Quantum Chemical Study of Ethynylfullerenes

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Abstract—DFT PBE0/cc-pVDZ method was applied to calculate the structural parameters of $C_{60}C(CCH)_2$, $C_{60}H_2$, $C_{60}H$(t-Bu), $C_{60}HCCH$, $C_{60}(CCH)_2$ molecules, and of the corresponding carbanions. The length of the carbon-carbon fullerene after the binding with the diethynylcarbene, atoms and/or radicals increases to 1.565, 1.577, 1.587, 1.591, 1.616 Å respectively, but in the relatively stable fulleride anions $C_{60}(t\text{-Bu})^-$ and $C_{60}CCH^-$ this bond has a normal length of 1.525 Å. Acetylenide anions $C_{60}HCC^-$, $C_{60}(CCH)CC^-$, and $C_{60}C(CCH)CC^-$ are weaker as Brønsted bases than the hypothetical dodecahedrane analogs, but stronger than $C_{60}(t\text{-Bu})^-$, $C_{60}CCH^-$, and $C_{60}H^-$ fulleride anions where the charge is localized on the fullerene core.

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