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Instability of molecular structure of non-IPR isomer 17984 (C_1) of the C_{76} fullerene and probable ways of its stabilization

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Abstract

It is well-known that non-IPR fullerenes are highly unstable. For this reason, they cannot be obtained as pristine fullerenes; however, some of them become stable as derivatives (exohedral or endohedral). In this article, we attempted to elucidate in detail molecular structure for such a non-IPR fullerene. Using theoretical approach supported by DFT calculations, the features of molecular structure of isomer 17894 (C_1) of fullerene C_{76} with data about distribution of single, double and delocalized π-bonds as well its structural formula has been determined for the first time. The instability of the studied fullerene molecule caused by its open-shell structure and significant local overstrains related to the high folding angle value of pentagons in pentalene fragment. The supposed synthesis of the endohedral molecule starts with the ionic pair formation, i.e. anionic fragment of fullerene cage and metal cation electrostatically bound with it. It would lead to closing of open electron shell of fullerene and local overstrain release at pentalene fragment. As to the exohedral derivatives the probable positions of addends are discussed. Both methods in their own demonstrate the possibilities to stabilize the molecule of the C_{76} isomer 17894. The elucidation and analysis of structural features along with electronic characteristics of non-IPR fullerene molecules appear to be useful for predicting the possibility of their synthesis as derivatives and will assist in determination of their reactivity. This will ensure the targeted production of fullerenes and their derivatives for the needs of medicine, electronics and other industries. The fundamental knowledge of the properties of nanoobjects, namely fullerenes, is actually developing as the independent direction with a long-term perspective.

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