

Sixth International Meeting on NMR Spectroscopy

University of Edinburgh

10 – 15 July 1983

SCIENTIFIC PROGRAMME

The Opening Ceremony will take place in George Square Theatre, on Monday 11 July, as well as the scientific sessions for that day. The scientific sessions on Tuesday, Wednesday, Thursday and Friday, will take place in the Appleton Tower Lecture Theatre. 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 posters sessions will be held, each of which will contain contributions associated with the various symposia topics. Contributions on other topics and late submissions have been included in a miscellaneous section.

The first exhibition, 'A', will be mounted between 16.00 and 18.00 on Sunday, and on Monday morning. The associated formal viewing sessions for these posters will take place at 15.30 on Monday and Tuesday. Posters for the second exhibition 'B', will be mounted on Wednesday with time-tabled viewing at 15.00 and 17.30 on Thursday.

MONDAY 11 JULY

09.00 Welcome
 E.A.V. Ebsworth, University of Edinburgh
 George Square Theatre

SYMPOSIUM : NMR METHODS

Chairman: Dr G.A. Morris, University of Manchester

09.10 INVITED LECTURE
 New Broadband Decoupling Experiments
 R. Freeman, University of Oxford

10.10 Sensitivity of FT NMR Experiments for Small Quantities of Material
 H.D.W. Hill and A.P. Zens, Varian Associates, Palo Alto, USA

10.40 COFFEE

11.10 INVITED LECTURE
 Laser Flash Photolysis NMR: Applications to Biological Systems
 R. Kaptein, University of Grøningen, The Netherlands

12.10 Composite Pulses and Composite Rotations
 M.H. Levitt, ETH, Zürich, Switzerland

SYMPOSIUM : RELAXATION STUDIES

Chairman: Professor K.J. Packer, University of East Anglia

- 14.00 INVITED LECTURE
The Interpretation of Nuclear Spin Relaxation in Complex Systems such as
Proteins and Lipid Bilayers
M. Bloom, University of British Columbia, Canada
- 15.00 Deuterium Spin Relaxation and Liquid Crystal Dynamics
R.R. Vold and R.L. Vold, University of California, San Diego, USA
- 15.30 TEA AND POSTER SESSION A
- 16.30 INVITED LECTURE
Relaxation in Solid Polymers: Some Interesting Case Histories
V.J. McBrierty, Trinity College, Dublin
- 17.30 Nuclear Spin Relaxation in Paramagnetic Systems Beyond the Solomon-
Bloembergen-Morgan Theory
L. Nordenskiöld, N. Benetis, J. Kowalewski, H. Wennerstrom
and P-O. Westlund, University of Stockholm, Sweden
- 20.00 University Reception in the Upper Library, Old College
Wines and soft drinks will be served

TUESDAY 12 JULY

SYMPOSIUM : APPLICATIONS IN ORGANIC CHEMISTRY

Chairman: Dr J.W. Emsley, University of Southampton

- 09.00 INVITED LECTURE
Applications of ^{13}C NMR in Whole-Cell Metabolism and Enzyme
Mechanisms
A.I. Scott, Texas A&M University, USA
- 09.55 Whole Cell NMR Studies of Formaldehyde Metabolism
J.K.M. Sanders, B.K. Hunter and K.M. Nicholls, University of Cambridge
- 10.30 COFFEE
- 11.10 INVITED LECTURE
NMR in Structural and Mode of Action Studies of Peptide Antibiotics
D.H. Williams, University of Cambridge
- 12.00 Structure Determination of Triterpenoids by 2D NMR Spectroscopy
W. Kraus, M. Bokel, S. Nieter and W. Weber, University of Hohenheim,
Stuttgart, West Germany
- 12.30 LUNCH in the Student Centre

SYMPOSIUM : APPLICATIONS IN INORGANIC CHEMISTRY

Chairman: Dr G.E. Hawkes, Queen Mary College, London

- 14.00 INVITED LECTURE
Cadmium -113 NMR Spectroscopy – The Complementary Nature of Liquid
and Solid State Approaches
P.D. Ellis, University of South Carolina, USA
- 15.00 Multinuclear NMR Studies of Organometallic Complexes
S. Aime, University of Turin, Italy
- 15.30 TEA AND POSTER SESSION 'A'
- 16.30 INVITED LECTURE
Inorganic Applications of Multinuclear NMR: From Chemistry to Medicine
P.J. Sadler, Birkbeck College, London
- 17.15 Tungsten-183 NMR: A Complete Assignment of the ^{183}W - ^{183}W Connectivities
in Heteropolytungstates via 2-Dimensional ^{183}W Techniques
C. Brevard, Bruker Spectrospin SA, Wissembourg, France
- 17.35 Thallium-205 Solid State NMR Spectroscopy
J.F. Hinton, University of Arkansas, USA
- 17.55 Close
- 20.00 Corporation Reception and Supper in the Assembly Rooms
Coaches will depart from the Pollock Halls of Residence at the Main Entrance
in Holyrood Park Road at 20.00

