



実験報告書様式(一般利用課題・成果公開利用)

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 Experimental Report 	承認日 Date of Approval 2016/06/20 承認者 Approver Jun-ichi SUZUKI 提出日 Date of Report 2016/07/11
課題番号 Project No. 2015A0038 実験課題名 Title of experiment Effects of Cation- π Stacking between Imidazolium and Benzene Rings on Heterogeneous State of Imidazolium-based Ionic Liquids-Benzene Derivative Mixtures 実験責任者名 Name of principal investigator Toshiyuki Takamuku 所属 Affiliation Saga University	装置責任者 Name of Instrument scientist Jun-ichi Suzuki 装置名 Name of Instrument/(BL No.) TAIKAN (BL15) 実施日 Date of Experiment 2016.June, 13 10:00 – June 15 9:00

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.

<p>1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.</p> <p>The present samples were binary mixtures of imidazolium-based ionic liquids $C_n\text{mimTFSA}$ (n: alkyl chain length) and deuterated dimethyl sulfoxide ($\text{DMSO}-d_6$) with various DMSO mole fractions x_{DMSO}.</p> <ol style="list-style-type: none"> 1. $C_2\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$ 2. $C_4\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$ 3. $C_6\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$ 4. $C_8\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$ 5. $C_{10}\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$ 6. $C_{12}\text{mimTFSA}-\text{DMSO}-d_6$ $x_{\text{DMSO}} = 0.5, 0.7, 0.8, 0.9$

<p>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。)</p> <p>Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.</p> <p>The small-angle neutron scattering (SANS) spectra for the 12 samples of $C_n\text{mimTFSA}-\text{DMSO}-d_6$ were measured at a room temperature using TAIKAN spectrometer to elucidate the microinhomogeneity of the ionic liquid-DMSO mixtures. However, all of the samples did not give significant SANS intensities. The present results suggested that $C_n\text{mimTFSA}$ and DMSO are homogeneously mixed with each other even on the molecular scale. This seems to be uninteresting information in the field of SANS experiments. Nevertheless, we could confirm the previous results from the NMR and IR measurements by the present SANS results; i.e., DMSO molecules with the high electron donicity are hydrogen-bonded with the three imidazolium ring hydrogen atoms at the positions of 2, 4, and 5 as shown in Fig. 1. The hydrogen bonding of the imidazolium ring hydrogen atoms with DMSO results in the homogeneous mixing of both liquids.</p> <p>As shown in Fig. 2, in the middle Q-range, a peak at $\sim 0.2 \text{ \AA}^{-1}$ appears in the SANS spectra for $C_n\text{mimTFSA}-\text{DMSO}-d_6$ mixtures with the alkyl chain length of more than 10. This peak may give us the.</p>

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

information on the liquid structure of ionic liquids and the change in the structure of the ionic liquids with increasing DMSO content. We will analyze the peak by some function to clarify the structure of the ionic liquids.

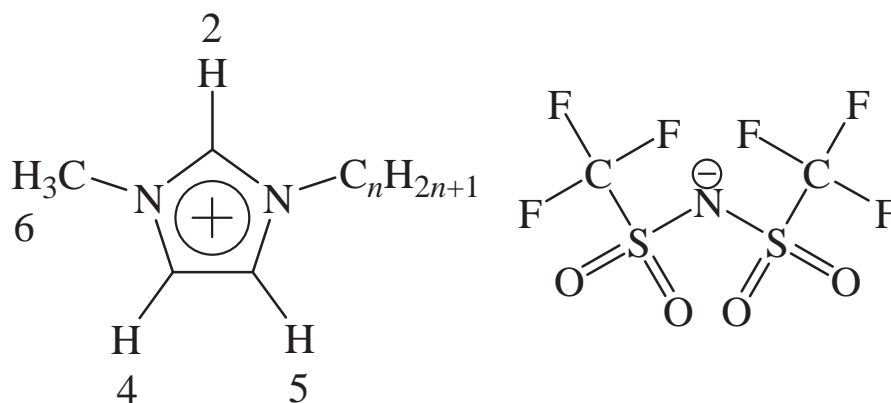


Fig. 1 Structure of imidazolium-based ionic liquid $C_n\text{mimTfSA}$.

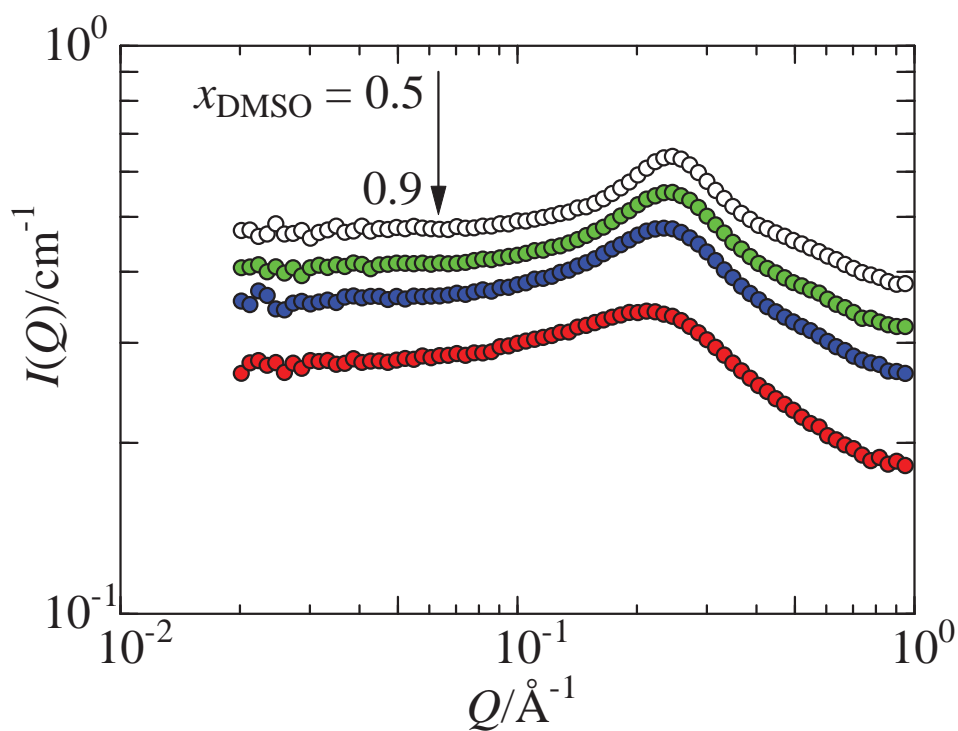


Fig. 2 SANS spectra for $C_{12}\text{mimTfSA-DMSO-d}_6$ mixtures as a function of $x_{\text{DMSO}} = 0.5, 0.7, 0.8,$ and 0.9 .