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Quantum-chemical study of the structure and energy of formation of isomeric structures $C_{60}N_2^q$ and $C_{60}N_2H^q$, q = 0, -1, -2, based on C_{60}

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Abstract

In this paper various intermediates of the fixation of molecular nitrogen in the presence of supramolecular complexes of C_{60} with γ -cyclodextrin under electrolysis were considered. Found structures have a relatively small increase of energy during the addition N₂.