

**Second International Symposium on Nuclear Magnetic Resonance
Spectroscopy
University of Surrey**

3 -7 July 1972

SCIENTIFIC PROGRAMME

Tuesday 4 July

Morning Session

Chairman: **Dr. L. H. Sutcliffe**

- 09.00 Plenary lecture: **^{13}C and ^{15}N Fourier NMR Techniques and Applications**
by E. W. Randall *Queen Mary College, London*
- 10.00 The Stereospecificity of Carbon-13 Proton NMR Coupling,
by D. Bencivenga, D. R. Clutter and K. L. Williamson *Mount Holyoke College, South Hadley, U.S.A.*
- 10.15 Carbon Magnetic Resonance Studies of Enriched Compounds. ^{13}C - ^{13}C
Coupling Constants of ^{13}C -7 Labelled Monosubstituted Benzene
Derivatives,
by A. M. Ihrig and J. L. Marshall *North Texas State University, Denton, U.S.A.*
- 10.30 Discussion
- 10.40 **Coffee**
- 11.00 A ^{13}C NMR Study of ^{13}C - ^{31}P Spin Coupling Constants in some
Arylphosphines,
by H. J. Jakobsen and S. Sørensen *University of Aarhus, Denmark*
- 11.15 The Nuclear Magnetic Resonance Spectra of Fluoroaromatics, Part V.
The ^{13}C Spectra of some Fluorobenzenes and Fluorobenzofurans,
by R. J. Abraham and D. F. Wileman *University of Liverpool* and G. R.
Bedford and D. Greatbanks *I.C.I. Pharmaceuticals, Macclesfield*
- 11.30 Discussion
- 11.40 The Application of ^{13}C NMR Spectroscopy to Organometallic
Compounds,
by A. J. Cheney, B. E. Mann, R. Pietropaulo and B. L. Shaw *University of Leeds*
- 11.55 Long-Range ^{13}C —F Couplings in Polycyclic Aromatic Compounds,
by P. E. Hansen *University of Aarhus, Denmark*

12.10 Discussion

12.30 **Lunch**

Afternoon Session

Chairman: **Dr. W. McFarlane**

14.00 Plenary lecture: **Analysis by Iterative Computer Programmes of Complex Spectra from Symmetrical Spin Systems**
by C. W. Haigh *University College, Swansea*

15.00 A Comparative ^{13}C NMR Study of Ethenes, Acetylenes, Allenes, Cumulenes, Butadienes and Diacetylenes,
by M. J. A. de Bie, J. P. C. M. van Dongen and R. Steur *University of Utrecht, The Netherlands*

15.15 ^{14}N NMR Studies of some 5- and 6- Membered Aromatic Heterocycles,
by H. Januszewski, L. Stefaniak and M. Witanowski
Polish Academy of Sciences, Warsaw, and G. A. Webb University of Surrey

15.30 Discussion

15.40 **Tea**

16.00 Tritium Nuclear Magnetic Resonance,
by D. E. Caddy, J. A. Elvidge, E. A. Evans, J. R. Jones and J. C. Turner *University of Surrey*

16.15 The Determination of Chemical Shifts Using Heteronuclear Magnetic Triple Resonance: ^{77}Se NMR Parameters in Organophosphorus Selenides,
by W. McFarlane and D.S. Rycroft *City of London Polytechnic*

16.30 Discussion

16.40 NMR Studies of Fluorocyclopentenes,
by L. Cavalli *Montecatini Edison S.p.A., Milan, Italy* and R. K. Harris
University of East Anglia

16.55 Participation of Hydrogen-Bonded Donor Molecules in Vicinal H-F Coupling,
by Soon Ng *University of Malaya, Kuala Lumpur, Malaysia*

17.10 Discussion

18.00-19.00 Informal Discussions, led by R. K. Harris *University of East Anglia*

