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Magnetic Endohedral Metallofullerenes with Floppy Interiors

MEICHUN QIAN, SHIV KHANNA, Virginia Commonwealth University, MARK KNICKELBEIN, Argonne National Laboratory — Investigations on the electronic structure and magnetic properties of a free Gd_3N and $\text{Gd}_3\text{N}@C_{80}$ have been carried out using to examine the stability and the electronic and magnetic properties of the endohedral species. Using a synergistic approach combining Stern-Gerlach experiments in beams and first principles electronic structure studies, it is demonstrated that an isolated Gd_3N has a ground state spin moment of $23 \mu\text{B}$ followed by a non-collinear state of $17.2 \mu\text{B}$ only 88 meV above the ground state. The large moment is largely due to localized f-electrons. As a Gd_3N is embedded inside a C_{80} cage, the localized f-electrons maintain the magnetic character while the hybridization between the s,d states of isolated Gd_3N and p-states of C_{80} leads to a strongly bound motif with an interaction energy of 13.63 eV and a large HOMO-LUMO gap of 1.48 eV. $\text{Gd}_3\text{N}@C_{80}$ is further shown to possess two isomers corresponding to the location of the N atom on either side of the Gd_3 triangle with an appreciable electric dipole moment and a low barrier of 91 meV for transition between them offering potential for a fluctuating dipole.

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