

11TH INTERNATIONAL MEETING, UNIVERSITY COLLEGE OF

SWANSEA,

4-9 July 1993

SCIENTIFIC PROGRAMME

The scientific sessions commence at 09.00 on Monday 5 July in the Taliesin Theatre on the University campus. Coffees and teas will be served in the Salad Bowl, First Floor, Fulton House at the times stated in the programme.

Eight symposia, which make up the meeting, have invited lectures as well as shorter contributed talks associated with them.

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 6 July (16.10-17.30) and Thursday 8 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 on the First Floor, Fulton House (South West end of Dining area).

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 5 JULY

09.00 Welcome and Opening Remarks

Symposium A - Experimental Techniques

Underlining denotes presenter

Chairman: Dr J C Lindon *Wellcome Research Laboratories*

09.10 I.1 New NMR Methods for the Structural and Conformational Analysis of Oligosaccharides. S W Homans *University of Dundee*

10.00 I.2 NMR with Ultrasound. J Homer *University of Aston in Birmingham*

10.30 COFFEE

11.00 I.3 Development of Coupled HPLC-NMR for Bioanalysis. J K Nicholson *Birkbeck College, London*

11.40 I.4 Quantified Maximum Entropy and Its Application to NMR. J Skilling
University of Cambridge

12.30 LUNCH

Symposium B - Structure and Dynamics - Biological Macromolecules

Chairman: Dr D L Turner *University of Southampton*

14.00 I.5 NMR Studies of Hydration and Surface Structure of Biological
Macromolecules in Aqueous Solution. K Wüthrich *Institut für
Molekularbiologie und Biophysik, ETH, Zürich. Switzerland*

15.00 O.1 How ^{15}N Relaxation Studies Helped to Define the Role of the (30-51)
Disulphide Intermediate in the Folding Pathway of Bovine Pancreatic
Trypsin Inhibitor. D Neuhaus *MRC Laboratory of Molecular Biology,
Cambridge*

15.30 TEA

16.00 I.6 Functionally Important Motions in Proteins. R J P Williams *University
of Oxford*

16.30 O.2 Conformational and Topological Analysis of Membrane -
Reconstituted Polypeptides from Amide Exchange Trapping and Selective
Pulse ^1H NMR Spectroscopy. C E Dempsey and P B Williams *University of
Bristol*

17.00 Close

TUESDAY 6 JULY

Symposium C - Biological NMR

Chairman: Professor J Griffiths *St George's Hospital Medical School, London*

09.00 I.7 Water-Macromolecule Proton Magnetisation Transfer. R S Balaban
NHLBI. Bethesda, Maryland, USA

09.50 O.3 Time-Resolved Solid-state NMR of an Enzyme in Action. J N S Evans
Washington State University, USA

10.10 O.4 Non-Invasive Characterisation of Ischemic Lesions in Rodent Brain by
 ^1H NMR P D Bookings, S E Rose, D G Reid, A Rothaul, S Patel, N I Wood,
S Crozier, W Roffman, J Hunter and D M Doddrell *University of
Queensland, Australia and SmithKline Beecham Pharmaceuticals, UK*

10.30 COFFEE

11.00 I.8 Neural Networks and Pattern Recognition in NMR Spectroscopy
R J Maxwell *St George's Hospital Medical School, London*

11.30 I.9 NMR and Neuroscience: Studies of the Functioning Human Brain in Vivo. J Frahm *Max-Planck Institut für Biophysikalische Chemie, Göttingen, Germany*

12.20 Discussion

12.30 LUNCH

Symposium D - Structure and Dynamics - Inorganic

Chairman: Dr M Schröder *University of Edinburgh*

14.00 I.10 Variable Pressure NMR Spectroscopy in Co-ordination Chemistry. A E Merbach *Université de Lausanne, Switzerland*

14.45 I.11 Dynamic Behaviour of Transition Metal Carbonyl Clusters in Solution and the Solid State. B T Heaton *University of Liverpool*

15.30 O.5 NMR Studies of Molecular Dynamics in Inorganic and Organometallic Solids. S. J Heyes *University of Oxford*

15.50 O.6 Multinuclear NMR Studies of Platinum Porphyrin Complexes. L R Milgrom and R J Zuurbier *Brunei University* and J M Gascoyne, B C Moor and D Thomsett *Johnson Matthey, Reading*

16.10 TEA AND POSTER SESSION 1 (ODD numbered posters)

Postgraduate Session

Chairman: Professor L H Sutcliffe *University of Surrey*

20.00 O.7 A High-Resolution Solid-State NMR Study of Layered Alkali Metal Silicates. G G Almond and R K Harris *University of Durham*

20.20 O.8 Measurement of Tracer Diffusion and Dispersion in Heterogeneous Media Using NMR Imaging. A E Fischer, B J Balcom, T A Carpenter and L D Hall James *Herchel Smith Laboratory for Medicinal Chemistry, Cambridge*

