The structures of non-IPR isomers 270 (D_3) and 271 (D_5h) of fullerenes C_{50}

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All empty fullerenes starting with C_{60} and higher ones, which were synthesized so far, satisfy the Isolated Pentagon Rule (IPR). So, the smaller fullerenes Cn (n<60) that do not obey this rule are highly unstable and can`t be obtained as empty molecules. However, they become stable as exohedral or endohedral derivatives. A good example is the successful production and characterization of small non-IPR fullerene C_{50} (isomer 271 (D_5h)) as chlorine exohedral derivative $C_{50}Cl_{10}$. Considering this experimental success, the purpose of our theoretical investigations are identify the causes of stabilization of smaller fullerenes in the form of their derivatives and expand to lower fullerenes the approach developed early by us for higher fullerenes to establish possibility of their production.In this report, we investigated the molecular structures of non-IPR isomers 270 (D_3) and 271 (D_5h) of fullerene C_50, that are the most energetically favourable isomers from possible 271 isomers. Quantum chemical calculations (DFT) show that both isomers have a closed electronic shells. The data about the distributions of single, double and delocalized π-bonds in researched isomer molecules are presented for the first time as well as their molecular formulas.It is found unusual for higher fullerenes chain of π-bonds delocalization passing through some cycles are appeared. It is shown that chlorine atoms in the exohedral derivative $C_{50}Cl_{10}$ of isomer 271 (D_5h) are attached to the indacene substructures, confirming our recent conclusions about preference of π-delocalized hexagons in radical addition reactions. Identified features in the structures of lower fullerene molecules can be predictive of the ability to their synthesis as derivatives and will assist in their structure determination.

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