

Third International Meeting on Nuclear Magnetic Resonance Spectroscopy

University of St Andrews

6 – 11 July 1975

SCIENTIFIC PROGRAMME

The lectures will take place in Theatre 300 in the Chemistry Department, Purdie Building of the University of St Andrews. Poster sessions will take place in the vestibule areas of the Chemistry Department, where coffees and teas will be served. There will be an exhibition of books also situated in the vestibule areas. Each of the six symposia which make up the meeting, has its plenary lecture(s) and shorter talks; each is in the charge of its Chairman.

In addition, two poster exhibitions will be held

Poster Exhibition A will be mounted on Sunday and will cover the first three symposia. The Exhibition may be viewed by participants at any time convenient to them. The exhibitions will be manned by the author(s) at the times shown in the programme. In addition, some general collective discussions will be held (as timetabled) in the Lecture Theatre.

Poster Exhibition B will be mounted on Wednesday, will cover the last three symposia, and will have a form and programme the same as for Exhibition A.

It is anticipated that last minute programme changes may have to be effected following the printing of this programme. The organisers wish to apologise in advance for any inconvenience this may cause.

The underlined name denotes the author presenting paper.

MONDAY 7 JULY - SYMPOSIUM 1

NMR of ^{13}C and Other Nuclei: Recent Applications to Chemical Problems

Chairman: **Dr R.K. Harris** (University of East Anglia)

09.00 Welcome

09.10 NMR in Chemical and Biosynthetic Studies of Natural Products
Professor A.R. Battersby (University of Cambridge)

10.10 Protonation and Covalent Hydration of Nitrogen Heterocycles by ^{13}C NMR
U. Ewers, H. Günther and L. Jaenicke (University of Cologne)

10.30 Coffee

- 11.00 ^{13}C NMR Studies of Butadiene Iron Tricarbonyl and Related Complexes
W. von Philipsborn and K. Backmann (University of Zürich)
- 11.25 ^{13}C Spin Lattice Relaxation. Some Applications to Chemical Problems
G.C. Levy (Florida State University)
- 11.50 The Experimental Application of the Forsen-Hoffman Method of NMR Double Resonance to Exchange in ^{13}C NMR Spectroscopy
B.E. Mann and B.F. Taylor (University of Sheffield)
- 12.10 Alkali and ^{13}C Resonance NMR of Alkali Radical Ion Pairs
E. de Boer, J.J. Mooij and G. von Velden, (University of Nijmegen)
- 13.00 Lunch

MONDAY 7 JULY - Symposium 1 (continued)

- 14.00 NMR Studies of ^{29}Si
Dr R.K. Harris (University of East Anglia)
- 15.00 Applications of ^3H NMR
J.A. Elvidge, J.R. Jones, R. Thomas, V.M.A. Chambers and E.A. Evans (University of Surrey)
- 15.20 ^{205}Tl Ft-NMR Spectroscopy of Substituted Mono- and Di-aryl Thallium Trifluoroacetates
J.E. Hinton and R. Briggs (University of Arkansas)
- 15.40 Solvation of Al^{3+} in Solutions of AlCl_3 and $\text{Al}(\text{ClO}_4)_3$ in Methanol and Ethanol. Ft Studies involving ^1H , ^{27}Al and ^{35}Cl NMR
J.W. Akitt and R.H. Duncan (University of Leeds)
- 16.00 Tea
- 16.30 **Poster Exhibition - A** Part I (see p 12-14)
- 17.00 **Poster Discussion - A**

TUESDAY 8 JULY - SYMPOSIUM 2

NMR Studies of Oriented Molecules

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

- 09.00 Some Trends and Traps in the NMR of Oriented Molecules
Professor P. Diehl (University of Basle)
- 10.00 Structures of Fluorinated Compounds
J.W. Emsley (University of Southampton)

- 10.30 Coffee
- 11.00 NMR Studies of Ordered Fluids and Disordered Solids
A. Pines (University of California, Berkeley)
- 11.30 NMR SPDE Studies of Thermotropic Liquid Crystals
N. Boden, Y.K. Levine, D. Lightowers and R.T. Squires
University of Leeds)
- 13.00 Lunch

TUESDAY 8 JULY - SYMPOSIUM 3

NMR Studies of Solids

Chairman: **Dr N. Boden** (University of Leeds)

