

15th International Meeting on NMR Spectroscopy
University of Durham
8 -12 July 2001

I - Invited Speaker; C - Contributed Oral, *= Presenter. Affiliation refers to the presenter A discussion period of 5 minutes has been allowed between each talk.

Monday 9 July

09:00-09:15 Welcome

Lecture Theatre CG93

SESSION I Symposium 1: New Experimental Techniques

Chair: **James Keeler.** *University of Cambridge, UK*

09:15 - 09:55 I.1 Higher Order Effects in the Solid State NMR of Quadrupolar Nuclei

Lucio Frydman

Weizmann Institute of Science, Israel and University of Illinois, Chicago. USA

10:00 –10:30 C.1 New NMR-Methods For Small Molecules; MBOB, J-HMBC and Broadband XLOC

Axel Meissner* and Ole W Sorensen

Carlsberg Laboratory. Denmark

10:30 – 11:00 **COFFEE IN POSTER ROOMS**

11:00 – 11:40 I.2 Structure, Dynamics and Interactions of Macromolecules in the Weakly Aligned State

Steven Homans

University of Leeds, UK

11:45 – 12:25 New Pulses. New Sequences and New Spectra using Filter Diagonalization

A J Shaka

University of California. Irvine. USA

12:30 **Close of Session and lunch**

PARALLEL SESSION II

Lecture Theatre CG85

Symposium 2: Unusual Nuclei

Chair: **Gerry Lawless**

University of Sussex. UK

14:00-14:40 I.4 Transition Metal and High-Pressure NMR Spectroscopy

C J Elsevier

University of Amsterdam. The Netherlands

14:45 -15:10 C.2 ^{13}C , ^7Li and ^{23}Na Solid State NMR of Organometallic Compounds: Information about Structure and Dynamic Behaviour
H Günther*, M Kühnen, A Repels and S Jost
University of Siegen. Germany

15:15 – 15:55 I.5 Molecular and Spin Dynamics of Some Crystalline Organometallic Compounds
Angelika Sebald
University of Bayreuth. Germany

Lecture Theatre CG93

Symposium 3: Structural Biology

Chair: David Neuhaus
MRC Lab of Molecular Biology. Cambridge, UK

I.6 How can We Trick Proteins to Behave Well for NMR Studies?
Gerhard Wagner
Harvard University. USA

C.3 Applications of NMR Spectroscopy for Structure-Based Inhibitor Design
S R Laplante
Boehringer Ingelheim (Canada) Ltd. Canada

I.7 Using NMR to Probe Ribosome Function
Joseph Puglisi
Stanford University School of Medicine. USA

16:00- 16:30 TEA IN POSTER ROOMS

Lecture Theatre CG93

Post Graduate Session

Chair: David Davies.
Birkbeck College. University of London. UK

16:30 – 16:45 C.4 Solid State NMR Study of Biopolymers
N McDougal* and M J Duer
University of Cambridge. UK

16:50 – 17:05 C.5 Determination of the Orientational Distribution in Disordered 1,2,3-trichloro-4,5,6-trimethylbenzene by Deuterium NMR Single Crystal Experiments
T Braeuniger*, R Poupko, Z Luz, D Reichert, H Zimmermann and U Haeberlen
Weizmann Institute of Science. Israel

17:10 – 17:25 C.6 Structure and Dynamics of an Unusual Metallothionein

C Blindauer
University of Edinburgh, UK

17:30 – 17:45 C.7 NMR Studies on Drug Glucuronide Reactivity
S Vanderhoeven
Imperial College. London, UK

17:50 **Close of Session**

POSTER SESSION 1 WITH REFRESHMENTS - **CG193 AND CG272**
Odd numbered posters to be manned

Tuesday 10 July

Lecture Theatre CG93

SESSION III

Symposium 4: Organic Small Molecules
Chair: Duncan Farrant. GlaxoSmithKline. UK

09:00 - 09:45 I.8 Small Molecule NMR Techniques: Ethanol and Beyond..
Tim Claridge
University of Oxford. UK

09:50 - 10:25 C.8 The Automated Structure Elucidation of a Series of
Cryptolepine Derivatives
**A Williams*, S Molodtsov, K Blinov, E Martirosian, M
Elyashberg, G Martin and C Madden**
Advanced Chemistry Development, Toronto, Canada

10:30 - 11:00 **COFFEE IN POSTER ROOMS**

11:00 - 11:40 I.9 Chiral Recognition through NMR in Liquid Crystal Solvents:
an Order Affair
Jacques Courtieu
Université Pans-Sud, France

11:45 - 12:25 I.10 High Resolution Spectroscopy of Protons in Solids
Lyndon Emsley
École Normale Supérieure de Lyon, France

12:30 **Close of Session - lunch and excursions**

Excursions - full details of coach departure points can be found on page 10.

