II-C 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 sperical 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-C-1 La@C_{82} Anion. An Usually Stable Metallofullerene

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The anion of the major isomer of La@C_{82} was electrochemically prepared and isolated. Anionic La@C_{82}(–) is very stable in water, even after exposure to air at room temperature. The high stability of La@C_{82}(–) is essentially due to its closed-shell electronic structure. As evidenced by the ESR analysis, La@C_{82}(–) is diamagnetic. These experimental findings are confirmed by density functional calculations. The cage structure of La@C_{82} was determined for the first time and shown to have C_{2v} symmetry based on the ^{13}C NMR measurements of the compound in its anionic form.

II-C-2 Transient Spectroscopic Properties of Endohedral Metallofullerenes, La@C_{82} and La_2@C_{80}

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Properties of the excited states of endohedral metallofullerenes (La@C_{82} and La_2@C_{80}) have been investigated by time-resolved absorption spectroscopy. Transient absorption bands of La@C_{82} showed two decay-components, which were attributed to excited states of different spin multiplicity. The properties of photoexcited states of La_2@C_{80} are also reported.

II-C-3 Vibrational Spectroscopy of Endohedral Dimetallofullerene, La_2@C_{80}

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The first FT-IR spectra of La_2@C_{80} are observed at temperatures from 353 to 83 K by dispersing the sample into the KBr pellet, which confirm that the C_{80} cage has I_h symmetry, as supported from theoretical calculations. Also discussed is the rotational motion of the C_{80} cage.