

Chairman: Professor R Freeman *University of Cambridge*

09.10 **New Angles in Solid-State NMR.** A Pines *University of California, Berkeley, USA*

10.05 **New Developments in Homonuclear Cross-Polarisation.** A J Shaka *University of California, Irvine, USA*

10.25 Multiple-Quantum NMR Experiments for Studying Spin 3/2 and Spin 5/2 Quadrupolar Relaxation. S C Wimperis *University of Manchester*

10.45 COFFEE

- 11.15 Gradients, Ramps and Transfer Functions: Separating the Sheep from the Goats. J H Keeler *University of Cambridge*
- 12.00 Absorption Mode Phase-Sensitive Zero-Quantum Spectroscopy. T H Norwood *University of Leicester*
- 12.20 CLOSURE OF SESSION

SYMPOSIUM B - Biological Macromolecules

Chairman: Professor G C K Roberts *University of Leicester*

- 14.00 **Structure-Function Studies in Solution by Isotope-Assisted NMR: Which Nuclei? How Many Dimensions?** J Markley *University of Wisconsin, Madison, USA*
- 14.50 NMR Structures of Two Different Protein DMA-Binding Motifs Based on Zinc: Fragments from Oestrogen Receptor and SW15. D Neuhaus, C van Mierlo, G Scott, N Darby and T Creighton* *IMB, Cambridge and *EMBL, Heidelberg, Germany*
- 15.10 3-D NMR Structure of an IgG-binding Domain of Streptococcus Protein G. L-Y Lian, J P Derrick, J C Yang, M J Sutcliffe and G C K Roberts *University of Leicester*
- 15.30 TEA
- 16.00 **Studies of Protein Ligand Interactions Using Isotopic Labelling and Multidimensional NMR.** J Feeney *NIMR, Mill Hill*
- 16.50 Drug-Calmodulin Interactions, and Phosphatidylinositol Headgroup Conformations, Viewed Through Protons and Deuterons. D G Reid *SmithKline Beecham*
- 17.10 Recent Improvements in the Solution Conformation Analysis of Carbohydrates. H van Halbeek and L Poppe *University of Georgia, Athens, USA*
- 17.30 CLOSURE OF SESSION

TUESDAY 9 JULY

SYMPOSIUM C - Solid State NMR

Chairman: Professor K J Packer *BP International*

- 09.00 **Rotational Resonance.** A McDermott, F Creuzet, L K Thompson, M Auger, R Gebhard, I van der Hoef, J Herzfeld, J Lugtenburg, M H Levitt and R G Griffin *MIT, Cambridge, USA, University of Leiden, The Netherlands and Brandeis University, Maryland, USA*

- 10.00 Polarisation Transfer Across Interfaces. N Zumbulyadis *Eastman Kodak, USA*
- 10.30 COFFEE
- 11.00 **Applications of NMR Spectroscopy to the Study of Catalyst Systems.**
A T Bell *University of Berkeley, USA.*
- 12.00 2D Solid State NMR Studies of Polymer Dynamics in Multicomponent Glass via ^{13}C and ^{31}P CSA Exchange Patterns. P T Inglefield, A A Jones and C Zhang *Clark University, Worcester, Massachusetts, USA*
- 12.30 CLOSURE OF SESSION

SYMPOSIUM D - Aspects of Computation

Chairman: Dr J H Keeler University of Cambridge

- 14.00 **Biomolecular Structure Refinement Based on NOE Data.** A Bonvin
University of Utrecht. The Netherlands
- 14.40 Simulation of Time-Domain Experiments. T Levante, S Smith, B H Meier and R R Ernst *ETH, Zurich, Switzerland*
- 15.10 Computer-aided and Automated Analysis of 2D and 3D Spectra of Biomolecules. S Boentges, C Griesinger and R R Ernst *ETH, Zürich. Switzerland*
- 15.40 NMR and Molecular Dynamics Simulations of Duplex DNA. P H Bolton
Wesleyan University, USA
- 16.10 TEA and **POSTER SESSION A** (even-numbered posters attended)

POSTGRADUATE SESSION A

Chairman; Dr P Meadows JEOL, London

- 17.00 Heteronuclear Isotropic Mixing 2D Correlation NMR. A Gibbs and G A Morris *University of Manchester*
- 17.20 Maximum Entropy Processing of PMRFI Spectra. J A Jones *University of Oxford*
- 17.40 ^{13}C NMR Relaxation Studies in Some Dicyclohexyl Compounds. S J Matthews *RHBNC, London*
- 18.00 CLOSURE OF SESSION

