A joint meeting between the

UK NMR Discussion Group

and the

Groupment Français d 'Etudes d e Resonance Magnétique

held at

University of Southampton
Wednesday September 4th to Saturday September 7th 2002

Organising Committee
Comité D'Organissation

NMRDG

David Neuhaus(Chair)
Harry Parkes (Treasurer)
Jim Emsley

GERM

Catherine Bessada (Chair)
Philippe Turek (Treasurer)
Florence Babonneau

Local Organisation

Jim Emsley, Malcolm Levitt, Matthew Crump, P.K. Madhu, Marina Caravetta, Jed Long, Ole Johannessen, Xin Zhao, Natala Ivchenko, Lindi Wai Cheu Lai, Stuart Findlow

Scientific Committees

NMRDG	T. Claridge, D. Davies, M. Dixon, D. Farrant, J. Griffin, G. Hawkes, I.P. Jones, D. Neuhaus
GERM	F. Babonneau, C. Bessada, S. Confort-Gouny, J. Emery, A. Guillermo, G. Guilot, J.-M. Neumann, I. Salliot-Maire, P. Turek

Scientific programme

Thursday September 5th 2002

09.99 – 09.40 G. Lippens
NMR study of Pin 1, a proline cis/trans isomerase involved in the eucaryotic cell cycle

09.45 – 10.05 F. Bontems
Study of the RegB endoribonuclease activity and of its regulation by the S1 ribosomal protein

10.10 – 10.30 Peter Nielsen
Complex of the chromodomain from HP l beta and the N-terminal tail of histone H3 methylated at lysine 9

10.35 – 11.00 Coffee

11.00 – 11.40 G. Martin
Application of SNIF-NMR and other isotopic techniques in the fight against counterfeiting of fine chemicals and pharmaceuticals

11.45 – 12.05 D. Uhrin
Measurement of small residual $^{1}D_{CH}$, $^{2}D_{CH}$ and $^{n}D_{HH}$ coupling constants in partially oriented samples of oligosaccharides

12.10 – 12.30 V. Michlova
Application of urea derivatives of calix(4)arene based ligands in anion recognition

12.35 – 14.00 Lunch

14.00 – 14.40 D. Williams
Volume reductions in receptors and enzymes as a source of binding energy and catalytic efficiency

14.45 – 15.05 F. Aussenac
Structural and dynamical investigation of bicelles model membrane and neu/erbB-2 transmembrane peptide by solid state NMR

15.10 – 15.35 Tea

15.35 – 15.55 R.K. Harris
Solid-state NMR studies of molecular systems

16.00 – 16.20 D. Middleton
Investigating molecular interactions using solid-state NMR and other methods

16.25 – 16.45 S.P. Brown
The direct detection of a hydrogen bond in the solid state via the observation and quantification of a hydrogen-bond mediated ^{15}N-^{15}N J coupling

16.50 - 18.30 Posters, Exhibitions

19.30 Conference Dinner in the University Staff Club

Friday September 6th 2002

Chairman:

09.00 - 09.40 M. Levitt
The symmetry-based approach for designing NMR experiments

09.45 - 10.05 B. Bechinger
Biophysical analysis of membrane-associated polypeptides by solid-state NMR spectroscopy

10.10 - 10.30 O. Soubias
High resolution 2D NMR on oriented lipid bilayers

10.35 - 11.00 Coffee

11.00 - 11.40 P. Tekely
Probing molecular geometry of solids by NMR: methods and applications

11.45 - 12.05 I. King
^{31}P solid-state NMR study of MP_2O_7 crystalline phosphates

12.10 - 12.30 C. Bonhomme
"Unusual nuclei" in solid-state NMR: ^{1}H and ^{35}Cl. The case of Al-O-P clusters

12.35 - 14.00 Lunch

Chairman:

14.00 - 14.40 J. Lindon
NMR-based metabonomic studies on biofluids and tissues for drug safety evaluation and disease diagnosis

