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Phenalenyl like substructures in fullerene molecules

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In our research we are developing an alternative approach in which a fullerene molecule is considered to contain a number of substructures incorporated in the fullerene shell and resembling aromatic analogues such as indacene, pyrene, perylene, corannulene, coronene, phenalenyl radical, etc. Our result shows that the presence of phenalenyl-radical substructures with unpaired electron leads to instability of whole fullerene molecule. For example, fullerene C_{74} is unstable due to the presence of two phenalenyl-radical substructures, four such radical substructures caused of instability of fullerene C_{76} too. Here we report the computational characterizations of non-planar polycyclic hydrocarbon species that can be cut from fullerene molecule – substructure from three symmetrically fused phenalenyl composed by nine fused benzenoid rings. The results of quantum-chemical calculations show that this structure has an open-shell ground state and a relatively small HOMO–LUMO gap. This is due to the fact that this molecule is derivative of the phenalenyl-radical. Analysis of row of isolated-pentagon-rule (IPR) isomers of higher fullerenes from C_{72} to C_{104} shows that this substructure is present in structure of some of them, for example, in IPR isomer 7 (C_{3v}) of C_{82} fullerene. Indeed, our researches show that this molecule has an open-shell structure due to containing radical substructures (like phenalenyl-radical substructure). It should be noted that spin densities in triplet configuration of isomer 7 (C_3) of C_{82} fullerene are mainly concentrated namely on radical substructures likewise the C_{74} biradical. Thus, our results shows that such fullerenes are unstable and can`t be obtained as empty molecules. However they become stable as exohedral or endohedral derivatives or in polymeric forms.

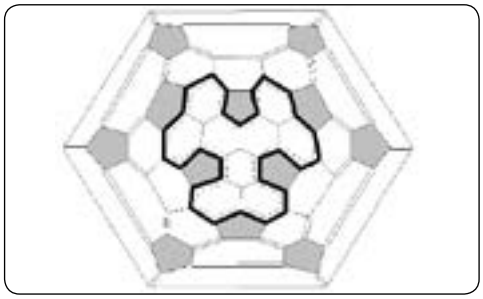

Figure 1: Schlegel diagram of isomer 7 (C_{3v}) of C_{82} fullerene with depicted phenalenyl-like substructure.

Recent Publications

1. Kovalenko V I and Khamatgalimov A R (2003) Open-shell fullerene C_{74}: Phenalenyl-radical substructures. Chem. Phys. Lett. 377:263-268.
2. Khamatgalimov A R and Kovalenko V I (2015) Stability of isolated-pentagon-rule isomers of fullerene C_{76}. Fuller. Nanotub. Car. Nanostruct. 23:148-152.
3. Khamatgalimov A R and Kovalenko V I (2016) Structures of unstable isolated-pentagon-rule fullerenes C_{72}-C_{86} molecules. Russ. Chem. Rev. 85:836-853.
4. Khamatgalimov A R and Kovalenko V I (2017) Stabilization of higher IPR fullerenes C_{74} (D_{3h}) and C_{76} (T_d) with open shell in radical addition reactions. Fuller. Nanotub. Car. Nanostruct. 25:128-132.
5. Khamatgalimov A R and Kovalenko V I (2018) Radical IPR fullerenes C_{74} (D_{3h}) and C_{76} (Td): dimer, trimer, etc. Experiments and theory. J. Phys. Chem. C. 122:3146-3151.

Biography

Ayrat R Khamatgalimov has completed his PhD from Kazan National Research Technological University, Russia and Postdoctoral studies from Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center of RAS, Russia. He is the Senior Researcher of Laboratory of Physical-Chemical Analysis in Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center of RAS, Russia. He is engaged in research in the field of physical chemistry and quantum-chemical calculations; in particular, he has expertise in calculations of electronic and geometric structures of higher fullerenes. He is an expert in the field of synchronic thermal analysis. The results of his research were published in more than 40 papers in reputed journals.

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