

Fourth International Meeting on Nuclear Magnetic Resonance Spectroscopy

University of York

2 – 7 July 1978

SCIENTIFIC PROGRAMME

The lectures in the seven symposia will take place in PX001 in the Physics Department, University of York, whilst the BRSG symposium on Friday will take place in PL002, also in the Physics Department. Poster sessions will be held in the Foyer of the Physics Department, where coffees and teas will be served 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 the charge of its Chairman.

In addition, two poster sessions will be held.

Poster Session A will be mounted on Sunday and Poster Session B will be mounted on Tuesday evening and Wednesday. Posters may be viewed by participants at any time convenient to them. The posters will be manned by the author(s) at the times shown in the programme.

The underlined name denotes the author presenting paper.

Monday 3 July

Symposium 1

NMR CONFORMATIONAL STUDIES

Chairman: Dr H. Booth, University of Nottingham

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| 09.00 | Welcome |
| 09.15 | Plenary Lecture
Conformational Analysis by Dynamic NMR Spectroscopy at Very Low Temperatures
F.A.L. Anet, University of California, Los Angeles, USA |
| 10.15 | Coffee |
| 10.45 | Plenary Lecture
Guest-Host Chemistry and Conformational Analysis
I.O. Sutherland, University of Liverpool |
| 11.25 | Ring Inversion in Compounds Containing Three and More 6-Membered Rings
D. Tavernier, State University of Gent, Belgium |
| 11.45 | The Conformational Analysis of Some Cyclic Derivatives of Hydroxylamine. Differentiation Between Ring and Nitrogen Inversion
F.G. Riddell, University of Stirling |

- 12.05 Conformation and Stereodynamics of Aminophosphorus Compounds: 2-Dialkylamino-1,3-Dimethyl-1,3,2-Diazaphospholanes
W.B. Jennings, University of Birmingham, with M.S. Tolley, J.H. Hargis and S.D. Worley, Auburn University, Alabama, USA
- 12.25 The Stereodynamics of Hindered Piperidine Derivatives
L. Lunazzi, University of Bologna, Italy, with D. Macciantelli, Laboratorio CNR, Bologna, Italy
- 12.45 Lunch

Symposium 2

NMR STUDIES OF LARGE MOLECULES

Chairman: Dr R.K. Harris, University of East Anglia

- 14.15 Plenary Lecture
Deuterium NMR of Membranes and Large Molecules
I.C.P. Smith, National Research Council, Ottawa
- 15.15 Use of ^{19}F and ^1H Labelling to Simplify Protein NMR Spectra
J. Feeney, National Institute for Medical Research, London
- 15.35 Tea
- 16.05 Plenary Lecture
Contribution of Proton NMR with Magic Angle Rotation to Studies of 'Internal Motions Restricted in Space'
B. Schneider and D. Doskočilová, Institute of Macromolecular Chemistry, Prague
- 16.45 High-Resolution NMR Studies of Solid Polymers
R.K. Harris and K.J. Packer, University of East Anglia
- 17.15 Proton and Carbon-13 Relaxation Studies of Motional Mechanisms in Synthetic Polymers
F. Heatley and M.K. Cox, University of Manchester
- 17.35 Close

Tuesday 4 July

Symposium 3

NMR STUDIES IN BIOLOGICAL SYSTEMS

Chairman: Dr J. Feeney, National Institute for Medical Research

- 09.00 Plenary Lecture
Studies of Proteins and Glycoproteins in Solution by Natural-Abundance Carbon-13 NMR
A. Allerhand, University of Indiana, USA

- 09.50 ^{13}C NMR Studies of Biosynthetically Enriched Membranes
I.C.P. Smith, National Research Council, Canada
- 10.10 Coffee
- 10.40 Plenary Lecture
NMR Studies of Some Calcium-Binding Proteins
R. J.P. Williams, University of Oxford
- 11.30 Conformational Features of Lysozyme in Solution
C.M. Dobson and F.M. Poulsen, Harvard University, USA
- 11.50 NMR Studies on the Structure of the Chromophore of Rhodopsin: A
Vertebrate Visual Pigment
G.D. Mateescu, J.W. Shriver, and E.W. Abrahamson, Case Western Reserve
University, Cleveland, USA
- 12.10 Metabolism and Transport in Red Cells Using ^1H , ^{13}C and ^{31}P NMR
I.D. Campbell, K.M. Brindle, F.F. Brown, C. Grathwohl and P.W. Kuchel,
University of Oxford

