

1st International NMRDG Meeting, Birmingham, 15-18 July

1969

SCIENTIFIC PROGRAMME

The plenary lectures and sessions A, C, E and G will be held in the Large Lecture Theatre of the Haworth Chemistry Building. Sessions B, D, F and H will be held in the Mechanical Engineering Building. Morning coffees and afternoon teas will be served in the Refectory at the times stated in the programme.

Tuesday, 15th July

9. 30 am WELCOMING ADDRESS, by Professor M. Stacey, CBE, FRS
(University of Birmingham)
9. 40 am THE NMR SPECTROSCOPY OF CARBANIONS, by L.M. Jackman
(University of Pennsylvania, USA)
- 10.45 am Coffee

Session A

- 11.15 am A1. Exchange phenomenon between a carbonium ion and its parent molecule,
by L. Lunazzi* and S.K. Brownstein (NRC, Ottawa, Canada)
- 11.35 am A2. PMR spectra of sulphonyl carbanions:thiopyranyl-1,1- dioxide anion and related species, by G.A. Pagani* and S. Bradamente Pagani (Istituto di Chimica Industriale dell'Universita di Milano, Italy)
- 11.55am A3. PMR spectra of heteroaromatic five -membered aza-anions, by S. Bradamente Pagani* and G.A. Pagani (Istituto di Chimica Industriale dell'Universita di Milano, Italy)
- 12.15 pm Discussion
- 12.30pm Lunch
- 2.00 pm A4. The effect of substituents on the vicinal coupling constants in X. CH₂CH₂. Y fragments, by G. Gatti* and R. J. Abraham (University of Liverpool). *To read paper
- 2.00 pm B4. A comparison between theoretically-predicted and experimentally-determined proton chemical shifts in non-planar

overcrowded benzenoid hydrocarbons, by C.W. Haigh and R.B. Mallion (University College, Swansea)

2. 20 pm B5 Steric effects in the PMR spectra of fluorenes and bifluorenyls, by K.D. Bartle, P.M.G. Bavin, D.W. Jones and R. L'Amie. (Institute of Analytical Chemistry, University of Stockholm, Sweden; Smith, Kline and French Laboratories Ltd., Welwyn Garden City; University of Bradford)
- 2.40 pm B6. Restricted rotation and magnetic non-equivalence in phenanthridinium compounds, by R.M. Acheson and I. A. Selby (University of Oxford)
- 3.00pm B7. A new iterative procedure to analyse NMR spectra, by P. Granger and D. Canet (Université de Nancy, France)
3. 20 pm B8. An investigation of the average energy and other approximation methods used in the calculation of nuclear spin-spin coupling constants, by R. V. Emanuel (University of Glasgow)
- 3.40pm Discussion
- 4.00 pm Tea
4. 30 pm NMR OF PARTIALLY ORIENTED MOLECULES IN THE NEMATIC PHASE OF LIQUID CRYSTALS, by P. Diehl (University of Basle, Switzerland)

Wednesday, 16th July

9. 30 am CONFORMATIONAL ANALYSIS OF SIX-MEMBERED RING COMPOUNDS BY NMR SPECTROSCOPY, by H. Feltkamp (Bayer AG, Elberfeld, Germany)

10.30 am Coffee

Session C

- 11.00 am C1. 220 MHz NMR spectroscopy in the cyclohexane series, by W. Naegele* and D. Wendisch (Farbenfabriken Bayer AG, Leverkusen, Germany)
- 11.20 am C2. Identification of stereoisomeric C₄ – cycloadducts by NMR spectroscopy at 220 MHz, by D. Wendisch and W. Metzner (Farbenfabriken Bayer AG, Leverkusen, Germany)
- 11.40 am C3. The proton magnetic resonance spectra of cyclopentadiene trimers at 220 MHz, by R. G. Foster and M. C. McIvor (ICI Petrochemical and Polymer Laboratories, Runcorn)