WEDNESDAY 10 JULY

SYMPOSIUM E - Non-Medical Imaging for non-specialists

Chairman: Professor L D Hall University of Cambridge

- 09.00 **The Development of NMR imaging.** R E Gordon *Bruker Instruments, Massachusetts, USA*
- 09.55 **Imaging Chemistry in Action.** T A Carpenter *University of Cambridge*
- 10.50 COFFEE
- 11.20 **Dynamic NMR Microscopy: Applications in Plant Physiology, Polymer Physics and Materials Science.** P T Callaghan *Massey University, Palmerston North, New Zealand*
- 12.15 CLOSURE OF SESSION

THURSDAY 11 JULY

SYMPOSIUM F - Structure and Dynamics I

Chairman: Dr K G Orrell *University of Exeter*

- 09.00 **CP/MAS Studies of the Structure and Dynamics of Complexes.** R Benn *Max Planck Institute, Mülheim, Germany*
- 10.00 ⁵⁹Co NMR: Temperature and Pressure Dependence of the Chemical Shift, ¹³C Isotope Shift, T₁ and Molecular Motion of [Co(CN)₆]³⁻
D G Gillies, L H Sutcliffe and A. Williams, *RHBNC, London*
- 10.30 COFFEE
- 11.00 **Stopped-Flow NMR and Analytical Chemistry.** G Hagele *University of Dusseldorf, Germany*
- 11.50 Studies of Anion Transport Through Membranes Using ³⁵Cl, ³⁷Cl, ⁷⁹Br and ⁸¹Br NMR. F G Riddell, S Arumugam, M A Chippa, A Patel and S Torapsett *University of St Andrews*
- 12.10 Studies of Interfacial Species in Clay Gels. J Grandjean and P Laszlo *University of Liege, Belgium*
- 12.30 CLOSURE OF SESSION

SYMPOSIUM G - In-Vivo Spectroscopy

Chairman: Professor D G Gadian *Royal College of Surgeons*

- 14.00 **A Multinuclear NMR Approach to the Chemistry of Living Systems.** J H Ackermann *Washington University in St Louis, Missouri, USA*
- 14.55 **NMR Proton Localised Spectroscopy and Metabolite Imaging of the Human Brain.** P R Luyten *University of Eindhoven, The Netherlands*

15.50 Human Brain Tumours: Evaluation by Localised ^1H NMR Spectroscopy. H Kugel, W Heindel, R-I Ernestus, J Bunke and G Friedmann *University of Cologne, Germany*

16.10 **TEA and POSTER SESSION B (odd-numbered posters attended)**

POSTGRADUATE SESSION B

Chairman: Professor L H Sutcliffe *RHBNC, London*

17.00 ^{93}Nb and ^1H NMR Study of the Stepwise Solvolysis of NbCl by Methanol. R Lee *University of St Andrews*

17.20 How Do the Ionophoric Antibodies Narasin and Salinomycin Accommodate Alkali Metal Ions? A 500 MHz ^1H NMR Study. S J Tompsett *University of St Andrews*

17.40 Interaction of Lysozyme with Water and with Trehalose by Solid-state NMR. A Gil, P Belton and S Tanner *AFRC, Norwich*

18.00 CLOSURE OF SESSION

FRIDAY 12 JULY

SYMPOSIUM H - Structure and Dynamics II

Chairman: Dr D L Turner *University of Southampton*

09.00 **Structure and Dynamics of Cyclic Peptides in Different Environments by NMR Spectroscopy and MD Calculations.** H Kessler *University of Munich, Germany*

09.55 Structure Determination of Cycle-[Arg-Gly-Asp-Ser-Lys], an Analogue Sequence of Fibronectin. M P Williamson, *J S Davies and **W A Thomas *University of Sheffield, "University College of Swansea, **Roche Products Ltd*

10.25 COFFEE

10.55 **NMR and Molecular Dynamics: From Small Molecules in Crystals to Proteins in Solution.** C M Dobson *University of Oxford*

11.50 Solution Conformation of the Neuropeptides NPY and $[\text{L}^{31}, \text{P}^{34}]$ -NPY in Deuteriomethanol by ^1H and ^{13}C NMR Spectroscopy. J Shocker, A E Aulabaugh and R Crouch *Burroughs Wellcome, USA*

12.15 **CLOSURE OF SESSION AND MEETING**
