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An Interest Group of the Royal Society of Chemistry
Charity Registration No. 207890

NMR Discussion Group 2017 Christmas Meeting

Date of meeting: Thursday 14th December 2017

Meeting venue*: Institute of Structural and Molecular Biology
Birkbeck College*
The Main Birkbeck Building
Torrington Square
London
WC1E 7JL

* Lecture theatre to be defined

Dear Member,

One of the principal objectives of the NMR Discussion Group is to provide mechanisms 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 diverse range of subjects, including recent developments in small molecule characterisation, structure based design in pharmaceuticals, molecular biology 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 **Thursday 14th December** at the easily accessed Institute of Structural and Molecular Biology, Birkbeck College, London. Relevant maps showing the venue location within London and also connections with the local underground stations are shown below. **Please note that details of the lecture theatre will be announced in due course.**

If you would like to attend the event, please complete the on-line registration form via the link <https://events.rsc.org/rsc/1303/register> . Additional details are available on the NMR DG website <http://www.nmrdg.org.uk> .

Registration will close on **Monday 4th December 2017** and the standard fee is £55.00 for non-RSC members or £45.00 for RSC members. However, if you are a student or retiree, then a concessionary rate of £30.00 will apply for non-RSC members or £25.00 for non-members. Members of affiliated groups, such as the Institute of Physics, will qualify for the same rates as RSC members. **Please note the following codes that are required to obtain discounted registration rates that are available to retirees or members of affiliate organisations:**

The code for retired members is: 17NMRXRET

The discount code for affiliate members is: 18921

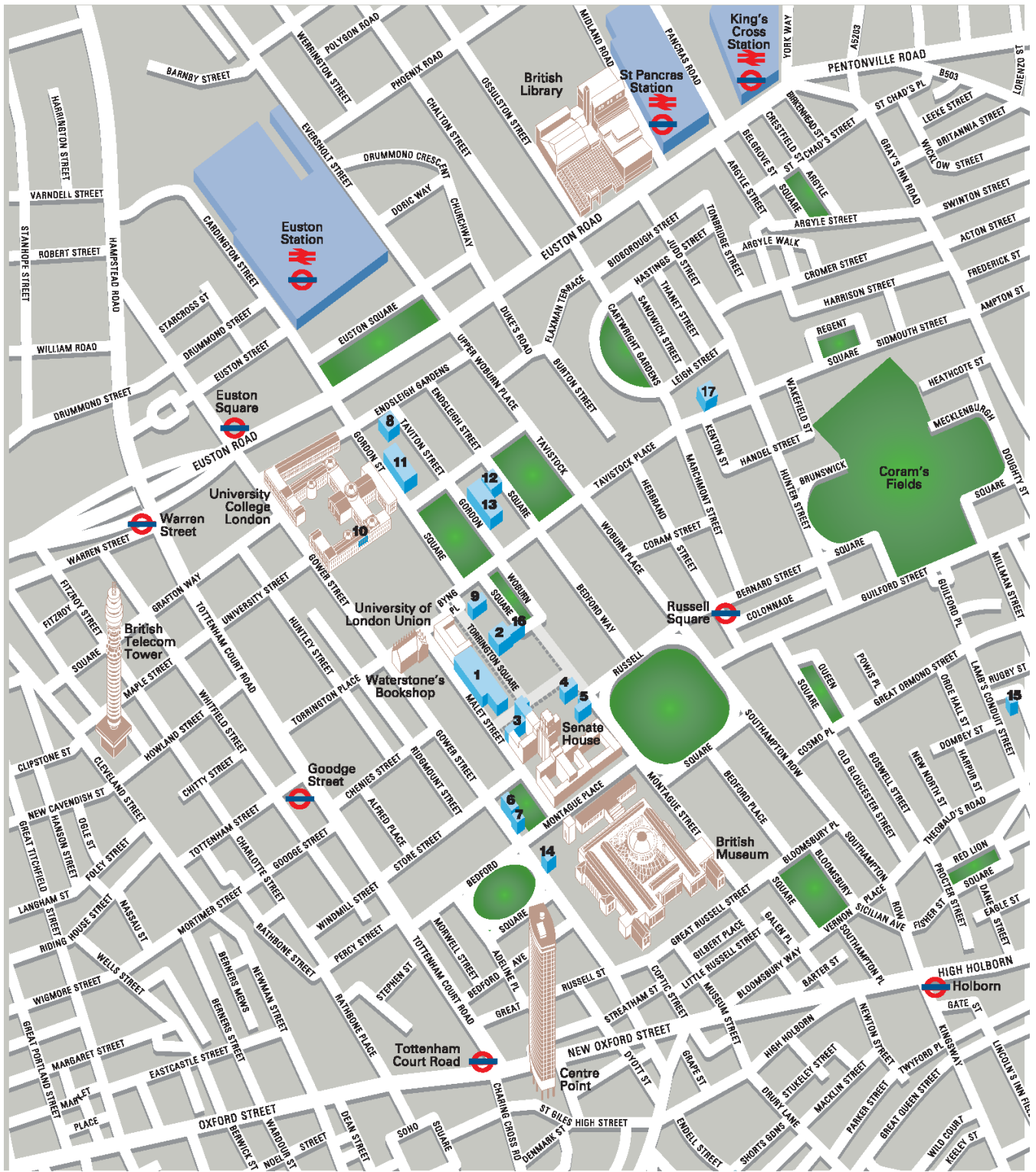
The NMR DG Christmas meeting has been organized in conjunction with the BRSG Christmas meeting, Wednesday 13th December (The day preceding the NMR DG Christmas meeting). Further details will be found on the Institute of Physics website using the link below:




