実験報告書様式（一般利用課題・成果公開利用）

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CROSS TOKAI **Experimental Report** J-PARC	承認日 Date of Approval 2017/5/3 承認者 Approver Jun-ichi Suzuki 提出日 Date of Report 2017/1/27
課題番号 Project No. 2016A0008 実験課題名 Title of experiment Relation between the Transition Metal Complex Formation and Aggregation of DMSO Molecules in Imidazolium-based Ionic Liquids 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 2017.Jan.21 10:00-Jan.23 10:00

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.

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

In the present experiments SANS measurements at 25 °C were conducted on four systems; A: imidazolium-based ionic liquid-alcohol mixtures including methanol and ethanol, B: hen egg white lysozyme (Lys) in 2-propanol-water and 1,1,1,3,3,3-hexafluoroisopropanol (HFIP)-water solutions, and C: 2,6-lutidine-D_2O-$NaBPh_4$ and water-$CDCl_3$-cetyltrimethylammonium bromide (CTAB).

System A:

1. C_2mimTFSA-Methanol-d_4 x_{MeOH} = 0.8, 0.9, 0.95, 0.97, 0.99
2. C_2mimTFSA-Ethanol-d_6 x_{EtOH} = 0.8, 0.9, 0.95, 0.97, 0.99
3. C_{12}mimTFSA-Ethanol-d_6 x_{EtOH} = 0.9, 0.95, 0.97, 0.99, 0.995

System B:

1. Lys/D_2O-2-Propanol-d_8 $x_{Alcohol}$ = 0, 0.1, 0.2, 0.25, 0.35
2. Lys/D_2O-HFIP $x_{Alcohol}$ = 0.05, 0.2, 0.6, 1
3. Lys/D_2O-H_2O-2-Propanol-d_8 $x_{Alcohol}$ = 0.1, 0.15, 0.2, 0.25
4. Lys/D_2O-H_2O -HFIP $x_{Alcohol}$ = 0.05, 0.2, 0.6

System C:

1. 2,6-Lutidine-D_2O-$NaBPh_4$ in the $NaBPh_4$ concentration range, 30-400 mmol dm^{-3}
2. Water-$CDCl_3$-CTAB at various water contents

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.

For system A reasonable SANS spectra could be measured for all of the samples as shown in the representative spectra (Fig, 1). The SANS spectra suggested that the inhomogeneity of the C_2mimTFSA–ethanol–d_6 solutions is higher than that of the C_2mimTFSA–methanol–d_4 solutions. Additionally, the inhomogeneous mixing of the C_{12}mimTFSA–ethanol–d_6 solutions is less remarkable compared to that of the C_2mimTFSA–ethanol–d_4 solutions. To quantitatively evaluate the inhomogeneity of the solution, the Ornstein–Zernike fits will be made on the spectra for the solutions.

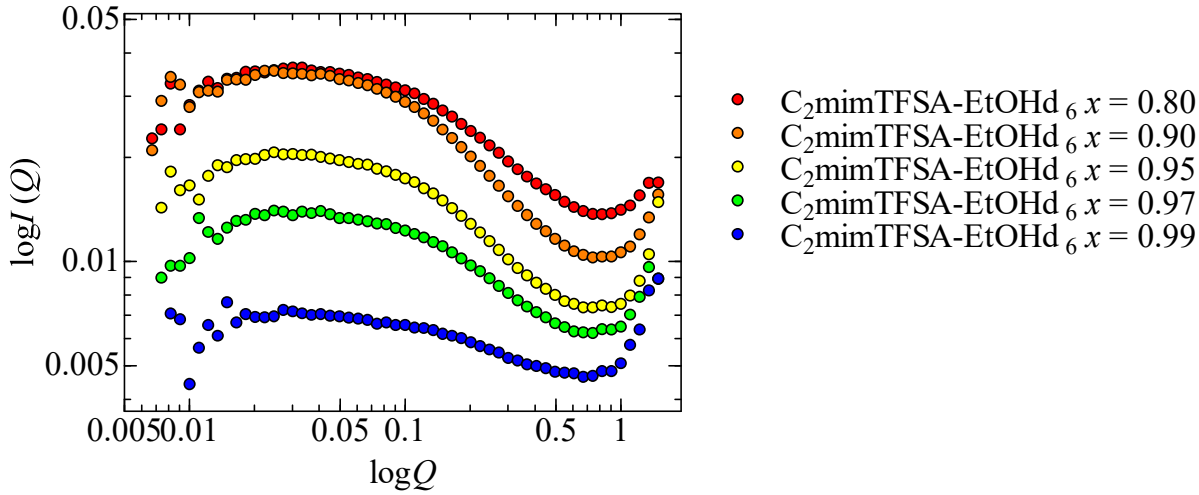

Fig. 1 SANS spectra of C_2mimTFSA–ethanol–d_6 solutions at various ethanol mole fractions.

