Experimental report

21/10/2016

Proposal:	**1-20-39**	**Council:**	4/2015
Title:	Wavelength dependence of the incoherent contribution to the total scattering in hydrogenous materials (containing 1H)		
Research area:	Chemistry		

This proposal is a new proposal

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Samples: D2O
H2O

Instrument	Requested days	Allocated days	From	To
D3	14	14	03/11/2015	19/11/2015

Abstract:

As a result of our previous experiments on D3, it is now demonstrated that the incoherent contribution to the total scattering from liquid water (as a prototype hydrogenous material) can be determined precisely at various H2O/D2O compositions by polarised neutron diffraction. A major area of application of this information would be the correction of non-polarised neutron diffraction data for hydrogenous samples. In order to confirm that this can be done for any neutron diffractometer (with an arbitrarily varying wavelength) by using D3 data, it must first be established if the incoherent contribution is strictly wavelength-independent (i.e., strictly Q-dependent). For this purpose, we propose polarised neutron diffraction experiments on liquid water samples containing 100, 64 and 0 % H2O at two additional wavelengths, 0.4 and 0.8 A, using the D3 instrument at the ILL.

Wavelength dependence of the incoherent contribution to the total scattering in hydrogenous materials (containing ^1H)

Introduction

Materials that contain hydrogen are undoubtedly among the most important substances in our world: it's sufficient to remember that life on Earth is based on water. For this reason, determining the structure of materials containing hydrogen is of utmost importance in various scientific fields, from basic chemistry and physics, through geochemistry, to biochemistry and soft-matter research.

X-ray diffraction is not a sufficiently sensitive probe for hydrogen in most of the cases (including the case of H_2O), so that neutron diffraction with H/D substitution seems to be the only feasible way of deriving more detailed information on the microscopic structure of hydrogenous (i.e., ones with ^1H) systems. The main difficulty with structure determination of ^1H-containing ('protonated') liquids is the huge incoherent inelastic scattering that arises due to the exceptionally high level of spin-incoherency of the proton (^1H). As a result, more than 90 % of the measured signal (using non-polarized neutron beams) from pure H_2O is useless ('background') from the structural point of view.

Spin-incoherence, however, can be bypassed if the neutron beam is polarized. We have recently shown that using the D3 instrument, it is possible to measure accurate (coherent) static structure factors of water samples, containing a varying proportion of ^1H, over a wide Q-range [1].

To determine the coherent and incoherent contributions to the total scattering of ^1H containing liquid water samples, we wished to measure the structure factor of H_2O-D_2O mixtures (protonated compound content: 0, 64 and 100 %), by separating the coherent and spin-incoherent parts of the scattering, using the D3 instrument at ILL. Measuring this series at two new wavelengths (previous experiments have all been conducted by using a neutron wavelength of 0.5 Å), 0.825 and 0.4 Å, would make it possible to make sure that the incoherent contribution is strictly only dependent on the magnitude of the momentum transfer, Q. This knowledge would facilitate the handling of spin-incoherent backgrounds of any hydrogenous materials, without actually performing polarisation analyses for every single sample. This would be valuable as polarisation analysis is very time consuming and can only be performed on D3.

The experiment

We have measured spin-flip and non-spin-flip intensities from pure D_2O, pure H_2O and "zero" water (64 % H_2O), in order to separate the coherent and spin-incoherent parts of the scattering, using the D3 instrument at ILL. Two wavelengths have been used: 0.4 and 0.825 Å. The separated coherent (for pure H_2O) and incoherent (for pure D_2O) contributions are shown in Figures 1 and 2, respectively, for the two wavelengths.

It can be established that results for the two (rather different) wavelengths coincide for the above examples. However, more detailed analyses are necessary for a full quantitative comparison.

