

Electronic structure and stability of C₇₆ fullerene IPR-isomers

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Only one isomer 1 (D₂) of two IPR-isomers of fullerene C₇₆ have been produced and characterized as empty molecule. This isomer also exists as various endohedral metallofullerenes and exohedral derivatives, whereas second isomer 2 (T_d) have been produced and characterized only as exohedral derivative C₇₆(CF₃)₁₂ [1]. To clarify instability reason of isomer 2 (T_d) as empty molecule, the analysis of energy and geometrical parameters of molecules of both C₇₆ fullerene IPR-isomers has been carried out on the basis of DFT calculations and earlier developed criteria [2].

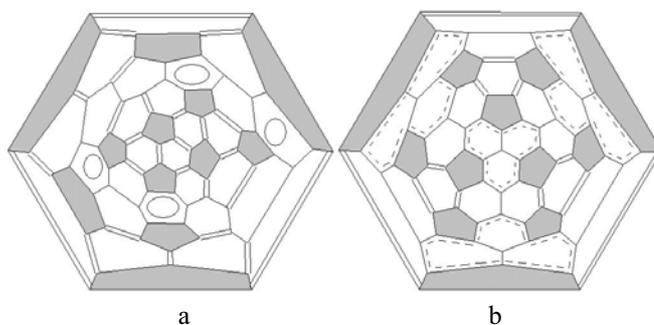


Figure. Schlegel diagrams of isomers 1 (D₂) (a) and 2 (T_d) of C₇₆ fullerene (b).

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_d) is presence of four phenalenyl-radical substructures whereas stable isomer 1 (D₂) have the closed electronic shell. The open-shell electronic structure of isomer 2 (T_d) 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 C₇₆(CF₃)₁₂ [1] occurs namely on those four phenalenyl-radical substructures. Thus isomer 2 (T_d) 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 (D₂) and 2 (T_d) show that local strains in both molecules are small, so instability of isomer 2 (T_d) is connected only with its radical nature.

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- [2] Kovalenko V.I, Semyashova M.V. Abstr.4thWorkshop «Fullerenes and Atomic clusters» (IWFAC'99), St.Petersburg, 234 (1999).
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