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, Li⁺@C₆₀.₁ The cationic Li⁺@C₆₀ has a high tendency to form ion-pair states with an anion such as SbCl₆⁻. The PF₆⁻ salt, [Li⁺@C₆₀](PF₆)⁻, that forms a rock-salt-type cubic structure has also been obtained.²

The electrostatic attraction between the off-centered Li⁺ and anions through the carbon cage implies that the position of the encapsulated 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 Li⁺ inside the carbon cage, the synchrotron-radiation X-ray structure analyses of [Li⁺@C₆₀](PF₆)⁻ under electric fields were performed in this study. The results are shown in this presentation.