

## 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  $\gamma$ -cyclodextrin under electrolysis were considered. Found structures have a relatively small increase of energy during the addition  $N_2$ .