Fullerenes with Confined Atoms

– The structure and dynamics of $Li@C_{60}$ and $La@C_{82}$

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Abstract

Fullerenes have attracted a lot of attention since their discovery, not only for their interesting fundamental properties, but also for their possible applications in nanotechnology devices. Insertion of metal atoms into the hollow interiors of fullerenes leads to drastic changes of stability, reactivity, and electronic properties of the molecule. This thesis presents results from investigations of the endohedral fullerenes $Li@C_{60}$ and $La@C_{82}$. Macroscopic amounts of $Li@C_{60}$ have been produced by ion bombardment of thin fullerene films. Characterization of chromatographically purified material with IR and Raman spectroscopy suggest that it exists as dimers $(Li@C_{60})_2$ and trimers $(Li@C_{60})_3$.

$La@C_{82}$ has been studied concerning ionization and fragmentation dynamics using time-of-flight mass spectrometry. When excited to several tens of electron volts of internal energy the molecule cools by radiative emission, loss of C_2-molecules, and electron emission. The radiative cooling plays a larger role for $La@C_{82}$ than it does for C_{60}. When $La@C_{82}$ is excited to internal energies above 65 eV the fullerene cage structure is lost and the La-atom is ejected from the molecule.

Thin films of $Li@C_{60}$ and $La@C_{82}$ have been measured to be significantly better conductors than similar films of C_{60}. The conductance was however shown to decrease at contact with air. The influence of air on $La@C_{82}$ thin films was studied with laser desorption mass spectrometry. The lanthanum atom was shown to escape the fullerene cage in a reaction involving molecular oxygen.

Keywords: fullerenes, endohedral fullerenes, delayed ionization, activation energy, UV-vis, IR, Raman, time-of-flight, laser desorption mass spectrometry, thermionic emission, transport measurements