For system B, SANS spectra for lysozyme in 2–propanol–water solutions showed that the three dimensional structure of lysozyme does not significantly change against the increase in the 2–propanol content (Fig. 2). In contrast, the structure of lysozyme in the HFIP–water solutions drastically changes with increasing HFIP content (Fig. 3). The present SANS results are consistent with the results of circular dichroism spectra. The structure of lysozyme in both alcohol–water solutions will be determined by fit on the SANS spectra using suitable model.

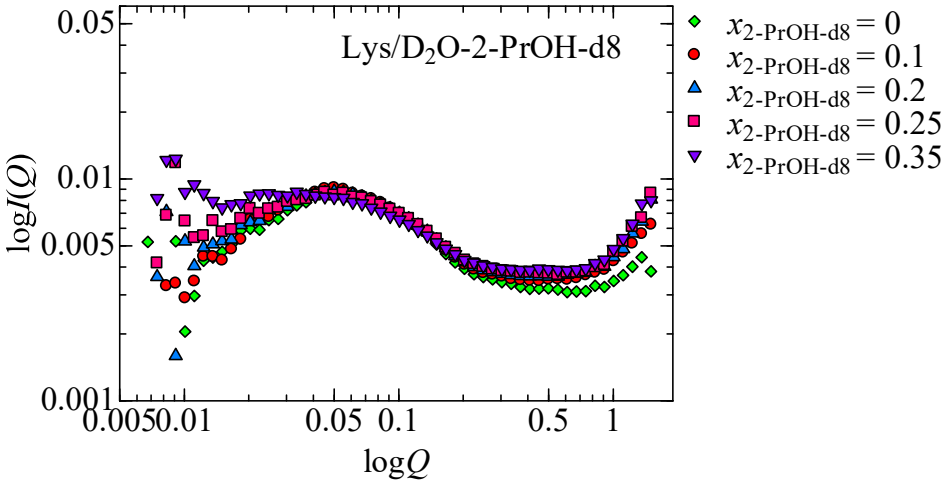

Fig. 2 SANS spectra of Lys/D_2O–HFIP at various 2–propanol mole fractions.

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

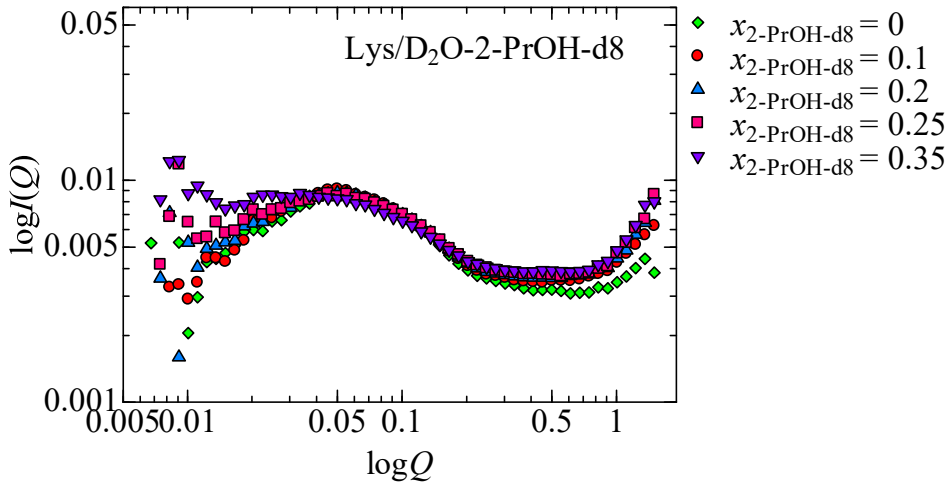

Fig. 3 SANS spectra of Lys/D_2O-HFIP at various HFIP mole fractions.

For system C, we could obtain the information on the change in lamella structure of 2,3-lutidine by SANS experiments using TAIKAN spectrometer. Furthermore, the SANS spectra for the water-$CDCl_3$-CTAB solutions were reasonably obtained. To elucidate the structure of aggregates formed in the solutions, the SANS spectra will be analyzed using suitable model equation.