References

[1] ILL Experimental Report 6-02-519 (by L. Temleitner); L. Temleitner et al., Phys. Rev. B 91, 014201 (2015)

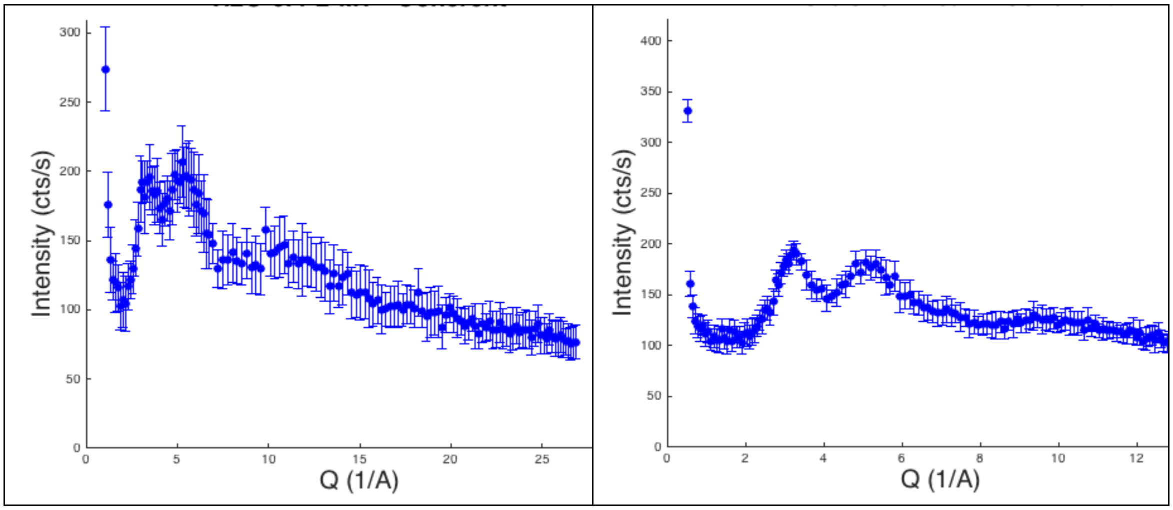

Figure 1: Measured coherent intensities for pure H_2O using neutrons of 0.4 (left panel) and 0.825 (right panel) $Å^{-1}$. The two curves coincide (note the different scales).

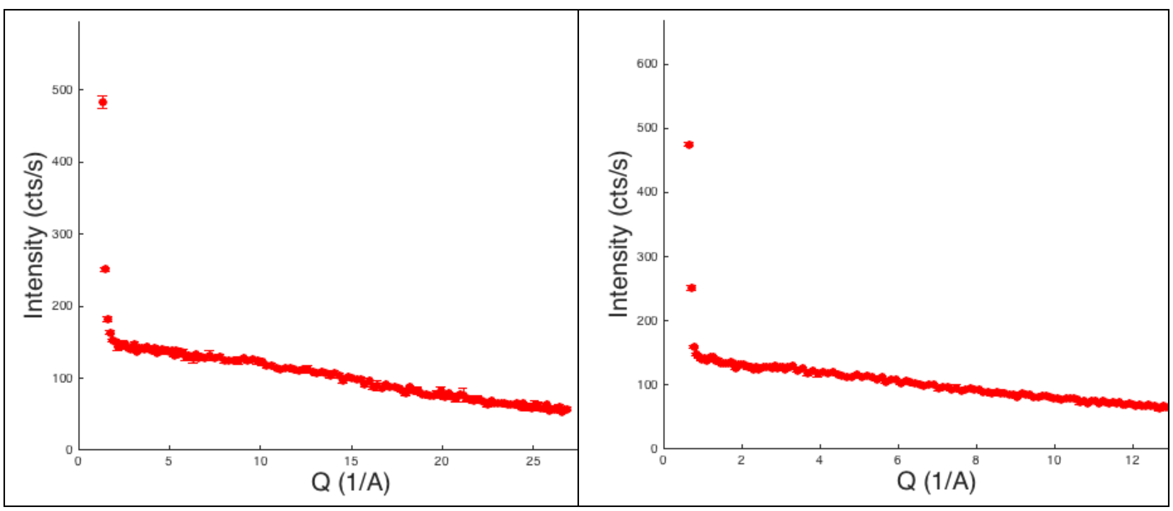

Figure 2: Measured incoherent intensities for pure D_2O using neutrons of 0.4 (left panel) and 0.825 (right panel) $Å^{-1}$. The two curves coincide (note the slightly different scales).