

Experimental report

19/02/2025

Proposal: 6-02-638

Council: 4/2023

Title: Exploring molecular segregation in methanol/water mixtures using polarized neutron diffraction

Research area: Physics

This proposal is a new proposal

Main proposer: Miguel Angel GONZALEZ

Experimental team: Ferdinando FORMISANO
Simone DE PANFILIS

Local contacts: Anne STUNAUULT

Samples: (CD₃OD)₇₀(D₂O)₃₀
(CH₃OH)₇₀(H₂O)₃₀
(CD₃OH)₇₀(H₂O)₃₀
(CH₃OD)₇₀(D₂O)₃₀
C₆H₈O₃

Instrument	Requested days	Allocated days	From	To
D3	5	8	15/11/2023	24/11/2023

Abstract:

The possible existence of molecular segregation in mixtures of methanol and water remains an open question. While the EPSR analysis of a complete series of neutron diffraction data using isotopic substitution led the authors to suggest an incomplete mixing of both species at the molecular level, recent simulation results complemented with neutron and x-ray diffraction experiments do not support this view. Tuning the model parameters in the potential employed in the simulation it is possible to favour the demixing of methanol and water. Using this approach we have generated two different liquid models for the methanol/water solutions (one perfectly mixed and another significantly demixed). Our results indicate that the differences between both models could be resolved experimentally by measuring the static structure factor of the H/D mixtures, i.e. $x(\text{CD}_3\text{OH}) \cdot (1-x)(\text{H}_2\text{O})$ and $x(\text{CH}_3\text{OD}) \cdot (1-x)(\text{D}_2\text{O})$. In order to explore this hypothesis, we ask for 5 days of beamtime in order to study the room-temperature structure of a methanol-water mixture with $x=0.7$.

ILL EXPERIMENTAL REPORT

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Instrument: D3

At the time of the experiment we were informed by the instrument responsible that the very same study on water/methanol mixtures was already completed few months earlier by Pusztai et al.

In agreement with the instrument scientist and local contact, then, we decided to use the beamtime to study pure dihydrolevoglucosenone (commercially known as Cyrene) and its water mixtures, attaching the allocated days to those also allocated on this same project for proposal 6-02-647. The preliminary results from this study are published on the experimental report of proposal 6-02-647.