20.40 O.9 Solution Structure of CD59 Antigen. C M Fletcher, R A Harrison, P J Lachmann and D Neuhaus *MRC Laboratory of Molecular Biology, Cambridge*

21.00 O.10 High Field ^1H NMR and Pattern Recognition Analysis as a Metabolic Tool in Renal Medicine. P J D Foxall G H Neild, J C Lindon and J K Nicholson *Birkbeck College, University College, London and Wellcome Research Laboratories*

21.20 O.11 ^{51}V , ^{183}W and ^{17}O NMR Spectroscopy of Polyoxotungstates in Aqueous Solution. J J Hastings and O W Howarth *University of Warwick*

21.40 O.12 NMR Studies of Silica-Siloxane Polymer Systems. M Turner and T Cosgrove *University of Bristol*

22.00 Close

WEDNESDAY 7 JULY

Symposium E - Solid-state NMR

Chairman: Professor R K Harris *University of Durham*

09.00 I.12 Magic Angle Spinning NMR of Quadrupolar Nuclei in Solids with Applications to Materials Research. H J Jakobsen *University of Aarhus, Denmark*

09.45 I.13 Quadrupole Effects in MAS NMR Spectra of Spin-% Nuclei Transmitted Through Dipolar and Scalar Interactions. A C Olivieri *Universidad Nacional de Rosario, Argentina*

10.30 COFFEE

11.00 I.14 High Temperature MAS NMR: Instrumentation and Phase Transition Studies on Inorganic Materials and Polymers. F Taulelle *Université Louis Pasteur, Strasbourg, France*

11.20 O.13 Spectral Spin Diffusion Under the $n = 0$ Rotational Resonance Condition: A Simple Physical Insight. R Challoner, J Kummerlen and C A McDowell *University of Bayreuth, Germany and University of British Columbia, Vancouver, Canada*

11.45 I.15 Characterization of Heterogeneous Polymers by Spatially Resolved NMR

B Blümich *Lehrstuhl für Makromolekulare Chemie der RWTH, Aachen, Germany*

12.30 LUNCH

PM **Excursions**

THURSDAY 8 JULY

Symposium F - NMR Imaging

Chairman: Professor P G Morris *University of Nottingham*

09.00 I.16 Ultra- and Hyper-fast Magnetic Resonance Imaging: Could the Dream Come True? Sir Peter Mansfield *University of Nottingham*

09.50 O.14 MRI of Rat Knee Pathology and the Effects of Treatment: A Longitudinal Study. T A Carpenter, J R Everett, L D Hall, G P Harper, R Hodgson and M F James *Herchel Smith Laboratory for Medicinal Chemistry, Cambridge and SmithKZine Beecham Pharmaceuticals*

10.20 COFFEE

10.50 I.17 Functional MR Imaging in the Brain. T J Brady *Massachusetts General Hospital, Harvard Medical School, USA*

11.40 1.18 Magnetic Resonance Functional Neuroimaging at High Field. R Turner *National Institutes of Health, Bethesda, Maryland, USA*

12.30 LUNCH

Symposium G – Structure and Dynamics – Physical

Chairman: Dr T Cosgrove *University of Bristol*

14.00 I.19 Association Phenomena, Studied by Magnetic Field Gradient NMR Methods. Application to Surfactant and Polymer Systems in Solution. P Stilbs *Royal Institute of Technology, Stockholm, Sweden*

14.45 I.20 Molecular Motion of Coupling Agents on Silica Surfaces. F D Blum *University of Missouri-Rolla, USA*

15.30 O.15 Self-Diffusion in Polymer Melt Blends. P C Griffiths and T Cosgrove *University of Bristol*

15.50 O.16 Intramolecular Motions in Crystalline Organic Solids Studied by ¹³C CP/MAS NMR Spectroscopy. F G Riddell and M Rogerson *University of St Andrews*

16.10 TEA AND POSTER SESSION 2 (EVEN numbered posters)

FRIDAY 9 JULY

Symposium H - Structure and Dynamics - Organic

Chairman: Dr D Neuhaus *MRC Laboratory of Molecular Biology, Cambridge*

09.00 I.21 Structural Studies using a Full NMR Parameter Matrix. P E Hansen *University of Roskilde, Denmark*

09.50 O.17 NMR Spectroscopy and the Fight Against Parasitic Worms: Structure Elucidation of Novel Natural Product Anthelmintics. J R Everett *SmithKline Beecham Pharmaceuticals*

10.10 O.18 Conformations and Dynamic Behaviour of Some Protein Kinase C Inhibitors

C H Hill, W A Thomas, and I W A Whitcombe *Roche Products, Welwyn Garden City*

10.30 COFFEE

11.00 O.19 Long-Range Heteronuclear Couplings - A Powerful Tool in Structure Elucidation. S M T D'Arcy, S E Morgan and W G Prowse *Lilly Research Centre, Windlesham, Surrey*

11.30 I.22 Improving Techniques for Organic Structure Determination. G A
Morris *University of Manchester*

12.20 Closing Remarks - End of Meeting

12.30 LUNCH
