



The Newsletter of the ISIS Molecular Spectroscopy User Group

Welcome!

It is time for the first issue of our Newsletter in 2017! Let us welcome back Samuel Jackson and say farewell to Raquel Álvarez Baños in the Mantid group.

A New Era for TOSCA

All sections of the TOSCA neutron guide have been successfully installed and, after initial commissioning, the beamline received its first users at the end of February 2017. The performance exceeds our expectations!



Mantid

A new Mantid release ([download](#)) includes an upgraded interface and a beta-version of AbINS (more info [here](#)) to calculate INS spectra from the CASTEP output.

The latest additions are also summarised [here](#).

IBEX on VESUVIO

After the IRIS experience, VESUVIO is the second instrument in TS-1 to upgrade the instrument-control software to [IBEX](#). A big thanks to the IBEX team and the [ISIS Computing Group](#) for their support.

Molecular Spectroscopy Science Meeting 2016

A great success! A fully-booked event at the Cosener's House in Abingdon (picture) with around 80 participants from all over the world. The proceedings are now published [here](#).

MDANSE 2016

We thank all the participants to the workshop on Molecular and lattice Dynamics to Analyse Neutron Scattering Experiments, jointly organised with ILL. The proceedings are now published [here](#). All data files used in the tutorials during the workshop can be found [here](#).

Sample Preparation Laboratories

New equipment is available in the [ISIS Support Laboratories](#), including a mass spec. system for the DSC/TGA instrument in the [hydrogen lab](#), a new VSM SQUID, and a Bruker benchtop diffractometer in the [materials lab](#). The second SMARTLAB (with the 2D detector) is now commissioned. Also, users should book bake-out furnaces as far in advance as possible through the local contact and [James Taylor](#).

IRIS Sample Changer

IRIS is now equipped with a new sample changer, especially useful for Xpress experiments. All our instruments accept Xpress proposals!

Please be reminded that the representatives of our group, [C.G. Salzmänn](#) and [R. Senesj](#), are always open for feedback.

Please inform us of your publications arising from ISIS-related work. Remember to include ISIS staff as co-authors on publications when deemed appropriate.

Next Proposal Round
Deadline: April 16th
Submit your proposals here

Science Highlights

- [Nuclear dynamics and phase polymorphism in solid formic acid](#)
- [Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework](#)
- [Unexpected cation dynamics in the low-temperature phase of methylammonium lead iodide – the need for improved models](#)
- [Unusual flexibility of mesophase pitch-derived carbon materials: An approach to the synthesis of graphene](#)
- [Intracellular water – an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons](#)
- [An assessment of hydrocarbon species in the methanol-to-hydrocarbon reaction over a ZSM-5 catalyst](#)
- [Structural and dynamic studies of substrate binding in porous metal-organic frameworks](#)
- [Proton Conduction in a Phosphonate-Based MOF Mediated by Intrinsic “Free Diffusion inside a Sphere”](#)
- [Nanostructuring of ionic liquids : impact on the cation mobility. A multi-scale study](#)



Forthcoming Events

- [Faraday Conference, 11-13 April 2017, Warwick](#)
- [ICANS XXII, 27-31 March 2017, Oxford, with four oral contributions from our group!](#)
- [Seeking Synergy between Dynamics and Statistics for non-Equilibrium Quantum Processes, 6-9 June 2017, Paris](#)
- [UK Neutron and Muon Science and User Meeting, 27 – 29 June 2017, Warwick; the Student day is on the first day!](#)
- [ICNS, 9-13 July 2017, Daejeon](#)
- [Gordon Conference in Neutron Scattering, 6-11 August 2017 Hong Kong](#)
- [Oxford School on Neutron Scattering, 3-15 Sept 2017](#)