


実験報告書様式（一般利用課題・成果公開利用）

（本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。  
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 <b>MLF Experimental Report</b>	提出日 Date of Report 27 June 2013
課題番号 Project No.2012B0086  実験課題名 Title of experiment Short and medium range order in pure alcohols  実験責任者名 Name of principal investigator PUSZTAI, László  所属 Affiliation Wigner Research Centre for Physics, Hungarian Academy of Sciences	装置責任者 Name of responsible person Prof. OTOMO, Toshiya  装置名 Name of Instrument/ (BL No.) BL-21 (NOVA)  実施日 Date of Experiment 24-26. March 2013

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表

添付のこと）

Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Deuterated methanol-heavy water mixtures,  $(CD_3OD)_x : (D_2O)_{100-x}$ ; x: 20,40,60,70,80,100

Deuterated ethanol-heavy water mixtures,  $(C_2D_5OD)_x : (D_2O)_{100-x}$ ; x: 20,40,60,80,100

Deuterated 2-propanol-heavy water mixtures,  $(C_3D_7OD)_x : (D_2O)_{100-x}$ ; x: 20,40,60,80,100

Deuterated 1-butanol-heavy water mixtures,  $(C_4D_9OD)_x : (D_2O)_{100-x}$ ; x: 2,60,80,100

Deuterated t-butanol-heavy water mixtures,  $(C_4D_9OD)_x : (D_2O)_{100-x}$ ; x: 20,50,80,100

Deuterated 1-hexanol  $C_6D_{13}OH$

Deuterated 1-octanol-heavy water mixtures,  $(C_8D_{17}OD)_x : (D_2O)_{100-x}$ ; x: 76,100

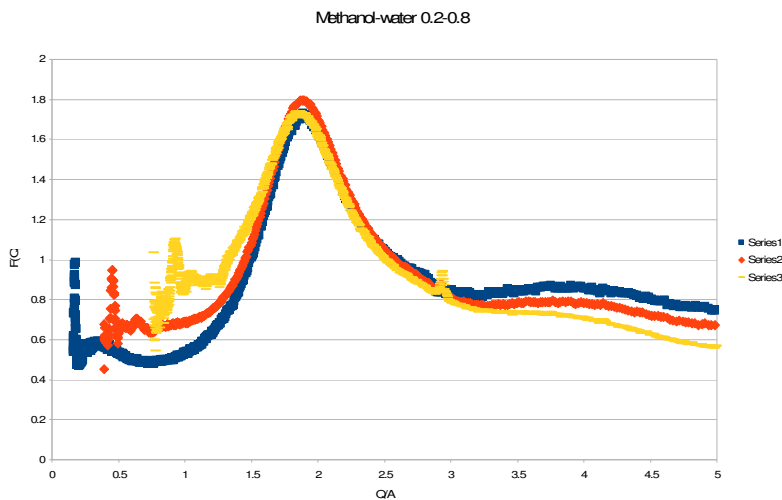
Deuterated 1-decanol  $C_{10}D_{21}OH$

## 2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。)

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

The liquid samples mentioned above were contained in 3 mm diameter vanadium sample holders and were taken to the NOVA (BL-21) total scattering instrument at J-PARC. The total scattering structure factors of the liquid mixtures have been determined over a very wide Q-range (up to at least 60 inverse angstroms). The main objective of this systematic study on alcohol-water mixtures was to establish if there is any visible sign of 'micro heterogeneities' on the total scattering structure factor: that is, definite small angle scattering signals and/or pre-peaks have been searched for.

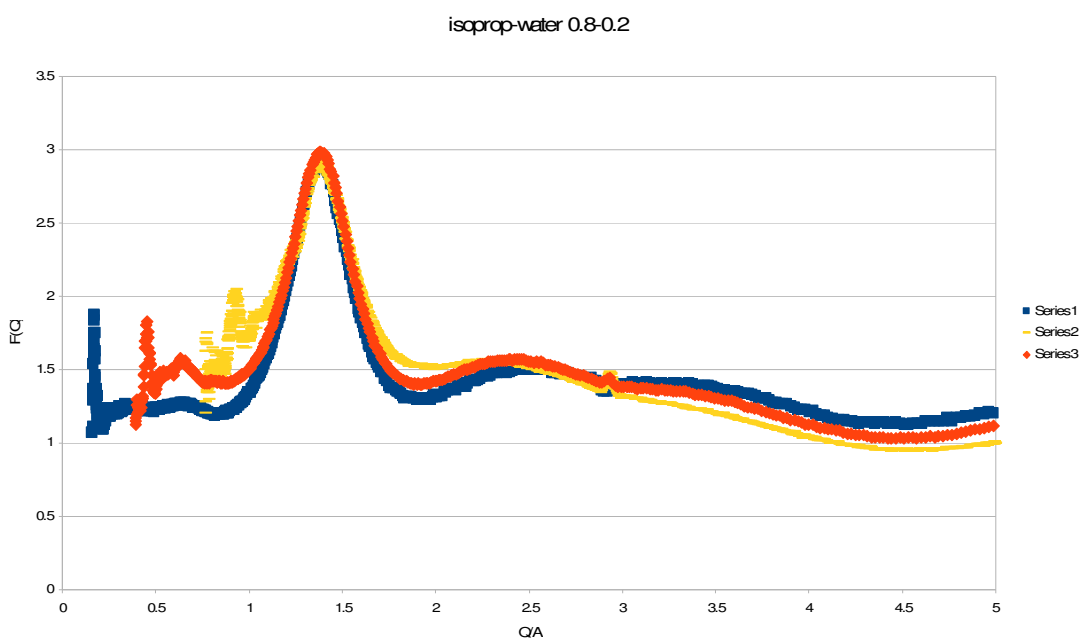
Each sample received 2 hours of beamtime on average, which proved to be providing reasonable statistical accuracy up to at least 20 inverse angstroms. Below some examples of the corrected total scattering signals are provided.



The picture above shows the total scattering structure factor of a water-rich methanol-water mixture, as measured by the 20 (blue), 45 (red) and 90 (yellow) degree detector banks. The emphasis here is on the low Q part of the curves. Although there is intensity preceding the main peak on each curve, since the position of these small maxima changes with changing the detector bank, the intensity at low Q should be considered as noise in this case.

Next, we consider an alcohol-rich isopropanol-water mixture (see below). Here, signals from the 20 and 45 degree detector banks both display a small hump at around 0.7 inverse angstroms, so that the small maximum should be considered as real. We note that out of the 4 isopropanol-water mixture, only this one exhibits any visible sign of a possible larger-than-atomic scale structural feature; the exact origin of this feature will be searched for in extensive computer modeling studies.

## 2. 実験方法及び結果 (つづき) Experimental method and results (continued)



In summary we have determined the total scattering structure factors of 20+ alcohol-water mixtures in the liquid state. Only very few of the datasets show clear signs of larger-scale structural features. The data measured on NOVA (at J-PARC) will be complemented by similar information from X-ray diffraction. It is also planned that X-ray and neutron weighted structure factors would be used as input for Reverse Monte Carlo structural modeling [1] studies.

[1] McGreevy RL, Pusztai L, Mol. Simul. 1, 359 (1988)