Wednesday 5 July
Morning Session
Chairman: **Dr. D. Shaw**

- 09.00 Plenary lecture: **Chemically-Induced Dynamic Nuclear Polarisation, an NMR Method for the Study of Radical Reactions**,
by H. Fischer *University of Zürich, Switzerland*
- 10.00 Chemically-Induced Nuclear Spin Polarisation in Products of the Reaction of Diphenylmethylene with Benzyl Fluoride and α , α -Bromofluorotoluene: Novel Effects Arising from Intramolecular Interaction of Polarized ^1H and ^{19}F Nuclei,
by D. Bethel, M. R. Brinkman and J. Hayes *University of Liverpool*
- 10.15 Studies of the Molecular Association between Lanthanide Shift Reagents and Organic Substrates,
by I. Armitage, L. D. Hall and A. G. Marshall *University of British Columbia, Vancouver, Canada*
- 10.30 Discussion
- 10.40 **Coffee**
- 11.00 Use of Europium Shift Reagent in NMR Spectroscopy of Tetrahydrofuran Derivatives,
by M. Holík *Brno, Czechoslovakia*
- 11.15 ^1H - and ^{13}C - NMR Spectrum of a Paramagnetic, Organometallic Europium - Complex,
by R. von Ammon *Kernforschungszentrum, Karlsruhe, Germany*
- 11.30 Discussion
- 11.40 Determination of some Carbon-13 - Proton Couplings from PMR Spectra of ^{15}N -Pyrrole,
by J. Briggs and E. W. Randall *Queen Mary College, London* and E. Rahkamaa *University of Oulo, Finland*
- 11.55 ^1H and ^{13}C NMR Studies of NADPH and Related Compounds,
by B. Birdsall and J. Feeney *MRC Pharmacology Unit, Cambridge*
- 12.10 Discussion
- 12.30 **Lunch**
- 18.00-19.00 Informal Discussions, led by M. R. Brinkman *University of Liverpool*

Thursday 6 July

Morning Session

Chairman: **Dr. J. Feeney**

- 09.00 Plenary lecture: **Proton and ^{13}C Studies of Biopolymers and Model Compounds**,
by F. A. Bovey *Bell Telephone Laboratories, New Jersey, U.S.A.*
- 10.00 The Application of Empirical Approximation Formulae in the Interpretation of the ^{13}C NMR Spectra of Polymers,
by L. P. Blaauw, A. D.H. Clague and A. M. Leonardi-Cattolica *Koninklijke/Shell Laboratorium, Amsterdam, The Netherlands*
- 10.15 NMR Studies on Viomycin,
by A. Lai *University of Cagliari, Italy*, C. Franconi and P. Viglino *Istituto Chimica Fisica, Venice, Italy*, and E. Brosio and F. Conti *University of Rome, Italy*
- 10.30 Discussion
- 10.40 **Coffee**
- 11.00 Carbon-13 NMR Conformational Study of the Ferrichromes, a Suite of Microbial Iron Transport Cyclohexapeptides,
by W. H. Horsley, M. P. Klein, M. Llinas, J. B. Neilands and D. M. Wilson *University of California, U.S.A.*
- 11.15 Conformations of Nucleotides in Solution by NMR Spectroscopy,
by S. S. Danyluk *Argonne National Laboratory, U.S.A.* and D. B. Davies *Birkbeck College, London*
- 11.30 Discussion
- 11.40 Proton Magnetic Resonance Study of the Histidine Residues of Sperm Whale and Horse Myoglobins,
by J. S. Cohen, H. P. Hagenmaier, H. Pollard and A. N. Schechter *National Institutes of Health, Bethesda, Maryland, U.S.A.*
- 11.55 NMR Studies of the Conformations of Decahydroquinolines,
by H. Booth and D. V. Griffiths *University of Nottingham*
- 12.10 Discussion
- 12.30 **Lunch**

Afternoon Session

Chairman: **Dr. G. R. Bedford**

- 14.00 Plenary lecture: **Relaxation Effects in Fourier Spectroscopy**,
by R. R. Ernst *ETH, Zürich, Switzerland*

