

II-E Endohedral Metallofullerenes: New Fullerene Molecules with Novel Properties

Encapsulation of one or more metal atoms inside hollow fullerene cages (endohedral metallofullerenes) has long attracted special attention because it could lead to new spherical molecules with novel properties unexpected for empty fullerenes. Great efforts have been made for the production and characterization of endohedral metallofullerenes. Up to now it has been demonstrated that group 2 and 3 metals and most lanthanide metals can be trapped inside the higher fullerenes to form soluble and relatively stable endohedral metallofullerenes. Because of the difficulty in producing pure samples in large quantities, the experimental characterization of endohedral metallofullerenes has been hindered. Recent important progress is marked by the successful isolation and purification of metallofullerenes in macroscopic quantities. This has made it possible to investigate the interesting electronic properties and chemical reactivities.

II-E-1 Structural Determination of the La@C₈₂ Isomer

cage is also studied based on the temperature dependence of the mean-square displacement of La–C.

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[*J. Phys. Chem. B* **105**, 2971 (2001)]

A stable diamagnetic monoanion of the La@C₈₂ isomer was electrochemically prepared and isolated in order to disclose its cage symmetry. By measuring the ¹³C NMR spectrum of the anion, it was determined for the first time that the isomer has C_s symmetry, as was also confirmed by density functional calculations.

II-E-2 Structure of La₂@C₈₀ Studied by La K-Edge XAFS

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[*Chem. Phys. Lett.* **335**, 163 (2001)]

The structure of La₂@C₈₀ is studied by La K-edge XAFS from 40 to 295 K. The distances between the La atom and the first nearest C atoms, and between the La atom and the second nearest C atoms have been determined to be 2.42(1) Å at 40 K and 2.44(2) Å at 295 K, and 2.97(2) Å at 40 K and 2.98(3) Å at 295 K, respectively. The La–La distance has also been determined to be 3.90(1) Å at 40 K and 3.88(2) Å at 295 K. The dynamical behavior of two La atoms in the C₈₀