12.00 noon C4. Nitrogen inversion rate of piperidines and piperazines by a competitive method of protonation, by J. J. Delpeuch, M. N. Deschamps, Y. Martinet, B. Bianchin and C. Beguin Université de Grenoble, France)

Session D

11.00 am D1. Trans-effects in transition metal complexes, W. T. Dixon (Bedford College, London)

11.20 am D2. Effect of molecular and local symmetry on the PMR spectra of temperature independent paramagnetic d^4 complexes, by D. Shaw (Varian Associates, Walton-on-Thames, Surrey)

11.40 am D3. Temperature dependence of PMR shifts in paramagnetic organometallic 4f and 5-f systems, by R. v. Ammon* and B. Kanellakopoulos (Institut für Heisse Chemie, Karlsruhe, Germany) and R. D. Fischer (Laboratorium für Anorganische Chemie, Munich, Germany)

12.00 noon D4. The temperature dependence of chemical shifts and nuclear spin couplings,
by D. B. Cook, A. M. Davies and W. T. Raynes, (University of Sheffield)

12.20 pm Discussion

12.40 pm Lunch

Thursday, 17th July

9.30 am NMR STUDIES OF THE NATURE OF GRIGNARD REAGENTS AND RELATED COMPOUNDS IN SOLUTION, by D. F. Evans (Imperial College, London)

10.30 am Coffee

Session E

11.00 am E1. NMR spectra and structures of some allyl complexes of iron and ruthenium,
by G. A. Fuchs and C. A. Reilly (Shell Development Company, California, USA)

11.20 am E2. $^1\text{H} - ^{31}\text{P}$ spin coupling constants in some heteroaromatic phosphines and their derivatives, by H. J. Jakobsen (University of Aarhus, Denmark)

11.40 am E3. Solvent dependence of $^2\text{J}(\text{P-H})$ and $^4\text{J}(\text{P-H})$ in allenic phosphines, by M-P. Simonnin (Ecole nationale Supérieure de Chemie, Paris, France). * To read paper

12.00 noon E4. Phosphorus-phosphorus coupling constants in transition metal complexes,

by J. F. Nixon (University of Sussex)

12.20 pm Discussion

12.40 pm Lunch

2.10 pm E5. The ^{19}F chemical shifts in oxygen containing fluorine products, by F. Ciampelli, M. Tacchi Venturi and D. Siansesi (Montecatini Edison S. p. A., Centro Ricerche de Milano, Italy)

2.30 pm E6. The effects of substituents on chemical shifts and coupling constants in three small ring systems, by K. L. Williamson* and L. H. Sutcliffe (University of Liverpool)

2.50 pm E7. Applications of field sweep, proton decoupling in ^{13}C resonance using the NSS technique, by R. R. Dean and M. Takeuchi (Jeolco Ltd., London and Tokyo, Japan)

3.10 pm E8. The application of noise decoupling to the study of ^{13}C resonance spectroscopy, by J. Feeney* and U. Scheidegger (Varian AG, Zürich, Switzerland) and L. F. Johnson (Varian Associates, Palo Alto, USA)

3.30 pm E9. A new NMR spectrometer and its accessories, by A. R. J. Arthur (Perkin-Elmer Ltd., Beaconsfield)

3.50 pm Discussion

Session F

11.00 am F1. Two new organometallic reference compounds for PMR spectroscopy at higher temperatures and in aqueous solutions, by B. Hampel*, M. Eckle and L. Pohl (E. Merck AG, Darmstadt, Germany). * To read paper

11.20 am F2. NMR studies of the tacticity of poly(vinylamine). I. Interpretation of the NMR spectra of meso and racemic forms of 2,4-pentanediamine and 2,4-diacetamidopentane, by M. Murano and H. J. Harwood (University of Akron, Ohio, USA)

11.40 am F3. Application of fluorine-19 chemical shifts in the study of bonding in tercovalent boron compounds, by K. Jones* and E. F. Mooney (University of Birmingham)

12.00 noon F4. Structural and solvent effects in ^{19}F NMR of substituted benzyl fluorides, by C. Beguin and J. J. Delpuech (Université de Grenoble, France)