- 14.00 Enhanced Detection and Resolved Dipolar Oscillations of Dilute Spins in Solids
Professor J.S. Waugh (M.I.T.)
- 15.00 Spin Decoupling in Solids
N. Hearing, E. Sinning (University of Dortmund) and A. Pines (University of California, Berkeley)
- 15.30 High Sensitivity Detection of Nuclear Quadrupole Resonance of the Light Nuclei and its Applications
D. Edmunds (University of Oxford)
- 16.00 Tea
- 16.30 **Poster Exhibition - A** Part II (see p 12-14)
- 17.00 **Poster Discussion - A**

WEDNESDAY 9 JULY - SYMPOSIUM 4

Theoretical Aspects of NMR

Chairman: **Mr C.W. Haigh** (University College, Swansea)

- 09.00 An Approximate Gauge-invariant Molecular Orbital Theory of Magnetic Shielding Constants
Professor P.P. Ellis (University of Southern Carolina)
- 10.00 Gauge Invariance of the Finite Basis Set of Coupled Hartree-Fock Calculations of Molecular Magnetic Properties
A.J. Sadlej (Academy of Sciences, Warsaw)
- 10.30 Coffee
- 11.00 Proton-Proton Coupling Constant in Ammonia; Geometry Dependence and Effect of Vibrations
J. Kowalewski and B. Roos (University of Stockholm)
- 11.30 Nuclear Relaxation in Coupled Spin Systems
A.D. Bain and R.M. Lynden-Bell (University of Cambridge)

12.00 Density Matrix Theory for NMR Line Shapes in Exchange Systems: Dynamic Behaviour of an Organo-lithium Compound
G. Fraenkel (Ohio State University)

12.30 Lunch

THURSDAY 10 JULY - SYMPOSIUM 5

Biological Symposium

Chairman: **Dr J. Feeney** (M.R.C., Mill Hill)

09.00 The Effects of Histone Interactions on the Structure of Chromatin

Dr E.M. Bradbury (Portsmouth Polytechnic)

09.50 Discussion

10.00 NMR Studies of the Unfolding of Ribonuclease G.C.K. Roberts (M.R.C., Mill Hill)

10.25 Discussion

10.30 Coffee

11.00 Phosphate Ester Hydrolysis by Alkaline Phosphatase; does ³¹P NMR see a catalytic intermediate?
B. Sheard (I.C.I., Macclesfield)

11.20 ¹³C Studies of Membrane Systems
N.J.M. Birdsall (M.R.C., Mill Hill)

11.40 ³¹P Studies of Oriented Phospholipid Membranes
P.R. Cullis, M. Hemmings, D. Hoult, A.C. McLauchlin, G.K. Radda and R.E. Richards (University of Oxford)

12.00 Discussion

13.00 Lunch

14.00 Structural Studies on the Antibody Combining Site

Dr R. Dwek (University of Oxford)

14.50 Application of Multiple Resonance Techniques to Protein NMR
I. Campbell (University of Oxford)

15.10 Structural Studies on Lysozyme
C.M. Dobson (University of Oxford)

15.30 Discussion

15.40 High Resolution NMR Studies of the Molecular Dynamics in Proteinase Inhibitors
K. Wüthrich, G. Wagner and A. de Marco (E.T.H., Zürich)

16.00 Tea
16.30 **Poster Exhibition - B** (see p 15-16)
17.00 **Poster Discussion - B**

FRIDAY 11 JULY - SYMPOSIUM 6

Correlation and Fourier Spectroscopy

Chairman: **Dr R. Freeman** (University of Oxford)

09.00 Correlation Spectroscopy
 Dr D. Ziessow (Technical University of Berlin)

09.45 Design of a very fast Fourier Routine
 M.J.A. de Bie (Rijksuniversiteit, Utrecht)

10.15 Discussion

10.30 Coffee

11.00 Saturation Behaviour and Equivalence Problems in
 Stochastic Resonance
 A. Wokaun, E. Bartholdi and R.R. Ernst (E.T.H., Zürich)

11.30 Chirp Pulse NMR Spectroscopy
 J. Delayre (Cameca, France)

11.50 The Elimination of Signals due to an Abundant Isotope:
 The Determination of ^{15}N - ^1H Coupling by Proton Fourier NMR
 J.-P. Marchal and D. Canet (University of Nancy)

12.20 **Discussion and close of meeting**
