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 2017/5/10 承認者 Approver Kaoru Shibata 提出日 Date of Report 2017/5/10
課題番号 Project No. 2016B0127. 実験課題名 Title of experiment Dynamics of water and glycine molecules in their mixture confined in MCM-41 実験責任者名 Name of principal investigator Koji Yoshida 所属 Affiliation Fukuoka University	装置責任者 Name of Instrument scientist Kaoru Shibata 装置名 Name of Instrument/（BL No.） DNA/BL02 実施日 Date of Experiment February 23, 2017 to February 27, 2017

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.

Samples

1. 18 wt% D-Glycine($C_2H_3D_2NO_2$)/H_2O solutions at pH=2 confined in MCM-41 C18
2. 18 wt% D-Glycine($C_2H_3D_2NO_2$)/H_2O solutions at pH=5 confined in MCM-41 C18
3. 18 wt% H-Glycine($C_2H_2D_3NO_2$)/D_2O solutions at pH=2 confined in MCM-41 C18
4. 18 wt% H-Glycine($C_2H_2D_3NO_2$)/D_2O solutions at pH=5 confined in MCM-41 C18

The hydration levels (mass of glycine / mass of dry MCM-41) of all samples are 0.6.

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.

Experimental method

Vacuum dried MCM-41 C18 powder (pore diameter is 32 Å) and 18 wt% glycine aqueous solution at pH=5 and 2 were put in Eppendorf tubes, and the mixtures were stirred for about 1 h using a vortex mixer. The powdery samples were wrapped with aluminum foil in a thin plate-like shape were inserted into a double cylindrical aluminum cell, which consist of cylinder of 18.0 mm outer diameter, 0.25 mm thickness, and 50 mm height. The thickness of samples was 2~4 mm, depending on the transmission of samples (more than 90 %). These cells were sealed with indium. The measurements were performed at 305, 290, 275, 260 and 245 K.

Results

Fig. 1 shows the temperature dependence of QENS spectra of 18 wt% D-glycine solution at pH=5 confined in MCM-41 at Q=1.0 Å^{-1}. The individual spectra are shifted for clarity. The instrumental resolution function was measured at 100 K since any motion of water molecules can be regarded as a standstill on the time scale of this spectrometer. QENS spectra were fitted by a Lorentzian function and a delta function.

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

Fig. 2 shows the fitting results of the half width half maximum (HWHM), Γ(*Q*), by a jump diffusion model for 18 wt% D-glycine solution confined in MCM-41. The self-diffusion coefficient, *D,* and the residence time, τ, were obtained from this model.

$$\Gamma(Q) = \frac{DQ^2}{1 + DQ^2\tau}$$

Fig. 3 shows the Arrhenius plots of *D* for glycine solutions confined in MCM-41. The activation energies of D-glycine at pH=5, D-glycine at pH=2, H-glycine at pH=5 and H-glycine at pH=2 solutions confined in MCM-41 C18 were 21.3, 24.5, 20.7 and 17.1 kJ/mol, respectivery. The values for H-glycine solutions could reflect the activation energy of the translatonal motion of glycine molecules since the neutrons scattering cross section of H is much larger than that of the other atoms. The results indicate that the activation energy of the translational motion of glycine moelcuels at pH=5 was larger than that at pH=2. It is consisttent with the X-ray diffraction results which indicate that the glycine molecules locate near the silica surface by forming the hydrogen bond of $NH_3CH_2COO^-$…HO-Si at pH=5.

On the other hand, the activation energy for D-glycine solutions could reflect that of the translational motion of water molecules. X-ray diffraction results imply that glycine molecules locate in the pore center at pH=2. Hence, glycine molecule could be hydrated at pH=2 more strongly. That is why the activation energy of the translational motion of water molecules at pH=2 was larger than that at pH=5.

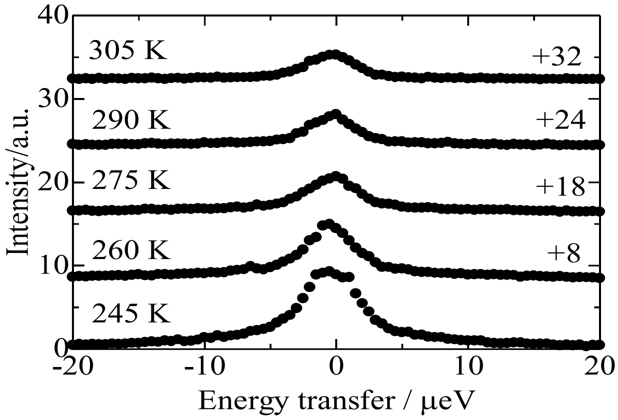

Fig. 1. The temperature dependence of QENS spectra of 18 wt% D-glycine solution at pH=5 confined in MCM-41 C18 at *Q* = 1.0 Å^{-1}.

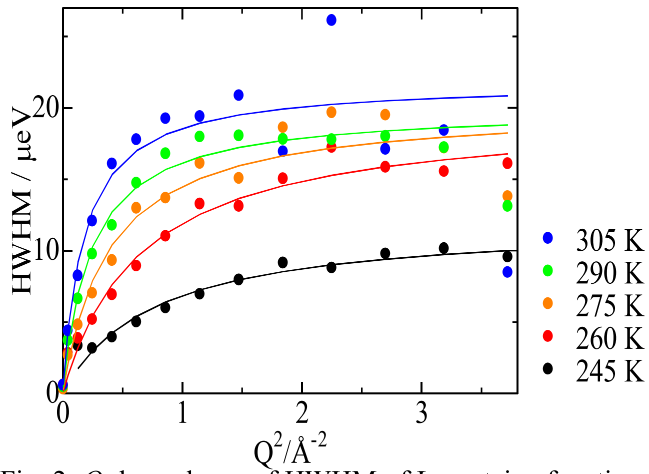

Fig. 2. *Q*-dependence of HWHM of Lorentzian function for 18 wt% D-glycine solution at pH=5 confined in MCM-41 C18 at 305, 290, 275, 260 and 245 K. The solid lines are fitting results by a jump diffusion model.

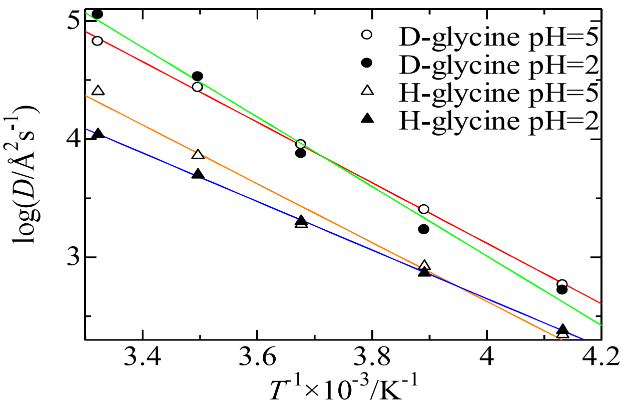

Fig. 3. Arrhenius plot of self-diffusion coefficient *D* for 18 wt% glycine solution confined in MCM-41 C18.