



# Good Vibrations

The Newsletter of the ISIS Molecular Spectroscopy User Group (MSUG)

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## News

### Welcome

Welcome to the final newsletter of 2014!

In this issue, we welcome two new faces who have recently joined the group: [Dr. Pedro Duarte Vaz](#), instrument scientist on TOSCA; and Daniel Nixon from the University of Newcastle-upon-Tyne, sandwich student to work on Mantid Data Analysis Software.

Please join us in a warm welcome to both of them.

### ISIS Molecular Spectroscopy Science Meeting 2015

29<sup>th</sup> & 30<sup>th</sup> January  
The Cosener's House, Abingdon

*We invite contributions in terms of oral or poster presentations from researchers willing to present their work in the supportive atmosphere of our user group.*

**Registration deadline is 30<sup>th</sup> November**

**Please register [here](#).**

We look forward to seeing you there!

### Data Analysis and Mantid

Current developments of data analysis on Mantid have been summarised in two reports, one [across all instruments](#) and another on [VESUVIO](#). A big thanks to Samuel Jackson, for all his work during his placement with us last year.

### Inelastic Neutron-Scattering Database

The [INS database](#) has now increased to near 700 entries thanks to the efforts of a work experience student, Jack Parker. Have a look!

### TOSCA Guide Project: Latest News

Tenders have been submitted for the design, manufacture, and supply of the shutter guide insert and surrounding shielding. A delivery schedule for the remainder of the guide is in preparation.

### Simultaneous Neutron-Raman Spectroscopy Facility Upgrade

The Raman spectrometer used for simultaneous neutron/Raman studies has been upgraded. By replacing the laser rejection filters, transitions as low as 45 cm<sup>-1</sup> are now readily observable. The addition of a second, software selectable, grating means that 3 cm<sup>-1</sup> resolution spectra over the range 45 – 1800 cm<sup>-1</sup> can be obtained with high signal-to-noise ratio. The ability to measure Raman and neutron data simultaneously from

the same sample is a capability that is unique to ISIS. To date, it has been used on [IRIS](#), [OSIRIS](#), [TOSCA](#), [VESUVIO](#), as well as [MAPS](#) and [SANDALS](#). It can be used on any instrument accepting a 100-mm diameter centrestick.



### An Introduction to Neutron Techniques in Catalysis

A joint ISIS Catalysis Hub at RCaH workshop to be held on 3<sup>rd</sup> and 4<sup>th</sup> November 2014 at the Research Complex at RAL.

There will be a mixture of talks describing capabilities in neutrons and what can be learned from them, together with examples where neutrons have played a key role in catalysis studies. Further information and enrolment is available from the [workshop website](#).

*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 REMINDER

**Deadline October 16th.**  
Submit your proposal [here](#)

## Science Highlights

- [INS Study of the Molecular Properties of Pure Hydrogen Peroxide ...](#)
- [Investigation of a Nano-composite of Nanoparticles with Polyethylene Oxide Linear Chains.](#)
- [Magnetic Spectra in the Tridimensional-icosahedron Fe<sub>9</sub> Nanocluster by INS](#)
- [Low Energy Structural Dynamics and Constrained Libration in Li\(NH<sub>3</sub>\)<sub>4</sub>](#)
- [Modelling the Luminescence of Extended Solids](#)

## Forthcoming Conferences

- [International Symposium on Chemical Theory for Complex Systems, Oct 30-31, Sweden.](#)
- [9th Int. Conference on Comput. Phys., Jan 7-11, Singapore.](#)
- [Temporally and Spatially Resolved Molecular Science, Faraday Discussions 177, Jan 12-14, India.](#)
- [Frontiers of First-principles Simulations, Feb 1-5, Germany.](#)
- [MRS Spring Meeting, April 6-10, USA.](#)