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 MLF Experimental Report	提出日 Date of Report 2012/07/20
課題番号 Project No. 2011B0010 実験課題名 Title of experiment Development of novel analysis of quasi-elastic neutron scattering and its application to dynamics of molecular liquids 実験責任者名 Name of principal investigator Tatsuya Kikuchi 所属 Affiliation J-PARC Center, JAEA	装置責任者 Name of responsible person Kenji Nakajima 装置名 Name of Instrument/(BL No.) BL14 AMATERAS 実施日 Date of Experiment 2012.2.15 – 2012.2.22

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. benzene, C ₆ H ₆ benzene-d ₆ , C ₆ D ₆ carbon tetrachloride, CCl ₄
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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. Three samples were loaded into the double cylindrical Al can and sealed with indium gasket respectively beforehand outside MLF. We used the standard cryostat of AMATERAS for the measurements. Each sample was measured at several temperatures in 160 - 320 K. The measurements mainly were carried out under the settings of low energy and high resolution with multi E_i set of 23.7, 5.9 and 2.6 meV. Data acquisition times were 6 – 10 h at the operation with 120 kW proton-beam power of J-PARC, respectively. Figure 1 shows the examples of $S(Q, \omega)$'s by the measurements. The statistics precision was not so good, but was an acceptable level for our new analysis method. We analyzed the data by the new analysis method of quasi-elastic neutron scattering (QENS) as wrote for the proposal of this experiment. In this method, $S(Q, \omega)$ can be described, $S(Q, \omega) = A(Q)\delta(\omega) + \int B(Q, \Gamma) \frac{1}{\pi} \left(\frac{\Gamma}{\omega^2 + \Gamma^2} \right) d\Gamma.$
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2. 実験方法及び結果(つづき) Experimental method and results (continued)

$B(Q, \Gamma)$ is an intensity distribution for HWHM of Lorentzian. This function can show the number of modes and distributions of the relaxation times in the modes and we call it as mode distribution function (MDF). In this new approach, we can obtain $B(Q, \Gamma)$ by using the maximum entropy method (MEM). Figure 2 shows the examples of obtained $B(Q, \Gamma)$'s by this method. From these results, we found that three relaxation modes were existed at least in liquid benzene in spite of a simple molecular liquid.

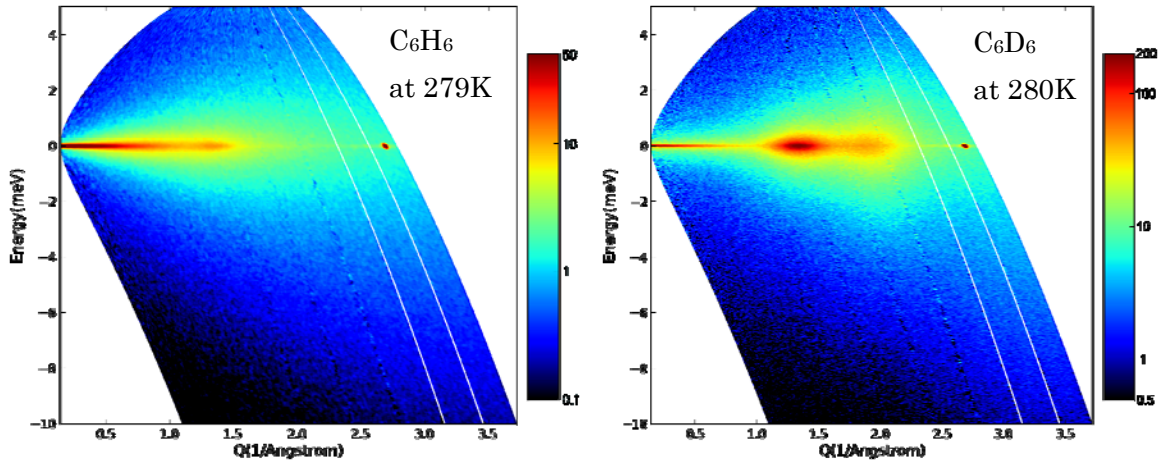


Fig. 1 $S(Q, E)$ maps of liquid benzenes at $E_i = 5.9$ meV.

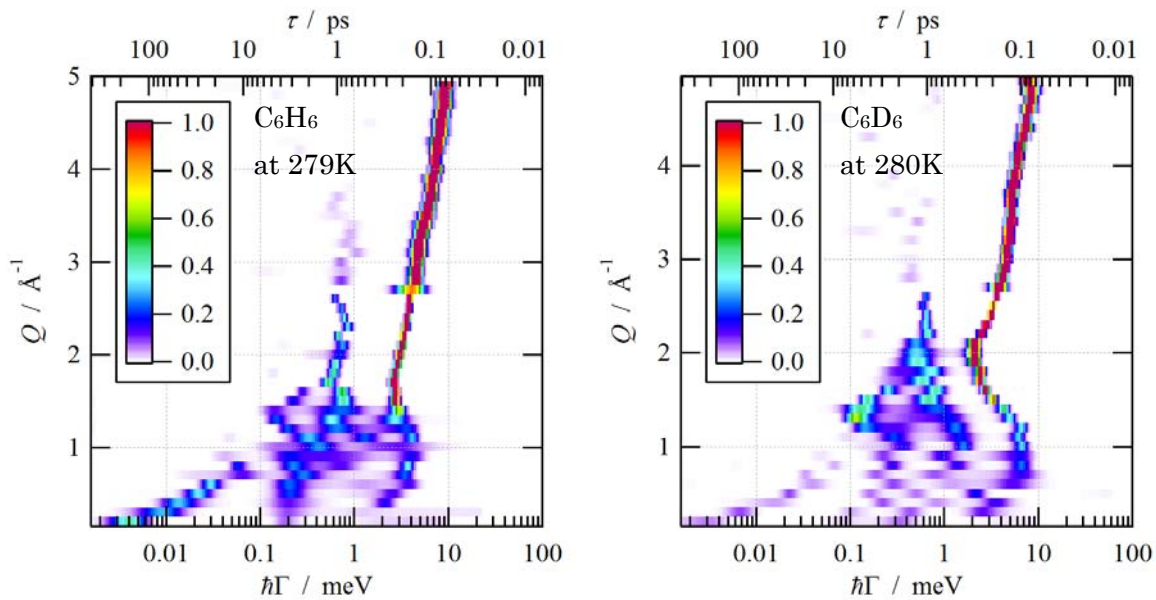


Fig. 2 $B(Q, \Gamma)$ maps of liquid benzenes.