<http://brsg2017.iopconfs.org/home>

Yours sincerely,

Prof Sharon Ashbrook – NMR DG Chairperson

Dr Stephen Byard - NMR DG Secretary



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|---|---|---|--|
|  Birkbeck buildings | 1 Birkbeck main building, Torrington Square | 8 Evening Nursery | 15 Knowledge Lab, 23-29 Emerald Street |
|  Stations (rail/tube) | 2 Clore Management Centre | 9 32 Torrington Square | 16 The Wolfson Institute for Brain Development and Function in the Henry Wellcome Building |
|  Stations (tube) | 3 Senate House (North Block) | 10 South Wing UCL (access via Gower Street) | 17 Egmont House |
|  Major landmarks and other buildings of interest | 4 25-26 Russell Square | 11 Gordon House | |
| | 5 30 Russell Square | 12 32 Tavistock Square | |
| | 6 10-16 Gower Street | 13 39-47 Gordon Square | |
| | 7 4 Gower Street | 14 7 Bedford Square | |



NMR Discussion Group Christmas 2017 Meeting

Thursday 14th December 2017

Institute of Structural and Molecular Biology, Torrington Square, London WC1E 7JL

10.00 – 10.25 Registration and refreshments

Morning session chair: tbd

10.25 – 10.30 Introduction and welcome

10.30 – 11.05 **Burkhard Luy, Karlsruhe Institut für Technologie (KIT)**

Fast and Broadband: New Developments in High Resolution NMR Spectroscopy

11.10 – 11.40 **Elisabetta Chiarparin, AstraZeneca, UK**

Free Ligand NMR Conformations: A New Perspective in Structure-Based Drug Design

11.45 – 12.05 **Vanessa Timmermann, University of Manchester**

Evaluating the Solution Structure of Uranium(IV) DOTA-type Complexes by ¹H NMR Spectroscopy

12.10 – 12.40 **Mathias Nilsson, University of Manchester**

Progress in Mixture Analysis of Small Molecules

12.45 – 13.55 Lunch and refreshments

13.55 – 14.10 NMR DG Business

Afternoon session chair: Sharon Ashbrook, University of St Andrews

14.10 – 14.40 **Tony Watts, University of Oxford**

Pushing the boundaries in solid state NMR of membrane-embedded proteins: DNP, fast MAS and proton detection

14.45 – 15.15 **Jonathan Iggo and Matthew Wallace, University of Liverpool**

Soups, Gels, Gradients and Images: NMR Methods for Studying NMR Invisible Soft Matter and other Things

15.20 – 15.45 **Michael Hope, University of Cambridge**

Investigating the Mechanism and Electronic Properties of Electrochemically Metallised VO₂ using Solid-state NMR

15.50 – 16.20 **Steven Brown, University of Warwick**

Characterising Structure of Organic Molecules in the Solid State: Combining Magic-Angle Spinning NMR, DFT Calculation and Powder X-ray Diffraction

16.25 – 16.30 **Closing remarks – Sharon Ashbrook**

16.30 - Refreshments and departure