Wednesday 11 July

Lecture Theatre CG93

SESSION IV Symposium 5: Materials

Chair:	Paul Hodgkinson University of Durham. UK
09:00 - 09:40	I.11 Solid-State NMR Methods for Studying Dynamics and Structure of Complex Polymer Systems Klaus Schmidt-Rohr <i>Iowa State University, USA</i>
09:45-10:05	C.9 Solid-State NMR Spectroscopy of Molecular Magnetic Materials F H Kohler* and H Heise <i>Technische Universität Munchen, Germany</i>
10:10 - 10:25	C.10 Structure and Dynamics of Water Soluble Monolayer Protected Gold Clusters (MPC's) by Means of NMR Methods and Computer Simulations C S Johnson Jr*, O Kohlmann, W Steinmetz, X-A Mao, W P Wuelfing, A C Tenpleton and R W Murray <i>University of North Carolina, USA</i>
10:30 - 11:00	COFFEE IN POSTER ROOMS
11:00 - 11:40	I.12 Dipolar Solid State NMR Strategies for Structural Studies of Disordered Materials Hellmut Eckert <i>University of Munster Germany</i>
11:45 - 12:25	I.13 Resolving a Crystallographic Structure on a Powder by NMR Francis Taulelle <i>University of Strasbourg. France</i>
12:30	CLOSE OF SESSION AND LUNCH
PARALLEL SESSION V Lecture Theatre CG93	
Symposium 6: industrial Applications	
Chair:	Mark Dixon <i>AstraZeneca R&D Charnwood. UK</i>
14:00 - 14:45	I.14 Coupling of Microseparations to NMR Detection Andrew Webb <i>University of Urbana at Champaign-Illinois, USA</i>
14:50 -15:05	C.11 Application of NMR and Hyphenated Techniques for the Study of Beer I F Duarte*, I Delgadillo, A Barros, P Belton, M Godejohann, U Braumann, M Spraul, E Humpfer and A M Gil <i>University of Aveiro. Portugal</i>
15:10 15:55	I.15 The Expanding Role of NMR in Drug Discovery and

Development
John Shockcor
Metabometrix Ltd, UK

Lecture Theatre CG85

Symposium 7: Theoretical/Physical
Chair: Jim Emsley
University of Southampton. UK

I.16 Are Cross-Correlation Effects too Complex to be Widely Accepted for Structural Studies?

Geoffrey Bodenhausen
École Normale Supérieure, Paris. France

C.12 Cross-Polarization Dynamics Involving Multiple Spin Baths in a Fluoropolymer

Paul Hazendonk*, S Pizzanelli and R K Harris
University of Durham. UK

I.17 Using Symmetry to Design Pulse Sequences in Solid-State NMR

Malcolm Levitt
University of Southampton, UK

16:00 - 18:00 **POSTER SESSION 2** WITH TEA + COFFEE - **CG193 AND CG272**
Even numbered posters to be manned

Thursday 12 July

Lecture Theatre CG93

SESSION VI Symposium 8: Biological NMR Spectroscopy
Chair: John Lindon
Imperial College, London. UK

09.00 - 09.35 1.18 Double Quantum Filtered NMR and MRI as New Methods for the Investigation of Connective Tissues

Gil Navon
Tel Aviv University, Israel

09.40 - 10.25 I.19 Resolution of Structural Details of Membrane-embedded Proteins and Peptides using Solid State NMR Methods

Anthony Watts
University of Oxford. UK

10.30 - 11.00 **COFFEE IN POSTER ROOMS**

11.00 - 11.25 C.13 Solid-State Fluorine NMR for Structural Studies in Biomembranes

S L Grage*, J Salgado, S E Afonin, U Duerr and A S Ulrich
Friedrich-Schiller-Universität Jena, Germany

11.30 - 12.15 I.20 High Resolution MagiC-angle-spinning NMR Studies of Biomaterials
Jeremy Nicholson
Imperial College, London, UK

12.20-12.30 **Closing Remarks**

CLOSE OF MEETING - LUNCH

Poster Presentations

Posters will be located in Rooms CG193 and 272 (on the 1st and 2nd floors of the Chemistry/Geology Building where the lectures will take place). Posters in CG193 will relate to Symposia 1-4 and those in CG272 to Symposia 5-8.
Two formal poster sessions are included within the scientific programme.

Monday 9 July at 19:45 - Poster Session 1 -Odd numbered posters

Wednesday 11 July at 16:00 - Poster Session 2 - Even numbered posters

Presenters must ensure that their posters are manned during the appropriate session.

Posters can be mounted from 08:30 on Monday morning.

Posters in CG272 must be removed at the end of the poster session on Wednesday evening. Posters in CG193 should be removed by coffee time on Thursday 12 July.