

8th International Meeting, University of Kent at Canterbury
6th – 10th July 1987

SCIENTIFIC PROGRAMME

The scientific sessions will take place in the Cornwallis Lecture Theatre. Coffees and teas will be served in the Rutherford College Dining Room 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 will be 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 7 July and Thursday 9 July with ODD numbered posters being attended on the Tuesday and EVEN numbered posters on the Thursday.

The detailed programme for the meeting is as follows:

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

SUNDAY 5 JULY

20.30 Inaugural Reception in Eliot College for all participants both resident and non-resident

MONDAY 6 JULY

09.00 Welcome to the University of Kent at Canterbury

SYMPOSIUM: NMR IN INORGANIC CHEMISTRY

Chairman: Dr J.W. Akitt (University of Leeds)

- 09.05 **INVITED LECTURE:** The Current Status of High Pressure NMR Spectroscopy. A.E. Merbach (University of Lausanne, Switzerland)
- 09.55 Magnetisation Transfer to Investigate Dynamic Processes in Organometallic Compound. M. Grassi, B.E. Mann, B.T. Pickup and C.M. Spencer (University of Sheffield)
- 10.20 COFFEE
- 10.50 **INVITED LECTURE:** NMR Studies of Poly-Oxo Anions. W. Klemperer (University of Illinois, Urbana, USA)
- 11.40 51 V and 17O NMR of Molybdovanadates. O.W. Howarth. and A. Hill (University of Warwick) and I. Andersson and L. Pettorason (University of Umea, Sweden)

12.05 The Interaction Between Peptides and Transition Metals Investigated by Metal NMR: ⁴⁵Sc NMR of Sc³⁺ Oligopeptide Complexes; ⁵¹V NMR of Vanadate (V)-dependent Peroxidase from Pigweed. W. Pribsch, D. Rahder and C. Weidemann. Institut für Anorganische Chemie der Universität Hamburg) and H.Vilter (Institut für Pharmazeutische Biologie der Universität Bonn, FRG)

12.30 LUNCH

SYMPOSIUM: LARGE MOLECULES NMR

Chairman: Professor G.C.K. Roberts (University of Leicester)

14.00 **INVITED LECTURE:** NMR-DG Studies of DNA Helices In Solution. D.J. Patel (Columbia University, New York, USA)

15.00 NMR Studies of Hen and Human Lysozymes. C.M. Dobson and C. Redfield (University of Oxford)

15.30 Tea

16.00 **INVITED LECTURE:** Conformation and Environment of Retinal In Rhodopsin and Bacteriorhodopsin - A Solid State ¹³C and ¹⁵N NMR Investigation. R.G..Griffin (Massachusetts Institute of Technology, USA)

17.00 Computer analysis of 2D NMR Spectra. B.U. Maier,. Z.L. Madi and R.R.Ernst (ETH, Zürich, Switzerland)

17.30 Close

20.00 EVENING ROUND TABLE
Discussion on Quantitative Aspects of NMR. Convener: Mr A. Ferrige (Wellcome Foundation). Full details will be announced at the Meeting.

TUESDAY 7 JULY

SYMPOSIUM: EXPERIMENTAL TECHNIQUES IN NMR

Chairman: Professor R. Freeman (University of Cambridge)

09.00 **INVITED LECTURE:** 2D NMR Studies of Protein/DNA Interaction. R. Kaptein (University of Groningen, The Netherlands)

10.00 Time-Domain Zero Field NMR and NQR with RF and DC Pulses. R. Kreis, M.A. Thomas and R. R. Ernst (ETH, Zürich, Switzerland)

10.30 COFFEE

11.00 **INVITED LECTURE:** Longitudinal and Transverse Relaxation Effects in 2-Dimensional Spectroscopy. G. Bodenhausen (University of Lausanne, Switzerland)

12.00 Selective Data Sampling: Application to 2D NMR. E.D. Laue (University of Cambridge)

12.30 LUNCH

SYMPOSIUM: NMR IN INDUSTRY

Chairman: Dr G. R. Bedford (ICI Pharmaceutical a Division, Alderley Park)

14.00 **INVITED LECTURE:** Conformation, Tacticity and Molecular Dynamics of Synthetic Polymers. L.W. Jelinski (Bell Laboratories, New Jersey, USA)

14.55 Liquid and Solid-State NMR In the Investigation of Catalyst Preparation. N.C.M. Alma-Zeestraten, O. Sudmeijer, A.E. Wilson, J.P. van Braam-Houckgeest, J. Dorrepaal, J. Keijsper and H. Gles (Koninklijke/ Shell-Laboratorium, Amsterdam, The Netherlands)