- 15.00 Barriers to Rotation around PN and SN Formal Single Bonds in Sulphinamides and Sulphonamides,
by W. B. Jennings *University of Birmingham* and W. R. Jackson, G. Kee and R. Spratt *University of Belfast*
- 15.15 Conformational Properties of N-Acyl Imino Acids and Dipeptides Investigated by ^{13}C and ^1H NMR Spectroscopy,
by W. A. Thomas and M. K. Williams *University College, Swansea*
- 15.30 Discussion
- 15.40 **Tea**
- 16.00 To be announced
- 16.15 A Study of "Geared" Intramolecular Rotation by NMR Using Liquid Crystalline Solvents,
by E. E. Burnell, P. Diehl and W. Niederberger *University of Basle, Switzerland* 16.30 Discussion
- 16.40 NMR Study of Ethylene Carbonate and Thiocarbonate and Cyclobutanone Partially Oriented in the Nematic Phase,
by P. F. Swinton *Istituto di Chimica delle Macromolecole del C.N.R., Milan, Italy*
- 16.55 Double Resonance Experiments on Partially Oriented Samples, by J. W. Emsley, J. C. Lindon and J. Tabony *University of Southampton*
- 17.10 Discussion
17. 40-18.40 Informal Discussions, led by Dr. J. Feeney *MRCPharmacology Unit, Cambridge*

Friday 7 July

Morning Session

Chairman: **Dr. E. W. Randall**

- 09.00 Plenary lecture: **Time-Averaged Intensive Parameters and Molecular Energetics in Acyclic Systems**,
by G. Binsch *University of Notre Dame, Indiana, U.S.A.*
- 10.00 NMR Bandshape Studies of Relaxation,
by R. K. Harris, N. C. Pyper and K. M. Worvill *University of East Anglia*
- 10.15 Determination of $J(^{14}\text{N}, \text{X})$ Values by a Carr-Purcell Spin-Echo Experiment, by N. Boden and R. Folland *University of Leeds*
- 10.30 Discussion
- 10.40 **Coffee**

- 11.00 Proton Shielding Functions for HCl and HBr,
by B. P. Chadburn and W. T. Raynes *University of Sheffield*
- 11.15 Water Proton Chemical Shifts in Electrolyte Solutions,
by J. W. Akitt *University of Leeds*
- 11.30 Discussion
- 11.40 The Inductive Effect in Open Chain Alkanes Studied by NMR
Spectroscopy,
by G. Schrumpf *University of Gottingen, Germany*
- 11.55 Empirical Parametrisations in "Ring Current" Calculations on
Conjugated Molecules,
by R. B. Mallion *University of Oxford*
- 12.10 Discussion
- 12.30 **Lunch and Close of Meeting**

RESERVE PAPERS

An Improved Density Matrix Formalism for Extracting Kinetic Data from NMR Line-Shapes, by G. Fraenkel *The Ohio State University, Columbus, U.S.A.*

Conformational Studies of Benzalaniline Type Compounds by NMR, by V. M. S. Gil and M. E. L. Saraiva *University of Coimbra, Portugal*

The Symmetry of Spin Liouville Space, by N. C. Pyper *University of Bristol*

Rapid Method of Analysis of ABX "Spectra", by R. Merenyi *University of Louvain, Belgium*

Trans Annular Long-Range Coupling Constants in Non-Planar Zig-Zag Configuration, by E. Dradi *Istituto Carlo Erba, Milan, Italy*

NMR Investigation of the Barriers to Ring Inversion in Methylated Cyclo-hexanones and Methylenecyclohexanes, by M. Bernard and M. St-Jacques *University of Montreal, Canada*

Nuclear Magnetic Resonance Studies of Retinal Isomers, by R. Rowan and B. D. Sykes *Harvard University, Cambridge, U.S.A.*

The Helix-Coil Transition of Polypeptides Studied by ^1H and ^{13}C Spectroscopy, by E. M. Bradbury, P. D. Gary, C. Crane-Robinson, L. Paolillo, T. Tancredi and P. Temussi *Portsmouth Polytechnic*

Biochemical Applications of Pulse Fourier Transform NMR Spectroscopy, by E. Breitmaier, G. Jung and W. Voelter *University of Tübingen, Germany*
 ^1H and ^{13}C Relaxation Studies of Lipid Bilayers and Biological Membranes, by A. G. Lee *MRC Unit of Molecular Pharmacology, Cambridge*

NMR Studies on Some $\text{Mn}(\text{CO})_3\text{Cr}(\text{CO})_3$ Organometallic Complexes, by C. K. Chu, C. S. Davies and N. J. Gogan *Memorial University of Newfoundland, Canada*

Some Recent Applications of Homonuclear INDOR, by R. A. Spragg *Perkin Elmer, Beaconsfield*