

On the ^{13}C -NMR chemical shift anisotropy patterns and aromatic character in strained fullerenes: Computational analysis of $\text{D}_{6\text{h}}/\text{D}_{2\text{d}}\text{-C}_{36}$ fullerene

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Abstract

The NMR characterization of small C_{36} hollow fullerene exposes a stable cage with structural features based on its strained curved π -surface in a $\text{D}_{6\text{h}}$ -symmetry. Our results indicate that planar-like aromatic properties of the $\text{D}_{6\text{h}}\text{-C}_{36}$ isomer decrease to a nonaromatic cage for $\text{D}_{2\text{d}}\text{-C}_{36}$ after Stone-Wales transformation of an equatorial [6.6] bond. This is given by the decrease of conjugation in the strained π -surface after Stone-Wales transformation. Calculated nuclear shielding shows that the main shielding component is always oriented perpendicularly to the cage π -surface despite the larger curvature degree, as a result of the sp^2 character of carbon atoms, resembling C_{60} . Moreover, the $\text{D}_{6\text{h}}$ - and $\text{D}_{2\text{d}}\text{-C}_{36}$ cages differ in their charge distribution properties, leading to charge accumulation in the strained cap of the former that leads to a polymerization-prone cage, which contrasts with that expected for the $\text{D}_{2\text{d}}$ structure. Hence, structural rearrangements of these non-Hirsch aromatic fullerenes show that their inherent global behavior requires considering the structural features besides electron counting rules.

Author keywords

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