Chairman:
Professor Sharon Ashbrook DPhil FRSC
School of Chemistry
University of St Andrews
North Haugh
St Andrews
KY16 9ST
Phone +44 (0) 1334 463779
Fax +44 (0) 1334 463808
Email: sema@st-andrews.ac.uk

Secretary:
Dr Stephen Byard CChem FRSC
ARCINOVA
Taylor Drive
Alnwick
Northumberland NE66 2DH
Tel: +44 (0) 1665 608544
Email: Stephen.byard@arcinova.uk

Treasurer:
Dr John Parkinson CChem FRSC
Department of Pure & Applied Chemistry
University of Strathclyde
Thomas Graham Building
295 Cathedral Street,
Glasgow G1 1XL
Tel: +44 (0) 141 5482820
Fax: +44 (0) 141 5484822
Email: john.parkinson@strath.ac.uk

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

* The lecture theatre will be signposted on entering the main Birkbeck Building from Torrington Square (see building marked **1** on map below).

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 directions for the lecture theatre will be clearly indicated on entering the Institute of Structural and Molecular Biology in the main Birkbeck Building, from the Torrington Square entrance. See building marked 1 on map below.**

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

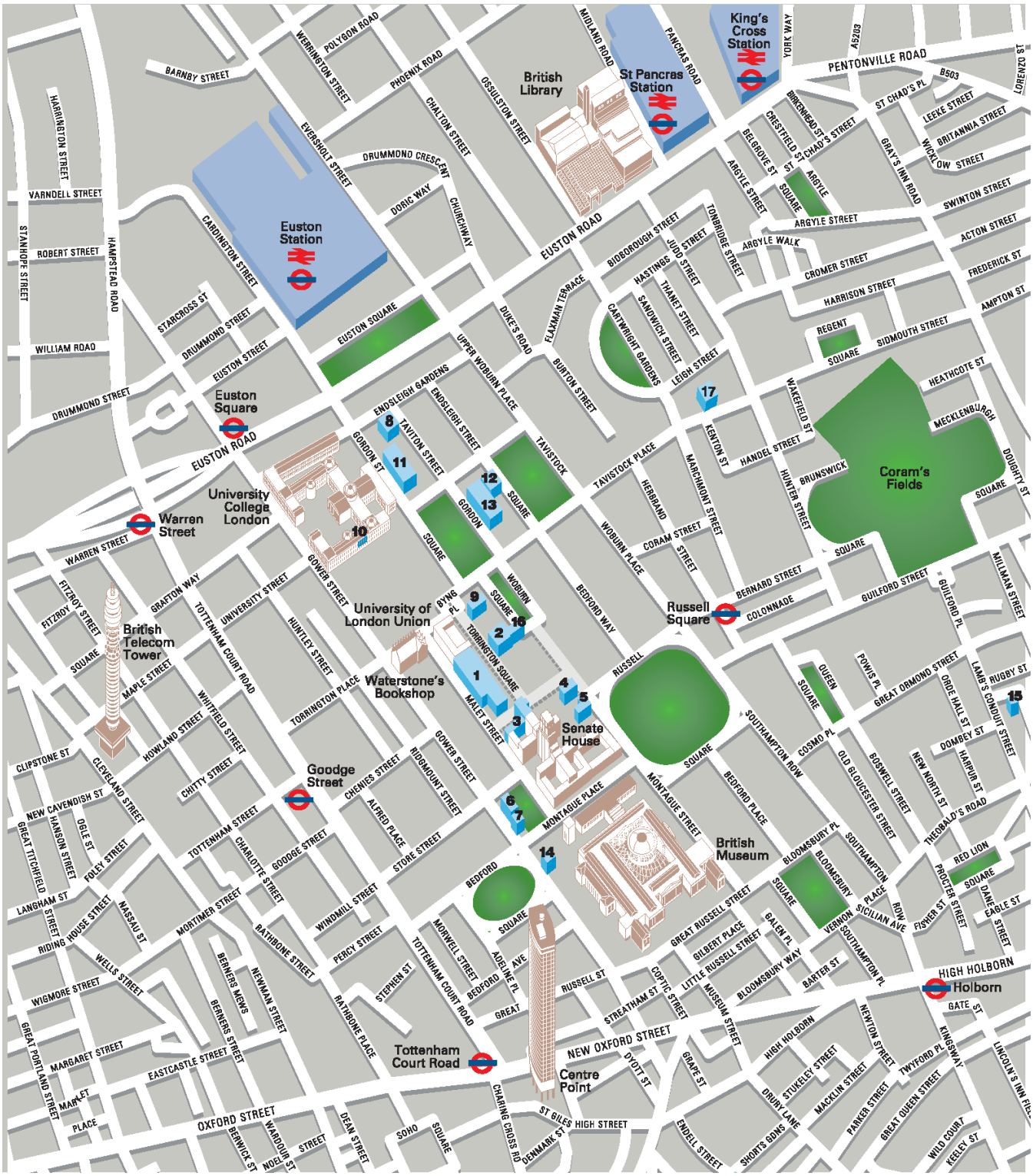
The NMR DG Christmas meeting has been organized in conjunction with the BRSG Christmas meeting, Wednesday 13th December (The day preceding the NMR DG Christmas meeting). Further details will be found on the Institute of Physics website using the link below:

http://brsg2017.iopconfs.org/home

Yours sincerely,

Prof Sharon Ashbrook – NMR DG Chairperson

Dr Stephen Byard - NMR DG Secretary


King's Cross Station
St Pancras Station
British Library
Euston Station
Euston Square
University College London
Warren Street
British Telecom Tower
University of London Union
Waterstone's Bookshop
Senate House
Goodge Street
Russell Square
Coram's Fields
British Museum
Tottenham Court Road
Centre Point
Holborn
HIGH HOLBORN
EUSTON ROAD
PENTONVILLE ROAD
OXFORD STREET
NEW OXFORD STREET
Birkbeck buildings
Stations (rail/tube)
Stations (tube)
Major landmarks and other buildings of interest
1 Birkbeck main building, Torrington Square
2 Clore Management Centre
3 Senate House (North Block)
4 25-26 Russell Square
5 30 Russell Square
6 10–16 Gower Street
7 4 Gower Street
8 Evening Nursery
9 32 Torrington Square
10 South Wing UCL (access via Gower Street)
11 Gordon House
12 32 Tavistock Square
13 39–47 Gordon Square
14 7 Bedford Square
15 Knowledge Lab, 23–29 Emerald Street
16 The Wolfson Institute for Brain Development and Function in the Henry Wellcome Building
17 Egmont House
N
0 100 200 300 Metres
0 0.1 0.2 Miles

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: Craig Butts, University of Bristol

10.25 – 10.30 Introduction and welcome

10.30 – 11.05 **Burkhard Luy*, Karlsruher 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 ^{1}H 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