14.45 - 15.05 F. Barbault
Lead optimisation of antifungal peptides with 3D NMR structures analysis

15.10 - 15.35 Tea

15.35 - 15.55 R.A. Atkinson
Structure determination and spectral interpretation without assignment

16.00 - 16.20 J. Trebosc
Frequency selective REDOR and J REDOR

16.25 - 16.45 P.K. Madhu

Radiofrequency modulations in quadrupolar nuclei

16.50 - 18.30 Posters, Exhibitions

19.00 Dinner in Highfield Hall

Saturday September 7th 2002

Chairman:

09.00 – 09.40 H. Desvaux
Dynamicy frequency shift in dia- and paramagnetic proteins

09.45 – 10.05 R. Thouvenot
^{31}P paramagnetic NMR: a tool for structural analysis of polyoxometalate sandwich complexes

10.10 – 10.30 P. Hodgkinson
Resolving ^{13}C-^{19}F interactions in the ^{13}C NMR of liquid-crystals and solids

10.35 – 11.00 Coffee

11.00 – 11.20 S. Wimperis
NMR of satellites: is it rocket science?

11.25 – 12.05 J. Keeler
Two short pieces

12.10 – 14.00 Lunch

14.00 Departure

Posters

1. ^{2}H NMR of solids: two-dimensional separation of quadrupolar and shift anisotropy interactions
   Sasa Antonijevic and Stephen Wimperis

2. Solid state NMR characterization of $CdPS_3$ intercalates
   J. Schmedt auf der Günne, H. Eckert, A., Léaustic and F. Babonneau

3. Investigation of seeds with high resolution solid-state ^{13}C NMR and pulsed field gradients NMR
   Michael Bardet, Armel Guillermo, Sébastien Maron, Marie Françoise Foray, Jacques Bourguignon and Pierre Alain Bayle

4. Quantification of the dynamic disorder in mixed chloromethylbenzenes by single crystal 2H-NMR
   Thomas Braüniger

5. Characterisation of sol-gel derived hybrid materials by solid state NMR.
   Lydie Camus, Christian Bonhomme, Jocelyne Maquet and Florence Babonneau

6. NMR studies by transferred NOE and STD experiments on the conformation of the 4l-62 hydrophilic region of HIV-I encoded virus protein U (Vpu) containing the phosphorylated sites Ser^{52} and Ser^{56} bound to β-TrCP protein and to its monoclonal antibody
   Gaël Coadou, Josyane Gharbi-Benarous, Gildas Bertho, Nathalie Evrard-Todeschi, Simon Megy, Thierry Delaunay, Richard Benarous and Jean-Pierre Girault

7. Solid State NMR studies of lemon and maize cellulose microfibrils
   Corinne Rondeau-Mouro, Bruno Pontoire and Alain Buleon

8. Comparative protein structure modeling of nsLTPs from Arabidopsis thaliana
   Pedro Da Silva, Céline Landon and Françoise Vovelle

9. New techniques in MAS NMR of quadrupolar nuclei: relative tensor orientation and rotor-synchronized excitation
   Nicholas G. Dowell, Sharon E. Ashbrook and S. Wimperis

10. Cholesterol dynamics in membranes of "raft" composition. A molecular point of view from ^{2}H and ^{31}P solid state NMR
    Fabien Aussenac, Marianne Tavares and Erick J. Dufourc

11. Quantitative NMR: minimising the errors for purity determination
    Sara J. Duncan, Richard J. Lewis, J. Mark Dixon and Michael A. Bernstein

12. X-STE: A new pulsed field gradient method for the measurement of ultraslow diffusion by NMR
    Fabien Ferragea, Manuela Zoonensb, Dror E. Warschawskib, Jean-Luc Popotb and Geoffrey Bodenhausen

13. Mechanical and microstructural study of new ultra high performance matrices
    Ph. Fonollosel, P.-C. Aïtcin, H .Zanni and Ph. Gégout