WEDNESDAY 13 JULY

SYMPOSIUM : NEW DEVELOPMENTS

Chairman: Dr N. Boden, University of Leeds

- 09.00 INVITED LECTURE
Exploring Solids by Polarization and Coherence Transfer
R.R. Ernst, ETH, Zürich, Switzerland
- 09.55 COFFEE
- 10.15 INVITED LECTURE
NMR Imaging of Non-Medical Objects
R.P. Hawker, University of Nottingham
- 11.10 INVITED LECTURE
Recent Developments in Multiple Quantum Spectroscopy
A. Pines, University of California at Berkeley, USA
- 12.05 LUNCH - in the Refectory at Pollock Halls of Residence

PM EXCURSIONS

THURSDAY 14 JULY

SYMPOSIUM : APPLICATIONS IN BIOLOGY (I)

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

- 09.00 INVITED LECTURE
Three Dimensional Protein Structures by Nuclear Magnetic Resonance
K. Wüthrich, ETH, Zürich, Switzerland
- 09.50 Structure of the DNA Binding Domain of Lactose-Repressor by 2D NMR
E.R.P. Zuiderweg, R. Kaptein and K. Wüthrich, ETH, Zürich, Switzerland
- 10.10 Solution Conformation of Glycoprotein Oligosaccharides as Revealed by One-
and Two-Dimensional NMR Techniques
H. van Halbeek and J.F.G. Vliegthart Rijksuniversiteit Utrecht, The
Netherlands
- 10.30 COFFEE
- 11.00 INVITED LECTURE
Methods for Studying Enzyme Kinetics in Intact Cells
I.D. Campbell, University of Oxford
- 11.50 Strategies in Drug Design Using NMR Studies on Dihydrofolate Reductase
B. Birdsall, C. Pascual, J. Feeney and G.C.K. Roberts, National Institute for
Medical Research
- 12.10 Protein Dynamics from ^1H NMR Studies of Lysozyme
C.M. Dobson, University of Oxford
- 12.30 LUNCH in the Student Centre

SYMPOSIUM : APPLICATIONS IN BIOLOGY (II)

Chairman: Dr D. Shaw, G.E. Medical Systems

- 14.00 INVITED LECTURE
Phosphorus NMR of Intact Tissues: From the Laboratory to the Clinic
G.K. Radda, University of Oxford
- 15.00 TEA AND POSTER SESSION 'B'
- 16.00 Imaging of the Foetus by NMR
M.A. Foster, University of Aberdeen and C.H. Knight Hannah Research
Institute, Ayr
- 16.25 Applications of ^{13}C -Multiplet Analysis to the Estimation of Metabolic
Flux During Nutritional Adaptions in Microorganisms
R.L. Baxter, University of Edinburgh

- 16.50 Photo CIDNP Study of Protein-Protein Interactions
K.A. Muszkat, The Weizmann Institute of Science, Rehovot, Israel
- 17.10 Structure and Motions of Lysozyme and Ribonuclease-A by ^{13}C NMR
O. Howarth, University of Warwick
- 17.30 POSTER SESSION 'B'
- 19.30 For 20.00. Conference Dinner in Holland House Hall, Pollock for Halls of Residence

FRIDAY 1st JULY

SYMPOSIUM : HIGH-RESOLUTION NMR OF SOLIDS

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

- 09.00 INVITED LECTURE
Analytical Applications of High-Resolution NMR of Solids
C.A. Fyfe, University of Guelph, Ontario, Canada
- 10.00 Multinuclear High-Resolution Solid-State NMR of Catalytic Systems
N.C.M. Alma and G.R. Hays, Koninklijke/Shell-Laboratorium, Amsterdam,
The Netherlands
- 10.25 COFFEE
- 10.55 High Resolution Proton NMR of Solids
B. Schnabel, Jena, GDR
- 11.25 INVITED LECTURE
Chemical Shift and Dipolar Tensors at Cryogenic Temperatures
D.M. Grant, University of Utah, USA
- 12.15 Closing Remarks

LUNCH in the Refectory at the Pollock Halls of Residence
