

Molecular structure of the two IPR isomers 234 (C_s) and 258 (C₁) of a higher fullerene C₁₀₄

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Abstract

An analysis of the molecular structures of two IPR isomers 234 (C_s) and 258 (C₁) of higher fullerene C₁₀₄ was carried out. The distribution of single, double and delocalized in some hexagons π -bonds in molecules of the two isomers are presented for the first time as well as their structural formulas. Quantum chemical calculations (DFT) show that both isomers have closed electronic shells, confirming in general the preliminary bond distribution according to the approach developed by us. Double bonds that connecting pentagons are most short ones in accordance to previously studied higher fullerenes. Some deviations of bond lengths from predicted ones may be connected with large size of C₁₀₄ molecule and, consequently, with a high ratio of the 42 hexagons to the 12 pentagon quantity. This fact determines an appearance of substructures, consisting of significant number of condensed hexagons up to 30. The application of the developed approach in combination with quantum chemical calculations appears to be effective in determining the structure of molecules of higher fullerenes in the researched structures of higher fullerenes with the number of carbon atoms greater than 90 keeping in mind very rare possibility to obtain such information by experimental methods. The features of structures of higher fullerene molecules can be precursory for a synthesis of higher fullerene isomer before experimental works. Correlating the features of electronic structures of fullerene molecules found by us with experimental data of their exohedral derivatives, which disclosed the positions of addends on fullerene cages, would open the way to estimate the most probable positions for different addition reactions in future. An important practical result is that the identified structures of fullerene molecules open a conscious way of chemical modification of fullerene molecules to obtain important derivatives.

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