14. A ^{31}P double quantum NMR of MIL-50. A nanoporous GaPO with a small water pool
A. Gansmüller, C. Huguenard, F. Taulelle, M. Henry, L. Beitone, T. Loiseau and G. Ferey

15. Structural and motional features of a layered sodium hydrous silicate as revealed by solid state NMR
Carole Gardiennet and Piotr Tekely

16. Solid-state ^{13}C NMR detection of deprotonated conformers of malonic acid
Roxane Colsenet, Carole Gardiennet, Bernard Henry and Piotr Tekely

17. ^{47,49}Ti solid-state NMR characterisation of titania-based materials
C. Gervais D. Veautier, P. Belleville, C. Sanchez F. Babonneau and M.E. Smith.

18. Hyperpolarized ^{129} Xenon NMR studies of mesoporous molecular sieves
A. Nossov, E. Haddad, F. Guenneau and A. Gedeon

19. NMR and MD conformational studies of the antibody-bound tyrosine phosphorylation site of the nicotinic acetylcholine receptor
C. Hemmerlin, A. Thureau, D. Krikorian, M . Sakarellos-Daitsiotis, V. Tsikaris, C. Sakarellos, M. Marinou, S.J. Tzartos and M.T. Cung

20. Measuring dissociation constants of protein:ligand complexes by water-exchange spectroscopy
Tom Harvey and Peter W.A. Howe

21. Modelling one and two-dimensional solid state NMR spectra
Dominique Massiot, Franck Fayon, Mickael Capron, Ian King, Stéphanie Calvé, Bruno Alonso, Jean-Olivier Durand, Bruno Bujoli, Zhehong Gan and Gina Hoatson

22. Structure determination of large DNA duplexes: impact of a small set of dipolar coupling constants
O. Mauffret, G. Tevanian and S. Fermandjian

23. Studies of the degradation of sulfonated polyimide membranes by liquid and solid state NMR
G. Meyer, M. Bardet, G. Gebel and P.-A. Ba1le

24. Continuous flow optical pumping ^{129}Xenon NMR: application on solid surfaces
A. Nossov, F. Guenneau, C. Mignon, A. Gedeon, E. Haddad, D. Grosso, F. Babonneau and C. Sanchez

25. NMR investigation of interaction between adsorbed molecules and surface of activated zeolites
M. Gaillard, J. Czyzniewska, V. Montouillout, C. Fernandez, F. Maugé and F. Thibault Starzyk

26. Blast furnace slag cement: microstructural study of hydration products
Sylvain Murgier and Hélène Zanni

27. ^{29}Si, ^{23}Na and ^{207}Pb solid state NMR study of lead silicates glasses in the systemNa_2O-PbO-SiO_2
Ioana Nuta, Catherine Bessada, Franck Fayon, Pierre Florian and Dominique Massiot

28. ^{1}H magnetic resonance spectroscopy of mouse spinal cord extracts in chronic relapsing experimental autoimmune encephalomyelitis (Crcae)
H. Parkes, R.A. Page, D. Baker, G. Giovannoni and C.A. Davie

29. Irradiation effects induced by swift heavy ions in $MgAl_2O_4$ and $ZnAl_2O_4$ spinels: ^{27}Al NMR study
N. Pellerin and D. Massiot

30. ^{19}F NMR investigation of solid and molten lanthanide fluorides
Aidar Rakhmatoulline, Catherine Bessada and Anne-Laure Rollet

31. Direct on-line hyphenation of capillary liquid chromatography to nuclear magnetic resonance spectroscopy: practical aspects and first applications to drug metabolite identification.
M. Sandvoss, D.A. Roberts and S.E. North

32. Aging of epoxide materials under γ irradiation: a solid state NMR and EPR study
M. Sebban, T. Devanne, N. Raguin, P. Palmas and A. Bry

33. Synthesis and characterization of a new class of energetic molecules
M. Sebban, J. Guillard, P. Palmas and D. Poullain

