

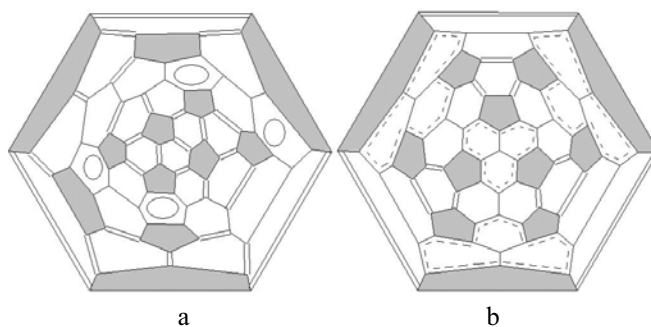
## Electronic structure and stability of C<sub>76</sub> fullerene IPR-isomers

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Only one isomer 1 (D<sub>2</sub>) of two IPR-isomers of fullerene C<sub>76</sub> have been produced and characterized as empty molecule. This isomer also exists as various endohedral metallofullerenes and exohedral derivatives, whereas second isomer 2 (T<sub>d</sub>) have been produced and characterized only as exohedral derivative C<sub>76</sub>(CF<sub>3</sub>)<sub>12</sub> [1]. To clarify instability reason of isomer 2 (T<sub>d</sub>) as empty molecule, the analysis of energy and geometrical parameters of molecules of both C<sub>76</sub> fullerene IPR-isomers has been carried out on the basis of DFT calculations and earlier developed criteria [2].



**Figure.** Schlegel diagrams of isomers 1 (D<sub>2</sub>) (a) and 2 (T<sub>d</sub>) of C<sub>76</sub> fullerene (b).

The distribution of single, double and delocalized pi-bonds in molecules of these isomers are shown (see Fig.). The reason of instability of isomer 2 (T<sub>d</sub>) is presence of four phenalenyl-radical substructures whereas stable isomer 1 (D<sub>2</sub>) have the closed electronic shell. The open-shell electronic structure of isomer 2 (T<sub>d</sub>) is confirmed by the results of quantum-chemical calculations of triplet state which energetically more favorable than the singlet one. Note that addition of trifluoromethyls in C<sub>76</sub>(CF<sub>3</sub>)<sub>12</sub> [1] occurs namely on those four phenalenyl-radical substructures. Thus isomer 2 (T<sub>d</sub>) cannot be obtained as a hollow molecule.

Generally, an instability of fullerenes can be caused not only by the presence of uncoupled electrons in a molecule (an open shell) but also by the strain of a molecule caused by cage distortions [3]. Analysis of geometry structures of isomers 1 (D<sub>2</sub>) and 2 (T<sub>d</sub>) show that local strains in both molecules are small, so instability of isomer 2 (T<sub>d</sub>) is connected only with its radical nature.

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