

Endofullerenes of lanthanides $\text{Ln}@\text{C}_{60}$: *ab initio* geometric and electronic structure calculation

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Endofullerenes are promising basic elements for quantum computer [1]. We have presented *ab initio* calculations of equilibrium geometric and electronic structure of lanthanide containing endofullerenes $\text{Ln}@\text{C}_{60}$. Stable position of metal atom is located on the C_3 -axis which connects the centres of the opposite six-membered rings. We found two types of $\text{Ln}@\text{C}_{60}$ structures. For the endofullerenes of the first type (La – Dy) the stable position of the lanthanide atom is located at the distance $0.67 R$ from the centre of the fullerene ($R=3.35 \text{ \AA}$ is the fullerene radius). The distance between lanthanide atom and the six nearest carbons coincides with 10 % accuracy with the sum of atomic radii of Ln and C. Similar interpretation of the off-centre position of lanthanide atom was recently presented for ion $[\text{Ce}@\text{C}_{60}]^+$ [2].

Potential energy surfaces of the second type of endofullerenes (Ho – Lu) have two minima. These minima correspond to the position of Ln in the centre and at the distance $0.5 R$ from the centre of fullerene. It results from qualitatively change of metal-cage interaction. Spinless lanthanide atom interacts weakly with the carbon cage and can occupy the equilibrium position in the centre of the fullerene. This is characteristic of the endofullerenes of the inert gases. Thus, the redistribution of the spin density is connected with the metall-cage interaction character change which results in the change of the equilibrium geometric and electronic structure of the endofullerene.

For all fullerenes the spin leakage effect is observed: partial or full transfer of the unpaired electrons to the carbon cage. Stability of lanthanoid's position depends on the degree of spin leakage. Transfer of 50% spin density from metal atom to cage results in stabilization of structure.

Analysis of the spin density makes possible estimating the relative stability of lanthanides endofullerenes. In the low-spin state $\text{Ho}@\text{C}_{60}$ and $\text{Tb}@\text{C}_{60}$ can have maximal reactivity. Other endofullerenes practically do not show radical character. In the high-spin state the endofullerenes $\text{Pm}@\text{C}_{60}$, $\text{Sm}@\text{C}_{60}$, $\text{Eu}@\text{C}_{60}$, $\text{Gd}@\text{C}_{60}$, $\text{Tb}@\text{C}_{60}$, $\text{Ho}@\text{C}_{60}$ show radical character, the most stable being $\text{Ce}@\text{C}_{60}$, $\text{Pr}@\text{C}_{60}$, $\text{Nd}@\text{C}_{60}$, $\text{Tm}@\text{C}_{60}$, $\text{Lu}@\text{C}_{60}$.

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