
COMPUTATIONAL SYNTHESIS OF THE C₆₀ HYDRIDES AND FLUORIDES

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The reactions of fullerene C₆₀ with molecular hydrogen and fluorine have been studied using HF SCF semi-empirical calculations (UHF versions of the AM1 technique of the CLUSTER-Z1 codes). The calculations are focused on a sequential addition of either hydrogen or fluorine molecule to the fullerene. Two families of species C₆₀X_{2k} + X₂ (X=H and F, x=0,...,30) have been studied. The preferred binding sites for sequential additions are selected by the largest value of the released electron density (RED) generated by partial exclusion of the molecule odd electrons from covalent bonding [1]. The relevant RED values are determined by using the broken symmetry approach [2] as suggested in [3]. As shown, any other sequential addition causes a remarkable change in the RED distribution over the C₆₀ core atoms. Following these changes and selecting atoms with the largest ERD values, new additions are created. Thus formed adducts are the most energetically stable. Among the other, species C₆₀H₃₆, C₆₀H₄₈, C₆₀F₂₄, C₆₀F₃₆, and C₆₀F₄₈ occurred to be of the highest possible symmetry. The obtained results are in good agreement with experimental data that convincingly exhibits a governing role of the RED values for the considered addition reactions.

The transitional metal atom (cobalt) effect on the formation of the C₆₀F₁₈ adduct is considered. The calculations have been performed using UHF versions of the NDDO-WF technique of the CLUSTER-Z2 codes. From the RED viewpoint, the presence of the metal atom fully blocks atoms of one of the C₁₀ fragments, so that the addition reaction may occur in one half of the C₆₀ core only. Energetically favorable structure of the C₆₀F₁₈ species is suggested.

Литература

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