15.25 **INVITED LECTURE:** NMR and Drugs: Some Examples of Conformational Analysis in Pharmaceutical Research. D. Neuhaus (Parks-Davis Research Unit, Cambridge)

16.15 TEA and POSTER SESSION

20.00 Concert in Canterbury Cathedral (Gratis)
Programme: Songs by: Schubert, Debussy, Ravel, Rodrigo, Guastavino, Turina, Granados.
Recital: Elly Aroeling (Soprano) Rudolf J risen Piano)
Coaches will operate a shuttle from Rutherford College Car Park, beginning 19.00 and ending at 19.30

WEDNESDAY 8 JULY

SYMPOSIUM: NMR IN ORGANIC CHEMISTRY

Chairman: Dr I.H. Sadler (University of Edinburgh)

09.00 **INVITED LECTURE:** Adventures with Spin-1 Nuclei. H. Giinther (University of Siegen, FRG)

09.55 Structural Studies on the Carbohydrate Moieties of Pituitary Glycoprotein Hormones by 1-D and 2-D NMR Spectroscopy. H. van Halbeek (University of Georgia, Athens, USA)

10.25 COFFEE,

10.55 The Assignment of Quaternary Carbons Using ^{13}C - $\{^1\text{H}\}$ Nuclear Overhauser Effects. A.G. Avent (University of Sussex)

11.15 **INVITED LECTURE:** NMR Techniques Inspired by Biosynthetic
 Studies
 J. Staunton (University of Cambridge)

12.10 Close

PM EXCURSIONS

THURSDAY 9 JULY

SYMPOSIUM: NMR IN SOLIDS

Chairman: Professor K.J. Packer (BP Research Centre, Sunbury on Thames)

09.00 **INVITED LECTURE:** Probing Metal Catalysts by NMR. C.P. Slichter
 (University of Illinois, Urbana, USA)

10.00 **INVITED LECTURE:** Nuclear Magnetic Resonance and Quadrupole
 Interactions in Solids. J.A.S. Smith (KQC, University of London)

10.30 COFFEE

11.00 **INVITED LECTURE:** Exploration with High-Resolution NMR
 Spectroscopy of Dynamically Polarised Nuclei. C.S. Yannoni (IBM
 Research, San Jose, California, USA)

12.00 Quantitation in Carbon-13 CP/MAS NMR. R.H. Newman (DSIR, New
 Zealand)

12.30 Close

SYMPOSIUM: NMR IN PHYSICAL CHEMISTRY

Chairman: Dr J.W. Emsley (University of Southampton)

14.00 **INVITED LECTURE:** How NMR is Used to Study Micelles and
 Lyotropic
 Liquid Crystals. N. Boden (University of Leeds)

15.00 **INVITED LECTURE:** Deuterium NMR Studies of Molecular Motion in
 Solids, Polymers and Liquid Crystals. R.L. Vold (University of
 California, San Diego, USA)

16.00 TEA and POSTER SESSION

19.30 for 20.00 Conference Dinner in Eliot College, preceded by a Sherry Reception

FRIDAY 10 JULY

SYMPOSIUM: BIOMEDICAL NMR

Chairman: Dr P.J. Sadler (Birkbeck College, University of London)

- 09.00 **INVITED LECTURE:** In Vivo NMR Spectroscopy of Animals and Humans
 J. Seelig (University of Basel, Switzerland)
- 09.50 Localised ³¹P Spectroscopy In-Vivo, Using Phase Encoding NMR Techniques
 D.R. Bailes, D.J. Bryant, G.M. Bydder, H.A. Case, A.G. Collins, I.J. Cox, R.R. Harman, A.S. Hall, S. Khenia, P. McArthur, B.D. Ross, I.R. Young (Hammersmith Hospital, London, and GEC Research, London)
- 10.10 Recent Applications of NMR to Plant Tissues. R.B. Lee, B.C. Loughman, H.D. Quiquampoix, R.G. Ratcliffe and T.E. Southon (University of Oxford)
- 10.30 COFFEE
- 11.00 NMR Studies of Body Fluids in Rheumatoid Arthritis. M.P. Williamson (Roche Products, Welwyn Garden City)
- 11.30 **INVITED LECTURE:** NMR Spectroscopy in Cancer Research. I.C.P. Smith (National Research Council, Ottawa, Canada)
- 12.30 CLOSURE AND LUNCH