34. Structural characterization of dia- and paramagnetic lanthanide derivatives of α_2-$P_2W_{17}O_{61}^{10-}$; NMR study of the racemisation of [Ce(α_2-$P_2W_{17}O_{61}$)$_2$] complexes
David Racimor, Sébastien Picart and René Thouvenot

35. A multinuclear NMR investigation of nitrogen derivatives of polyoxometalates.
Céline Dablemont, Pierre Gouzerh, Chrris Hamaker, Haidoo Kwen, Eric A. Maatta, Anna Proust and René Thouvenot

36. Frequency Selective REDOR
J. Trebosc, J.P. Amoureux, M. Pruski and J. Wiench

37. Structure and dynamics of lipopeptides from *Bacillus subtilis* in micelles by NMR
Benoît Rigard, Pascale Tsan, Laurent Volpon, Xavier Trivelli, Françoise Besson and Jean-Marc Lancelin

38. Alternate Ca^{2+}-calmodulin binding of the microtubule-associated STOP protein
Cécile Vanhaverbeke, Denis Bouvier, Jean-Pierre Simorre, Pierre Gans, Vincent Forge, Robert Margolis and Jean-Philipp Kleman

39. Solvent suppression for diffusion measurements in drug-protein systems
W.S. Price, C. Vigouroux, F. Elwinger and P. Stilbs

40. The three-dimensional structure of the gallium complex of azoverdin, a siderophore of *Azomonas macrocytogenes* ATCC 12 334, by NMR using residual dipolar coupling constants
Emeric Wasielewski, R. Andrew Atkinson, Mohamed A. Abdallah and Bruno Kieffer

41. Solid-state NMR studies of phospholipid bilayers supported on mesoporous anodic alumina
Olivier Wattraint, Catherine Sarazin and Christian Bourdillon

42. Conformational analysis of 2-halocyclohexanones: An NMR, theoretical and solvation studv
F.Yoshinaga, C.F. Tormena, M.P. Freitas, R.Rittner and R.J. Abraham

43. Laser-polarized xenon for NMR
Patrick Berthault, Hervé Desvaux and J. Gaspard Huber

44. Structural studies and protein interactions of polyketide synthase ACPs
Stuart Findlow and Matthew Crump

45. Using NMR to determine the structure and binding of chemokines
Jed Long and Matthew Crump

46. Mode of insertion of a fusogenic peptide into flat lipid membranes as determined by solid state ^{19}F-NMR
Sergii Afonin, Ulrich Dürr, Ralf W. Glaser and Anne S. Ulrich

47. Experimental considerations for using CF_3-groups as labels for solid state ^{19}F-NMR of biomembranes
Ulrich Dürr, Talf W. Glaser, Stephan L. Grage and Anne S. Ulrich

48. Susceptibility correction in high resolution solid state NMR experiments with macroscopically oriented membrane samples
Ralf W. Glaser, Reinhard Ulrich and Anne S. Ulrich

49. Orientational re-alignment of gramicidin S in lipid membranes: influence of lipid composition and experimental conditions screened by solid state ^{19}F-NMR
Sergii Afonin, Ulrich Dürr, Jesus Salgado, Parvesh Wadhwani, Stephan Grage, Anne S. Ulrich

50. 4-Fluorophenylglycine: a label for the structure analysis of membrane active peptides using ^{19}F-solid state NMR
Parvesh Wadhwani, Sergii Afonin, Ralf W. Glaser, Marina Berditchevskaja, Ute Möllmann and Anne S. Ulrich

51. Investigations of structural changes in plasma-sprayed hydroxy apatite coatings
P. Hartmann, J. Vogel and Anne S. Ulrich

52. Characterisation of oxo-metallic clusters by solution and solid state NMR spectroscopy
Stéphanie Le Calve, Bruno Alonso, Laurence Rozes, Clément Sanchez, Françoise Archaimbault, Laurent Duclaux, Marie-Noël Rager and Dominique Massiot