Experimental report

08/03/2019

Proposal: **6-02-584**

Council: 4/2017

Title: Structural properties of aqueous solutions of D-fructose

Research area: Chemistry

This proposal is a resubmission of 6-02-571

Main proposer: **Laszlo PUSZTAI**

Experimental team: Gabriel Julio CUELLO
Szilvia POTHOCZKI
Laszlo PUSZTAI
Laszlo TEMLEITNER

Local contacts: Anne STUNAULT
Andrew WILDES

Samples: 1 mol % D-(-)-Fructose (C6H12O6)/H2O
3 mol % D-(-)-Fructose (C6H12O6)/H2O
7 mol % D-(-)-Fructose (C6H12O6)/H2O
1 mol % D-(-)-Fructose (C6H12O6)/D2O
3 mol % D-(-)-Fructose (C6H12O6)/D2O
7 mol % D-(-)-Fructose (C6H12O6)/D2O

Instrument	Requested days	Allocated days	From	To
D3	14	14	19/03/2018	02/04/2018
D7	2	2	13/04/2018	15/04/2018

Abstract:

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 H2O, and more than cca. 70 % from pure C6H12O6 (fructose) 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 proportions of 1H, over a wide Q-range. The incoherent 'background' could also be determined precisely. Here we propose an analogue experiment for investigating the structure of an aqueous solution, as a function of concentration, of vital importance: that of D-fructose. In order to complete the coverage of the scattering vector range, we wish to complement the D3 experiment with measurements using cold polarized neutrons of the D7 instrument.

A new approach to the structure of ^{1}H-containing materials using polarised neutrons: aqueous solutions of fructose and glucose

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 ^{1}H) systems. The main difficulty with structure determination of ^{1}H-containing ('protonated') liquids is the huge incoherent inelastic scattering that arises due to the exceptionally high level of spin-incoherency of the proton (^{1}H). 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 ^{1}H, over a wide Q-range [1].

Here we considered aqueous solutions of prominent members of the family of sugars: fructose and glucose.

The experiment

For being able to determine the coherent and incoherent structure factor of ^{1}H containing liquid samples in which the chemical environment of the protons varies, we have measured structure factor of 1, 3, 7 m% fructose in aqueous solution with pure D_2O and with pure H_2O, as well as 1, 3, 5 m% glucose in aqueous solution with pure D_2O and with pure H_2O, by separating the coherent and spin-incoherent parts of the scattering, using the D3 and D7 instruments at ILL.

The separated coherent intensities (which are important from the aspect of the atomic level structure) are shown in Figures 1.

The effect of increasing sugar concentration is apparent on the functions corresponding to heavy water solutions, whereas it is hardly visible for light water solutions. This statement is valid particularly for solutions of glucose in light water; the reason for this difference is, at the time of writing, now known.

The next step will be to provide structural models via Molecular Dynamics simulations; this work is in progress. From these (molecular dynamics computer generated) models the coherent intensities can be calculated. We aim at comparing measured and simulated coherent total scattering intensities for each solution.

References

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

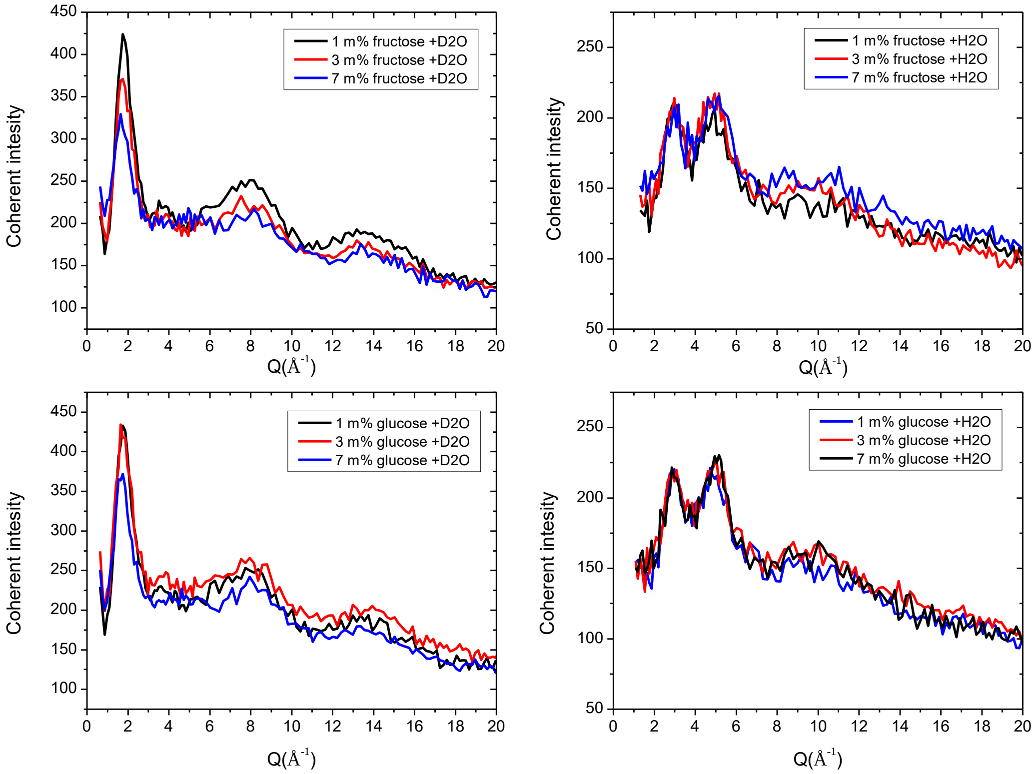

Figure 1: Measured coherent intensities for aqueous solutions of fructose and glucose, in pure heavy (left panels) and light (right panels) water.