


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。)

 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2013A0109 実験課題名 Title of experiment Nuclear density analysis of lithium cation encapsulated in C ₆₀ 実験責任者名 Name of principal investigator Shinobu Aoyagi 所属 Affiliation Nagoya City University	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/(BL No.) iMATERIA/BL20 実施日 Date of Experiment 4/27~4/28

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.
hexafluorophosphate salt of lithium endohedral fullerene $\text{LiC}_{60}\text{PF}_6$

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.
<p>The standard experimental setup of iMATERIA was used in this experiment. The TOF neutron diffraction pattern of 10 milligrams of $[\text{Li}^+\text{C}_{60}](\text{PF}_6)^-$ powder sample in a vanadium holder was measured at 4, 25, 50, 75 and 100 K by using three kinds of detector bank for back, 90-degree and low-angle scattering. The maximum measurement time for one data was 12 hours. The Rietveld structure refinement and nuclear density analysis are in progress to reveal the temperature dependence of the position and site occupancy of the lithium cation inside the fullerene cage. Weak nuclear density peaks probably due to the lithium cation were observed in the differential Fourier map at 4 K. However, the lithium cation barely contributes to the total scattering intensity. The measured scattering intensities were very weak due to the tiny amount of sample. The ratio of the strongest peak intensity (I_{max}) to the background intensity (I_{bg}) is about $I_{\text{max}}/I_{\text{bg}} = 3$. Additional experiment with larger sample amount and longer measurement time should be conducted to obtain higher intensity data.</p>

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