

Fifth International Meeting on Nuclear Magnetic Resonance Spectroscopy

University of Exeter

12 – 17 July 1981

SCIENTIFIC PROGRAMME

The lectures in the eight symposia will take place in the large lecture theatre in the Newman Building (adjacent to the Chemistry Department), at the University of Exeter. Poster sessions will be held in the Lower Examination Hall of the University Great Hall, 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 Monday 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.

* Denoted Presenter

Monday 13 July

Symposium 1

MULTINUCLEAR MAGNETIC RESONANCE: SPIN-1/2 NUCLEI

Chairman: **Dr. R.J. Goodfellow** (University of Bristol)

09.00 Welcome

09.15 **Invited Lecture**

Multinuclear Magnetic Resonance - a Synthetic Chemist's View
E. A. V. Ebsworth (University of Edinburgh)

10.15 COFFEE

10.45 **Invited Lecture**

^{57}Fe , ^{59}Co and ^{103}Rh NMR of Olefin Complexes
W. von Philipsborn (University of Zürich)

11.30 ^{205}Tl NMR of Organothallium(III) Derivatives
F. Brady, P. J. Burke, K. Henrich, R.W. Matthews*, B.J. Podesjma
(Polytechnic of North London), M.J. Forster and D.G. Gillies (Royal Holloway College, London)

12.00 High-field ^{29}Si NMR Studies of Aqueous Silicate Solutions
R.K. Harris*, C.T.G. Knight (University of East Anglia) and W. E. Hull
(Bruker GmbH)

12.20 LUNCH

Symposium 2

INTACT BIOLOGICAL SYSTEMS

Chairman: **Dr. I.A. Stenhouse** (PCMU, Harwell)

14.00 **Invited Lecture**

High Resolution NMR Studies of Cells and Tissues
R.G. Shulman (Yale University)

14. 55 NMR Studies on Plant Tissues
M.J. Kime, R.B. Lee, B.C. Loughman, R.G. Ratcliffe* and R. J. P. Williams
(University of Oxford)

15. 20 ^{31}P NMR of Perfused Hearts
R .L. Nunnally (University of Texas)

15.45 TEA

16. 15 T(Topical)MR Studies of Biological Tissues
R.E. Gordon* and D. Shaw (Oxford Research Systems Ltd)

16.40 **Invited Lecture**

High Speed Imaging
P. Mansfield (University of Nottingham)

17.35 CLOSURE

Tuesday 14 July

Symposium 3

HETEROGENEOUS SYSTEMS

Chairman: **Dr. W. Derbyshire** (University of Nottingham)

09.15 **Invited Lecture**

The Brønsted Acidity of Zeolites and the Microdynamic Behaviour of
Adsorbed Pyridine
H. Pfeifer (Karl Marx University, Leipzig)

10.10 COFFEE

10.40 **Invited Lecture**

The Hydrogen Spill-over Process as Revealed by NMR in H_xMoO_3 and
 H_xWO_3
J.J. Fripiat (CNRS, Orleans)

11.35 NMR Spectroscopy in Lamellar Solids - Effects of Anisotropy
L.G. Banks, G.R. Miller, M.J. Moran and H.A. Resing* (Naval Research

Laboratory, Washington)

12.30 LUNCH

Symposium 4

MULTINUCLEAR MAGNETIC RESONANCE: QUADRUPOLEAR NUCLEI

Chairman: **Dr. D. Shaw** (Oxford Research Systems)

14.00 The Solution Structure of Simple Inorganic Salts Studied by High-field ^9Be , ^{27}Al , ^{45}Sc , $^{69,71}\text{Ga}$ NMR
F.W. Wehrli* and S.W. Wehrli (Bruker Instruments Inc., USA)

14.40 Applications of ^{95}Mo NMR
R.T.C. Brownlee, S.F. Gheller, A.F. Masters, M.J. O'Connor* and A.G. Wedd (La Trobe University, Australia)

15.00 ^{17}O NMR Studies in Natural Abundance of Orthophosphates, Condensed Phosphates and Some Biophosphates
I. P. Gerothanassis* and N. Sheppard (University of East Anglia)

