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。 ）

CROSS TOKAI **Experimental Report** J-PARC	承認日Date of Approval 2014/6/23 承認者Approver Kaoru Shibata 提出日Date of Report 2013/11/10
課題番号 Project No. 2013A0162 実験課題名 Title of experiment Dynamics of methanol confined in mesoporous silica MCM-41 and ordered mesoporous carbon OMC78 実験責任者名 Name of principal investigator Toshio Yamaguchi 所属 Affiliation Fukuoka University	装置責任者 Name of responsible person Kaoru Shibata 装置名 Name of Instrument/（BL No.） DNA 実施日 Date of Experiment 3 May 2013 – 8 May 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.

Methanol, CH_3OH

Mesoporous silica MCM-41 C18, SiO_2

Ordered mesoporous carbon OMC78, C

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 capillary condensed methanol confined in MCM-41 C18 and OMC78 was prepared on an adsorption apparatus installed at Fukuoka University. The powder samples were inserted in cylindrical double aluminum cells previously used for QENS measurements at DNA spectrometer, J-PARC.

The energy range: -25 ~ +45 μeV with an energy resolution of 1.3 μeV.

The Q-range: 0.07 - 1.98 A^{-1} which covers the first peak of the structure factor of methanol in MCM-41 an OMC.

The temperature range: 315, 300, 285, 270, 255 K. The data at 150 K were used as resolution function.

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

Figure 1 shows the typical QENS spectra of methanol molecule in OMC at various temperatures. Since the energy resolution of DNA is several μeV, only the translational motion of a methanol molecule will contributes to the QENS data of methanol in Ph-PMO and OMC. Thus, the QENS data were analyzed by Eq.

$$\boldsymbol{S(Q,\omega) = \{A_1\delta(\omega) + A_2 L_{\mathrm{Trans}}(Q,\omega)\} \otimes R(Q,\omega) + BG} \qquad (1)$$

δ(ω) is a δ function and corresponds to the elastic component. $L_{\mathrm{trans}}(Q, \omega)$ is a contribution from translational diffusion of the capillary-condensed methanol molecules. BG is the background and $R(Q, \omega)$ is the resolution function.

The obtained half-width at half-maximum, Γ, was analyzed with a jump diffusion model given by Eq. (2).

$$\Gamma = \frac{D_T Q^2}{1 + D_T \tau_0 Q^2} \qquad (2)$$

Γ is HWHM (half width at half maximum). D_T is translational diffusion constant. τ_0 is residence time of translational diffusion. Q is the momentum transfer.

The translational diffusion constant, D, of a methanol molecule in Ph-PMO and OMC was plotted as a function of 1/T. The activation energy of the translational diffusion of a methanol molecule in Ph-PMO and OMC was obtained as 14.6 kJ/mol and 5.76 kJ/mol, respectively. The present results suggest that methanol molecules strongly bind to the pore wall of Ph-PMO probably due to the hydrogen bonding between the methanol OH and the silanol Si-OH groups. In the case of the hydrophobic wall of OMC, methanol molecules are less retarded than in Ph-PMO since the interactions between methanol molecule and the carbon wall of OMC.

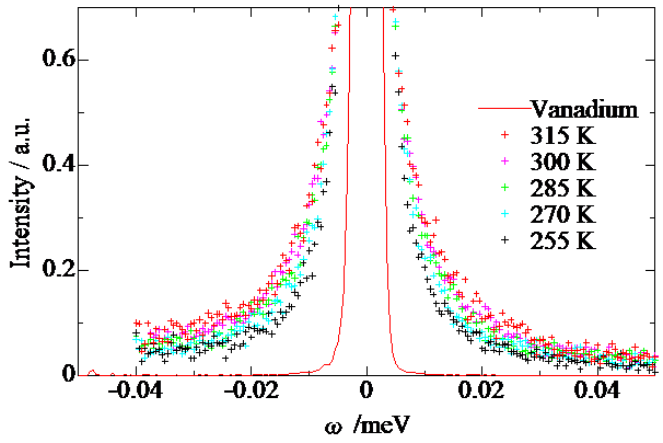

Fig. 1. QENS spectra of methanol confined in Ph-PMO at various Temperatures, together with that of vanadium for resolution function.