J-PARC　**MLF Experimental Report**	提出日 Date of Report 25th Mar. 2013
課題番号 Project No 　2012B0026 実験課題名 Title of experiment 　Mixing State of Imidazolium-based Ionic Liquids in Benzene 　Derivative Solutions on Meso- and Microscopic Scales 実験責任者名 Name of principal investigator 　Toshiyuki Takamuku 所属 Affiliation 　Saga University	装置責任者 Name of responsible person 　Prof. Toshiya Otomo 装置名 Name of Instrument/（BL No.） 　NOVA (BL21) 実施日 Date of Experiment 　2013. 1.25-2013. 1.28

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.
Ionic Liquid-DMSO, C2mimTFSA-DMSO-d6 at x_{DMSO} = 0.8, 0.9, 0.99, liquid state Ionic Liquid-DMSO, C12mimTFSA-DMSO-d6 at x_{DMSO} = 0.8, 0.9, 0.99, liquid state Ionic Liquid-Toluene, C12mimTFSA-Toluene-d8 at $x_{toluene}$ = 0.8, 0.9, 0.95, 0.97, 0.98, 0.99, 0.995, liquid state

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.

　To clarify the mixing states of imidazolium-based ionic liquid with deuterated DMSO-d6 ($(CD_3)_2SO$) and toluene-d8 ($C_6D_5CD_3$), neutron diffraction measurements were made on the sample solutions at the ambient temperature and pressure using the NOVA spectrometer. The ionic liquids included C2mimTFSA and C12mimTFSA with the ethyl and dodecyl chains, respectively. The machine time was given for 3 days.

　The sample solutions were kept in a cylindrical cell made of Ni-Ti null alloy with an indium-wire packing. The diameter of the cell was 6 mmϕ.

　The sample solutions were exposed to neutron beams for 2−6 h. The irradiation times were determined depending on the hydrogen-atom contents. The scattering intensities of ^0H_2O were also measured for the correction of incoherent scattering intensities of the sample solutions. Our original plan of the NOVA experiments was completed without beam dumps. However, the data at the small-angle bank for vanadium and C2mimTFSA-DMSO-d6 at x_{DMSO} = 0.3 and 0.8, and C12mimTFSA-DMSO-d6 at x_{DMSO} = 0.8 (4 samples) could not be saved because there are not enough storage space of the hard-disk drive.

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

The $S(q)$s were obtained from the scattering intensities measured for the sample solutions using the intensities of background, empty cell, and vanadium and the number densities tentatively calculated from the sample compositions. In the $S(q)$s of all the solutions, oscillations were well observed. Moreover, small-angle scattering intensities were significantly observed in the $S(q)$ of the deuterated toluene systems, showing the heterogeneous mixing of the ionic liquids and toluene. This agrees with the previous results of the SANS-U experiments. In contrast, significant small-angle scattering intensities of the deuterated DMSO systems were not observed. This is consistent with our expectation on the homogeneous mixing of the ionic liquids and DMSO.

To elucidate the structure of the solutions, radial distribution functions $g(r)$s will be calculated by Fourier transform on the $S(q)$s obtained from the scattering intensities corrected for incoherent ones. We would like to ask the NOVA group to obtain the final $S(q)$s according to the number densities of the sample solutions experimentally determined.