15.20 **Invited Lecture**
Calcium and Magnesium NMR: Chemical and Biological Applications
S. Forsén (University of Lund)

16.15 TEA and **Poster Session A**

17.45 CLOSURE

Wednesday 15 July

Symposium 5

APPLICABLE THEORY

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

09.15 **Invited Lecture**
The Derivation of Molecular Information from Measurement of Relaxation Times
R.L. Vold (University of California, San Diego)

10.15 COFFEE

10.45 **Invited Lecture**
Automated Analysis of Spectra
G. Binsch (University of Munich)

11.35 Non-empirical Calculations of Nuclear Spin-Spin Coupling Constants: Recent Advances
A. Laaksonen and J. Kowalewski* (University of Stockholm)

11.55 Recent Progress in the Theory and Application of L.I.S. Analysis of Molecular

Structures and Energies

R.J. Abraham, H.E. Burgen, D.J. Chadwick (University of Liverpool) and
F. Sancassan* (University of Genoa)

12.15 LUNCH

AFTERNOON FREE

Thursday 16 July

Symposium 6

DYNAMIC PROCESSES

Chairman: **Dr. B.E. Mann** (University of Sheffield)

09.15 **Invited Lecture**

Ion-Molecule Reactions: Thermodynamics, Chemical Dynamics and
Microdynamics

P. Laszlo (University of Liège)

10.15 The Use of Dynamic NMR Spectroscopy in the Study of Proton and Deuteron
Exchange Reactions in Solution

D. Gerritzen, J. Hennig, H.H. Limbach* and W. Seiffert (Albert-Ludwigs -
University, Freiburg)

10.35 COFFEE

11.00 NMR Studies of Some Dynamic Effects in Drug-Receptor Complexes

B. Birdsall, A.S.V. Burgen, M.G. Clore, J. Feeney*, A. Gronenborn, E.I.
Hyde and G.C.K. Roberts (National Institute for Medical Research, London)

11.20 Configurational Non-rigidity in Platinum(IV) Complexes with Sulphur and
Selenium Ligands

K.G. Orrell (University of Exeter)

11.40 **Invited Lecture**

Chemical Kinetics by High Pressure Multinuclear Magnetic Resonance

A.E. Merbach (University of Lausanne)

12.30 LUNCH

Symposium 7

TECHNIQUES

Chairman: **Dr. L.H. Sutcliffe** (University of Liverpool)

14.00 **Invited Lecture**

Instrumentation of NMR Imaging

D.I. Hoult (Health, Education and Welfare, Bethesda)

14.40 Measurement Techniques at Different Magnetic Fields

D.G. Gillies (Royal Holloway College, London)

- 15.05 Relaxation and Exchange in Two-dimensional NMR
G. Bodenhausen (ETH, Zürich)
15. 30 New Strategies for Resolving and Assigning the Proton NMR Spectra of
Complex Organic Molecules - Synergistic Use of One- and Two- Dimensional
Methods
L.D. Hall*, B.K. Hunter, G. Pouzard, J.K.M. Sanders and S. Sukumar
(University of British Columbia)
- 15.55 TEA and **Poster Session B**
- 17.25 **Invited Lecture**
Solid State High Resolution ^{29}Si NMR of Silicates and Aluminosilicates
E. Lippmaa (Estonian Academy of Sciences)

CLOSURE

At the Conference Dinner, Sir Rex Richards will give a talk in lighter vein.

Friday 17 July

Symposium 8 **TECHNIQUES**

Chairman: **Dr. W. McFarlane** (City of London Polytechnic)

- 09.15 **Invited Lecture**
High-field Hydrogen-2 and Nitrogen-14 NMR of Single Crystals
U. Haeberlen (Max Planck Institute, Heidelberg)
- 10.10 Some New Applications of Resolution Enhancement in FT NMR
J.C. Lindon (Wellcome Research Laboratories)
- 10.30 COFFEE
11. 00 FSU NMR Spectral Data Processing System and WARPATH Computer
Networks
G.C. Levy (University of Syracuse)
- 11.30 **Invited Lecture**
Two Dimensional Spectroscopy for the Chemist
R. Freeman (University of Oxford)
- 12.30 **CLOSURE AND LUNCH**
