

Structure and Electronic Properties of Endohedral
Metallofullerenes

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In this communication, we report the most recent results of our group on the electronic and structural properties of endohedral metallofullerenes. Among other properties we will discuss the relevance of thermal effects in the stabilization of specific isomers in cages with 70 carbon atoms or more. Like for larger cages small fullerenes are stabilized by charge transfer from the internal metal to the carbon cage. We will discuss this behaviour for the family of compounds $M@C_{2n}$, with $M = Ti, Zr$ and Hf and $26 < 2n < 50$.

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