( ※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.	装置責任者 Name of responsible person
2015A0135	Toru Ishigaki
実験課題名 Title of experiment	装置名 Name of Instrument/(BL No.)
Nuclear density analysis of lithium cation encapsulated in $\mathbf{C}_{60}$	iMATERIA/BL20
実験責任者名 Name of principal investigator	実施日 Date of Experiment
Shinobu Aoyagi	3/23/2016-3/29/2016
所属 Affiliation	
Nagoya City University	

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  $\mbox{LiC}_{60}\mbox{PF}_{6}$ 

## 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.

The standard experimental setup of iMATERIA was used in this experiment. TOF neutron diffraction patterns of 30 milligrams of  $[Li^+@C_{60}](PF_6)^-$  powder sample in a vanadium holder were measured at 20, 50, 80, and 110 K using three detector banks for back, 90-degrees, and low-angle scattering. The measurement time at each temperature was about 36 hours. The powder diffraction patterns taken by the 90-degrees detector bank are shown in the following figure. The scattering intensities and the ratio of the Bragg peak intensities to the back ground intensities of the data are much higher than that of the previous data obtained in 2013A0109 and 2014A0257. The present data is promising to reveal temperature dependence of the position and site occupancy of the lithium cation moving inside the fullerene cage.