12.30 Lunch

Symposium 4

STUDIES OF DYNAMIC PROCESSES

Chairman: Professor E.W. Randall, Queen Mary College, London

- 14.00 Plenary Lecture
Recent Advances in the Analysis of Complex NMR Bandshapes
G. Binsch, University of Munich, West Germany
- 5.00 Plenary Lecture
 ^{13}C and ^1H Dynamic NMR Studies of Benzaldehydes Acetophenones and
Other Protonated Analogues
T. Drakenberg, University of Lund, Sweden
- 15.30 Ring and Pyramidal Site Inversion Processes in Transition Metal Complexes
Involving Sulphur and Selenium Ligands
K.G. Orrell, University of Exeter
- 15.45 A Study of Cooperative Proton Jumping and Tunnelling in Meso-
Tetraphenylporphine by NMR Line Shape Analysis and Selective T1p
Measurements
H.H. Limbach and J. Hennig, University of Friburg, Germany
- 16.00 Tea
- 16.30 Poster Session A

17.30 Close

Wednesday 5 July

Symposium 5 RELAXATION STUDIES

Chairman: Dr I.D. Campbell, University of Oxford

- 09.00 Plenary Lecture
Nuclear Relaxation in Coupled Spin Systems and Molecular Dynamics and Structure
D.M. Grant, University of Utah, USA
- 09.50 Discussion
- 10.00 Temperature and Field Dependent Relaxation Studies in Benzonitrile
F.W. Wehrli, Varian AG, Switzerland
- 10.20 Coffee
- 10.50 Plenary Lecture
Proton Spin Lattice Relaxation - A Structural Probe for Both the Chemist and Spectroscopist
L.D. Hall, University of Vancouver, Canada
- 11.35 Discussion
- 11.40 Quantifying Internal Motions in Proteins and Peptides
O. Howarth, University of Warwick .
- 12.00 ¹³C T1 Studies of Molecular Motions
R.K. Harris and R.H. Newman, University of East Anglia
- 12.30 Lunch

AFTERNOON FREE

Thursday 6 July

Symposium 6 NEW EXPERIMENTAL TECHNIQUES AND APPLICATIONS

Chairmen: Dr J.W. Emsley, University of Southampton, and Dr K.J. Packer, University of East Anglia

- 09.00 Plenary Lecture
Exploring Imperceptible Spectral Features by Two-Dimensional NMR
R. Ernst, ETH, Zürich, Switzerland
- 10.15 Coffee
- 10.45 Plenary Lecture

Two Dimensional Fourier Transformation
R. Freeman, University of Oxford

- 11.45 J-Scaling: An Alternative to Off-Resonance Decoupling in the Assignment of Carbon-13 NMR Spectra
G. Morris, University of Oxford
- 12.15 NMR at 140 kG and 600 MHz
J. Dadok, Carnegie-Mellon University, Pittsburg, USA
- 12.45 Lunch
- 14.00 Plenary Lecture
Recent Applications of Coherent Averaging Effects in NMR
J.S. Waugh, MIT, USA
- 15.00 Plenary Lecture
NMR Imaging
E.R. Andrew, University of Nottingham
- 16.00 Tea
- 16.30 Poster Session B
- 17.30 Close

Friday 7 July

Symposium 7 REVIEW LECTURES

Chairman: Dr D. Shaw, Oxford Instruments

- 09.00 Plenary Lecture
Liquid Crystals
J.W. Emsley, University of Southampton
- 10.00 Coffee
- 10.30 Plenary Lecture
Is CIDNP Dynamic or Not?
K.A. McLauchlan, University of Oxford
- 11.30 Plenary Lecture
Recent Applications of Fourier Transform NMR for the Solution of Chemical Problems
J.N. Shoolery, Varian Associates, Palo Alto, USA
- 12.30 Lunch

Friday 7 July - BRSG Symposium
MOTIONAL EFFECTS IN MAGNETIC RESONANCE

Lecture Theatre: PL002, Physics Department

- 09.00 Invited Paper
 The Study of Motions in Solids by 2D NMR
 H.W. Spiess, Mainz
- 09.50 Molecular Motion in Mixed Molecular Crystals
 A.R. Briltcher and J.H. Strange, Kent
- 10.10 NMR Studies of Hydrogen Self-Diffusion in Hydrogen Molybdenum Bronzes
 R.C.T. Slade and T.K. Halstead, York
- 10.30 Proton Magnetic Relaxation in Solid Proteins
 E.M. Cashell, E.R. Andrew and D.J. Bryant, Nottingham
- 10.50 Coffee
- 11.10 Invited Paper
 A Review of Direct Measurements of Diffusion Coefficients with NMR
 R.M. Cotts, Cornell and Warwick
- 12.00 Nuclear Magnetism of Some Physiological Fluids in Low Fields
 G.J. Bené, B. Borcard, E. Hiltbrand and P. Magnin, Geneva, Switzerland
12. Biodynamics and NMR
 R. Lenk, Mo. Bonzon, P. Desouts and H. Greppin, Geneva, Switzerland
- 12.40 Lunch
- 14.10 Invited Paper
 NMR Spin Echoes in Solids
 N. Boden, Leeds
- 15.00 Motions in Anisotropic Fluids Studied by 2D NMR
 S.B.Ahmad and K.J. Packer, East Anglia
- 15.20 Close of meeting
