

Crystal Structure Analysis of Cationic Lithium  
Endohedral Fullerene under Electric Field

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Metallofullerenes encapsulating metal atoms within the hollow carbon cage are promising materials for molecular devices such as a single molecular memory. Recently, we have achieved the macroscopic synthesis and structure determination of metallofullerenes encapsulating a lithium cation,  $\text{Li}^+\text{@C}_{60}$ . [1] The cationic  $\text{Li}^+\text{@C}_{60}$  has a high tendency to form ion-pair states with an anion such as  $\text{SbCl}_6^-$ . The  $\text{PF}_6^-$  salt,  $[\text{Li}^+\text{@C}_{60}](\text{PF}_6)^-$ , that forms a rock-salt-type cubic structure has also been obtained. [2]

The electrostatic attraction between the off-centered  $\text{Li}^+$  and anions through the carbon cage implies that the position of the encapsulated  $\text{Li}^+$  can be switched by an external electric field. To reveal the effects of external electric fields to the position and thermal motion of the  $\text{Li}^+$  inside the carbon cage, the synchrotron-radiation X-ray structure analyses of  $[\text{Li}^+\text{@C}_{60}](\text{PF}_6)^-$  under electric fields were performed in this study. The results are shown in this presentation.

[1] S. Aoyagi, E. Nishibori, H. Sawa, K. Sugimoto, M. Takata, Y. Miyata, R. Kitaura, H. Shinohara, H. Okada, T. Sakai, Y. Ono, K. Kawachi, K. Yokoo, S. Ono, K. Omote, Y. Kasama, S. Ishikawa, T. Komuro, H. Tobita, *Nature Chem.*, **2** (2010) 678-683.

[2] S. Aoyagi, Y. Sado, E. Nishibori, H. Sawa, H. Okada, H. Tobita, Y. Kasama, R. Kitaura, H. Shinohara, *Angew. Chem. Int. Ed.*, **51** (2012) 3377-3381.