



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。)

 <b>Experimental Report</b> 	承認日 Date of Approval 2014/06/03 承認者 Approver Takanori Hattori 提出日 21st May 2014
課題番号 Project No. 2013B0066 実験課題名 Title of experiment Orientation of Water Molecules around Ca <sup>2+</sup> and Cl <sup>-</sup> Ions in Aqueous CaCl <sub>2</sub> Solutions at High Temperatures and Pressures 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 Dr. Takanori Hattori 装置名 Name of Instrument/(BL No.) PLANET / (BL11) 実施日 Date of Experiment 21st Mar. 2014-23rd Mar. 2014

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.
1. CaCl <sub>2</sub> /10D <sub>2</sub> O solution in Al-cell (15×15×15 mm) 2. CaCl <sub>2</sub> /25D <sub>2</sub> O solution in Al-cell (15×15×15 mm)

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.
<p>To clarify the hydration structure of Ca<sup>2+</sup> and Cl<sup>-</sup> under high pressures, neutron diffraction measurements were made on aqueous calcium chloride solutions with the PLANET spectrometer. Calcium chloride was dissolved in D<sub>2</sub>O at the molar ratios of <math>R = [D_2O]/[CaCl_2] = 10</math> and 25. During the measurements, the sample solutions of CaCl<sub>2</sub>/RD<sub>2</sub>O were kept in a cubic aluminum cell with the dimension of 15×15×15 mm. The dimension of sample in the aluminum cell was a cylinder with 6 mmφ in diameter and 6 mm in height. The pressure was loaded to the aluminum cell using the 6-axis multi-anvil press, ATSUHIME, installed at PLANET. The temperature was kept at the ambient of 298 K.</p> <p>For the CaCl<sub>2</sub>/10D<sub>2</sub>O solution, Bragg peaks appeared in the neutron scattering pattern above ~0.5 GPa. The Bragg peaks can be assigned to CaCl<sub>2</sub>·6D<sub>2</sub>O. Crystals of hydrate precipitated in the solutions above this pressure.</p>

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

For the  $\text{CaCl}_2/25\text{D}_2\text{O}$  solution, on the contrary, Bragg peaks did not appear in the scattering pattern until  $\sim 1.2$  GPa. However, crystals of  $\text{CaCl}_2 \cdot 6\text{D}_2\text{O}$  also precipitated from the solution above this pressure. In the future experiments, we should change the concentration of sample solution and the pressures to reach our goal for the observation of the hydration structure of  $\text{Ca}^{2+}$  and  $\text{Cl}^-$  in the solution at high temperatures and high pressures.

In the present experiments, we measured the diffraction intensities of both solutions at the ambient pressure and temperature using the vanadium cell. These results should be the references for  $\text{CaCl}_2/\text{RD}_2\text{O}$  solutions at high temperatures and high pressures in the near future.