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Structure and IR spectra of Me@C_{60} (Me = Cu, Ag, Au, Sc, Y, La) endofullerenes according to quantum-chemical calculation data

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Abstract

The results Ib- and IIIb-groups metal endofullerenes Me@C_{60} DFT-simulation are presented. It has been found that the copper subgroup metals are positioned in the center of the carbon cage without forming chemical bonds to carbon atoms, while the scandium subgroup metals are linked to six-membered ring forming a structure with C_s symmetry. With the encapsulation of Cu, Ag and Au atoms in C_{60}, IR spectrum endofullerene consists of four lines, as well as pure C_{60}. The spectra of scandium subgroup metal endofullerenes includes lines forbidden by symmetry for pure fullerene, which makes their experimental determination by IR spectroscopy in mixture with C_{60} possible.