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Structure of non-IPR isomer *4169* (C_s) of C_{66} fullerene and the reason of its stabilization as derivatives

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Abstract

In this paper, the analysis of the molecular structure of non-IPR isomer *4169* (C_s) of C_{66} fullerene is carrying out. The data on distribution of single, double and delocalized bonds are presented for the first time. Quantum chemical calculations (DFT) have shown that this isomer has a closed electronic shell. The local strains in the hexagons and pentagons adjacent to the linear combination of three conjugated pentagons are the reasons for its instability.