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

Endohedral metallofullerenes (fullerenes containing metal atoms inside hollow carbon cage) have long attracted special interest as new spherical molecules with novel properties. Recent important progress has been marked by successful isolation and purification in macroscopic quantities. With the availability of such purified samples, it has been possible to investigate the electronic properties and chemical reactivities.

II-D-1 Endohedrally Metal-Doped Heterofullerenes: La@C₈₁N and La₂@C₇₉N

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The first evidence of the gas-phase formation of endohedrally La-doped azafullerene ions La@C₈₁N and La₂@C₇₉N was obtained by the fast atom bombardment mass fragmentation of the adducts, La@C₈₂(NCH₂Ph) and $La_2@C_{80}(NCH_2Ph)$.

II-D-2 Isolation and Characterization of a Pr@C₈₂ Isomer

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A minor isomer of Pr@C₈₂ (Pr@C₈₂-II) has been isolated with an efficient two-step HPLC method, accompanied with a major isomer (Pr@C₈₂-I). The isolated Pr@C₈₂-II was well identified as a stable endohedral metallofullerene molecule. Mass spectra of both isomers confirmed that they were Pr@C₈₂. Visible and near-IR absorption spectra, and cyclic and differential pulse voltammograms for Pr@C82-II showed characteristic features different from those for Pr@C₈₂-I. Chemical derivatization of both isomers were also accomplished. These data reveal that Pr@C₈₂-II is a carbon-cage isomer of Pr@C₈₂-I.