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Quantum-chemical modeling of the reaction of C_2H_2 molecule intercalated with C_{60}

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Abstract

Reactivity of C_{60} was investigated by DFT/PBE/SBK with respect to acetylene intercalated into fullerite Formation of new chemical compounds between C_{60} and C_2H_2 in the octahedral pore fullerite was predicted. Spectral properties (IR-spectrum and the NMR chemical shifts) of the compounds were calculated.