

NMR DISCUSSION GROUP

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A Subject Group of the Royal Society of Chemistry
Charity Registration No. 207890

NMR Discussion Group Christmas Meeting

Date of meeting: Wednesday 12th December 2012

Meeting venue: Institute of Child health
Guilford Street
London WC1N 1EH

Dear Member,

One of the principal objectives of the NMR Discussion Group is to provide a forum for educating, sharing ideas and promoting recent developments in NMR and related disciplines. The group continues to provide such opportunities for scientists that work in many different areas associated with magnetic resonance. This is achieved through, in addition to other means, the popular Christmas meeting.

The forthcoming Christmas meeting comprises presentations covering a range of subjects, including recent developments in small molecule characterization and the continually developing discipline of solid-state characterisation. It is intended that the presentations will be of interest to the majority of spectroscopists of differing backgrounds, either through direct relevance or through potential applicability. An agenda is attached for your information.

The meeting will take place on Wednesday 12th December at the easily accessed Institute of Child Health, London.

A map of the venue for the NMRDG meeting is shown below, with an arrow indicating the location of the main building. Alternatively, a map of the location can be found at:

<http://www.streetmap.co.uk/newmap.srf?x=530518&y=182154&z=0&sv=wc1n+1eh&st=2&pc=wc1n+1eh&mapp=newmap.srf&searchp=newsearch.srf>

The Institute of Child Health is within 10 minutes walk of Euston, King's Cross and St Pancras main line stations. Russell Square on the Piccadilly line (dark blue) and Holborn on the Piccadilly and Central lines (red) are the nearest underground stations, and are within walking distance.

If you would like to attend please complete the on-line registration form via the link:
<http://www.rsc.org/Membership/Networking/InterestGroups/NMR/ForthcomingEvents.asp>
Registration will close on **Friday 30th November** and the standard fee is £45.00.
However, if you are a student or retiree, then a concessionary rate of £25.00 will apply.

The BRSG will be hosting a Christmas meeting on Tuesday 11th December at the Institute of Physics, London and further details will become available using the link
www.iop.org/conferences.

Yours sincerely,

Dr James Keeler – NMR DG Chairperson
Dr Stephen Byard - NMR DG Secretary



NMR Discussion Group Christmas 2012 Meeting

Wednesday 12th December 2012

Institute of Child Health, 30 Guilford Street, London WC1N 1EH

Morning session chair:

- 10.00 – 10.25 Registration and refreshments
- 10.25 – 10.30 Introduction and welcome
- 10.30 – 11.10 **Teodor Parella, *Universitat Auto`noma de Barcelona***
On the Accurate Determination of the Sign and the Magnitude of Small Heteronuclear Coupling Constants in Small Molecules
- 11.10 – 11.45 **Peter Howe, *Syngenta Limited, Bracknell, UK***
One-bond Proton-Carbon J-couplings: Useful Information for Xenobiotic Metabolite Identification
- 11.45 – 12.10 **Smita Odedra, *University of Glasgow***
Improved Background Suppression in ¹H MAS NMR using Composite Pulses
- 12.10 – 12.45 **John Morton, *University of Oxford***
2012 BRSG-NMRDG Prize Winner for Excellent Contribution to Magnetic Resonance by an Early Career Researcher
Electron and nuclear spin qubits in the solid state
- 12.45 – 14.00 Buffet Lunch

Afternoon session chair:

- 14.00 – 14.10 NMRDG Business
- 14.10 – 14.45 **Yaroslav Khimyak, *University of East Anglia***
Understanding Complex Heterogeneous Materials using Solid-state NMR: Structure and Dynamics
- 14.45 – 15.20 **Tran Pham, *GlaxoSmithKline, Stevenage, UK***
Solid-state NMR Analysis of Pharmaceuticals
- 15.20 – 15.45 **Scott Sneddon, *University of St Andrews***
Exploiting the ³¹P Chemical Shift Anisotropy of Aluminophosphates
- 15.45 – 16.25 **Jeremy Titman, *University of Nottingham***
Proton Shift Anisotropies in Solids: Measurement, Calculation and Applications
- 16.25 – 16.30 Closing remarks
- 16.30 - Refreshments and departure
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