Direct Observation of a H_2 Molecule Swallowed by Open-mouthed C_{60}

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Various types of endohedral fullerene complexes are known to date. However the metallofullerenes are generally produced by arc-discharge method, but the use of such extremely drastic conditions is apparently not suitable for encapsulation of unstable molecules or gases. We recently succeeded in incorporation of a H_2 molecule in 100% into a derivative of an open-cage C60 [1]. In order to observe the endohedral H_2 molecule directly, the X-ray diffraction analysis using synchrotron radiation were carried out. We observed a single H_2 molecule encapsulated in fullerene cage using structure analysis and maximum entropy method [2]. This H_2 molecule is floating inside of the hollow cavity and considered to be completely isolated from the outside (Fig.1).

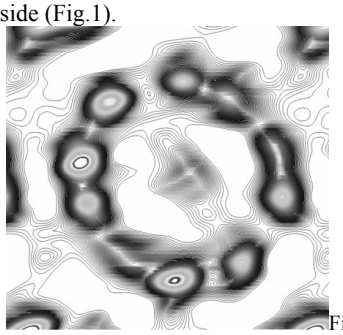

Fig.1. The MEM electronic density distributions of H2 endohedral open-cage C60.

[1] a) Murata Y., Murata M., Komatsu K., *J. Am. Chem. Soc*., 2003, **125**, 7152-7153; b) Murata Y., Murata M., Komatsu K., *Chem. Eur. J*., 2003, **9**, 1600-1609. [2] Sawa H., Wakabayashi Y., Murata Y., Murata M., Komatsu K., *Angew. Chemi.*, 2005, 13.

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