12.20 pm Discussion

12.40 pm Lunch

- 2.10 pm F5. NMR studies of hindered internal rotation of N, N –disubstituted amides. Solvent effects on the N-methyl resonance shifts and on the activation parameters, by A. Calzolari, F. Conti and C. Franconi (Universita di Roma and Universita di Cagliari, Italy)
- 2.30 pm F6. Rotational isomerism of vinylcyclopropanes studied by NMR spectroscopy, by G. Schrumpf (Universität der Göttingen, Germany)
- 2.50 pm F7. Intramolecular nuclear Overhauser effect as means of determination of structure and conformation of alicyclic and aromatic compounds, by J. Lugtenburg (Rijks Universiteit, Leiden, The Netherlands)
- 3.10 pm F8. Rotational isomerism in some chloropropenes, by K. Parry* and R. J. Abraham (University of Liverpool). * To read paper
- 3.30 pm F9. NMR spectra, configuration and conformation of diastereomeric 3-substituted and 2,3-diphenylproanoic acids and esters, by S. L. Spassov (Bulgarian Academy of Sciences, Sofia, Bulgaria)
- 3.50 pm Discussion
- 4.10 pm Tea
- 4.40 pm TECHNIQUES AND APPLICATIONS OF CARBON-13 MAGNETIC RESONANCE TO MOLECULAR STRUCTURE, by D. M. Grant (University of Utah, USA)

Friday, 18th July

- 9.30 am SOME BIOLOGICAL APPLICATIONS OF NMR, by K. A. McLauchlan (University of Oxford)
- 1030 am Coffee

Section G

- 11.00 am G1. PMR investigation of neurohypophyseal peptides, by LeRoy Johnson, I. L. Schwartz and R. Walter (Varian Associates, Palo Alto, USA)
- 11.20 am G2. Correlation of NMR and GLC data in lipid biochemistry: Isomerism of mono- and diglyceride trimethylsilyl ethers, by R. Watts and R. Dils (University of Birmingham)
- 11.40 am G3. The structure of the phenylboronates derivatives of glucose, by G. Kennedy*, M. J. How and E. F. Mooney, (University of Birmingham)
- 12.00 noon G4. NMR studies of heterocyclic compounds of boron, by W. G. Henderson* and E. F. Mooney (University of Birmingham). *To read paper

- 12.20 pm Discussion
- 12.40 pm Lunch
- 2.00 pm G5. Dynamic properties of Dimedone-aldehyde adducts, by P. Laszlo* and W. E. Frankle (Princeton University, USA) and S. Forsen (Lund Institute of Technology, Sweden)
- 2.30 pm G6. An NMR study of rotational isomerism and barriers to internal rotation in substituted ethanes and propanes, by A. B. Dempster, K. Price and N. Sheppard (University of East Anglia)
- 3.00 pm Discussion

Session H

- 11.00 am H1. A study of ^{15}N NMR shifts liquid $^{15}\text{NH}_3$ –solvent mixtures, by Mohammed Alei and A. E. Florin (Los Alamos Scientific Laboratory, Los Alamos, New Mexico, USA)
- 11.20 am H2. Nitrogen-14 resonance studies of fluorinated nitrobenzenes, by E. F. Mooney and P. H. Winson (University of Birmingham)
- 11.40 am H3. The electrical field effects of highly charged cations upon the chemical shifts and spin couplings of coordinated solvent molecules, by T. A. Sutherley, W. T. Raynes and T. H. Lilly (University of Sheffield)
- 12.00 noon H4. A nuclear magnetic resonance study of complexes present in aqueous solutions of phosphoric acid with aluminium and fluoride ions, by J. W. Akitt, N. N. Greenwood and G. D. Lester (University of Newcastle upon Tyne)
- 12.20pm Discussion
- 12.40 pm Lunch
- 3.15 pm SUMMING UP OF THE SYMPOSIUM, by J. A. Elvidge, Chairman of the Nuclear Magnetic Resonance Discussion Group (University of Surrey)
- 3.45 pm Tea
