Ionization Properties of Endohedral Fullerenes: Experimental and Computational Approaches

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Ionization properties of various endohedral metallofullerenes, including mono- and dimetallic species, as well as novel trimetallic nitride template (TNT) compounds, were studied experimentally by means of Knudsen Cell Mass Spectrometry - Ion-Molecule Equilibria method and theoretically, employing DFT calculations. We present some considerations concerning the metal atoms positions in the fullerene cages, the degree of participation of carbon cage and atoms entrapped in the ionization properties formation in different cases, the differences in carbon cage isomerism between empty and endohedral molecules, and the possibility of IPR violation for the endohedral structures.