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 承認者 Approver 提出日 Date of Report
課題番号 Project No. 2012B0254 実験課題名 Title of experiment Dynamics of water confined in ordered mesoporous carbon 実験責任者名 Name of principal investigator Toshio Yamaguchi 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/(BL-02) 実施日 Date of Experiment 30 Nov.-3 Dec. 2012

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.

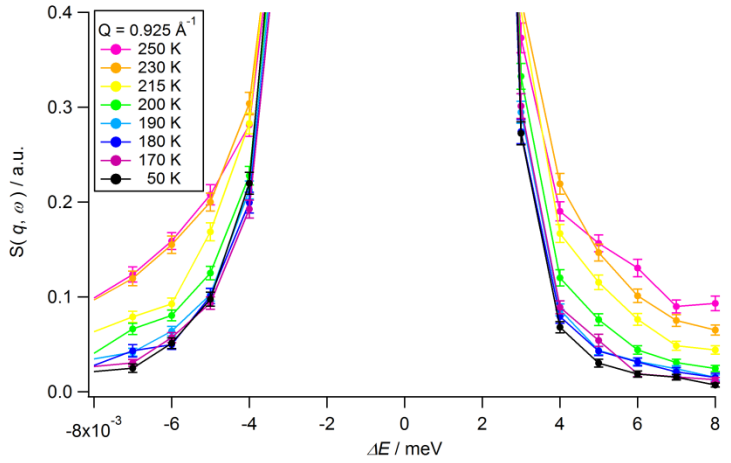
Water in ordered mesoporous carbon (H_2O in C)

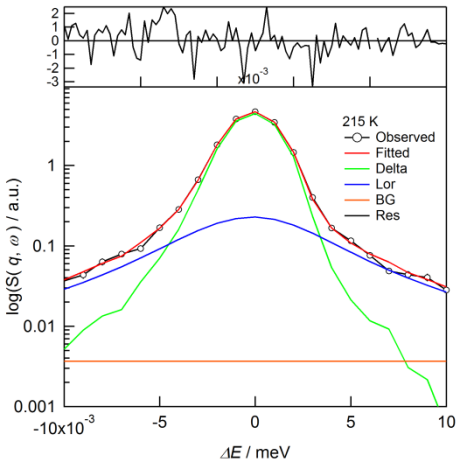
2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Water was adsorbed in a capillary condensed state at P/P_0 =0.68 (P and P_0 are the vapor pressure and the saturated vapor pressure of water, respectively) in mesoporous carbon OMC on an adsorption apparatus installed at Fukuoka University. The powder sample thus prepared was inserted in a cylindrical double aluminum cell (of 16.0 mm outer diameter, 0.25 mm thickness, and 45 mm height and an outer cylinder of 18.0 mm inner diameter, 0.25 mm thickness, and 50 mm height) previously used for QENS measurements at the AGNES spectrometer, JRR3. The measurements were performed at temperatures of 300, 250, 230, 215, 200, 190, 180, 170 and 50 K in a range of scattering vector, Q, from 0.18 to 1.70 $Å^{-1}$. The QENS spectra were successfully obtained.

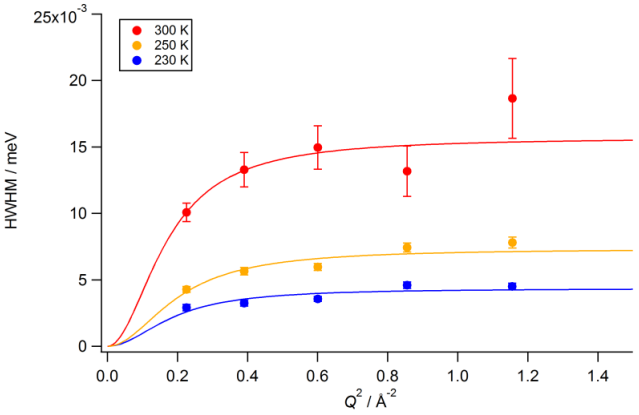
2. 実験方法及び結果（つづき） Experimental method and results (continued)





The left-hand side figure shows the temperature dependence of the QENS spectra of water confined in OMC prepared at P/P_0 =0.68 and at Q =0.925 Å^{-1}. The values measured at 50 K were used for instrument resolution. The right-hand side figure shows the fitting results of the corresponding QENS data of water confined in OMC at 215 K. The open circles denote the experimental data, the green line the elastic component, the blue line quasi-elastic component (translation) and the red line the fitted data.

The QENS spectra were analyzed by $S(Q,\omega) = \{A_1\delta(\omega) + A_2 L(\omega,\Gamma) + BG\} \otimes R(Q,\omega)$.

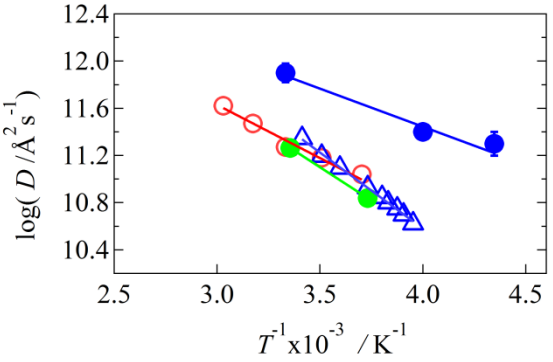


$$L(\omega,\Gamma) = \frac{1}{\pi}\frac{\Gamma}{\left[\omega^2 + \Gamma^2\right]}$$

The Q^2 dependence of the half-width at half-height (HWHM) of the Lorentzian component for water confined in OMC at 300, 250 and 230 K. The data were analyzed by a jump diffusion model,

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

$$D = A\exp\left(\frac{-E_a}{RT}\right)$$



The HWHM decreases with lowering temperature, showing that the motion of water molecules becomes slower.

The Arrhenius plot of diffusion coefficient D of translational diffusion for water confined in OMC (blue circle), Ph-PMO (red circle) and in MCM-41 C14(green circle), and in bulk (blue triangle).

The QENS data showed the self-diffusion coefficient of confined water in OMC at 300 K is larger than those for MCM-41, Ph-PMO and bulk water. This result suggests that the hydrophobicity of OMC surface is the highest in that of MCM-41 and Ph-PMO.