

The structure and stability of higher fullerenes C₁₀₄: IPR isomers 812 (D₂) and 822 (D_{3d})

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Abstract

An analysis of the molecular structures of two IPR isomers 812 (D₂) and 822 (D_{3d}) of higher fullerene C₁₀₄ is carrying out. The data about the distribution of single bonds, double bonds, and delocalized in hexagon π -bonds in studied isomer molecules are presented for the first time as well as their structural formulas instead of conventional molecular graphs. Quantum chemical calculations (DFT) show that isomer 812 (D₂) have a closed electronic shell, whereas isomer 822 (D_{3d}) contains a pair of equivalent radical substructures, each one consists of three condensed phenalenyls. The calculated energy difference between the two molecules is ca. 25 kcal/mol in favor of 812 (D₂) isomer. It is found that double bonds connecting pentagons in pristine isomer 812 (D₂) are most short ones similarly to previously studied higher fullerenes which is important for understanding the synthesis process of fullerene derivatives. The preliminary bonds distributions according to the developed approach are confirmed in general by DFT calculations. Some differences between calculated bond lengths and predicted ones should be explained in terms of great fullerene size and, consequently, great number of condensed hexagons (compared with constant number of pentagons, which are equal to 12). These bond lengths deviations are belonging to fragments of molecules that similar to nanotubes without pentagons. Our previous analysis of the addend distribution in a series of higher IPR fullerenes up to C₉₀ showed the additions were essentially to hexagons with delocalized π -bonds. We suppose that a similar picture of addends distribution would be in exohedral derivatives of higher fullerene C₁₀₄. The important practical result is that the disclosed structures of fullerene molecules open a conscious way of chemical modification of fullerene molecules to obtain important derivatives.

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