X-ray Charge Density Studies of $Sc_2@C_{66}$, $Sc_3N@C_{68}$ and $Gd@C_{82}$

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The structure of an IPR-violated metallofullerene $Sc_2@C_{66}$ has been determined in the electron density level[1)] by the MEM/Rietveld method[2,3)] using synchrotron radiation powder data. The fundamental structure has been obtained by the Rietveld analysis. The cage structure of C_{66} has been unambiguously identified as that of Isomer No.**4348**. The obtained charge density by the MEM analysis shows that the encapsulated two Sc atoms form the covalent bonded Sc_2 dimer and that the charge density of dimer is overlapping with that of C_{66} cage, indicating the existence of a covalent bond character between Sc_2 and the carbon cage.

It should be noted that the recent theoretical study suggested a different structural model of $Sc_2@C_{66}$ based on the isomer **4059**[4)]. The best fit of the Rietveld refinement based on this theoretical model gives the reliability factors R_{wp}=9.1% and R_I=57.6%. The extremely large discrepancy between the calculated and observed X-ray powder pattern should be caused by the burger-shaped cage structure of **4059** and the difference of Sc-Sc inter-atomic distance. Even at the Rietveld analysis level, it is concluded that the X-ray diffraction data obviously can not be explained by the **4059** structure based on the simple ionic bonding model between Sc atoms and the cage.

The charge densities of $Sc_3N@C_{68}$ and $Gd@C_{82}$ will be also presented.

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4)K.Kobayashi and S. Nagase, *Chem. Phys. Lett.* **362** (2002)373.