

IONIZATION POTENTIALS AND OXYDATIVE PROPERTIES OF SEVERAL NANOSTRUCTURES

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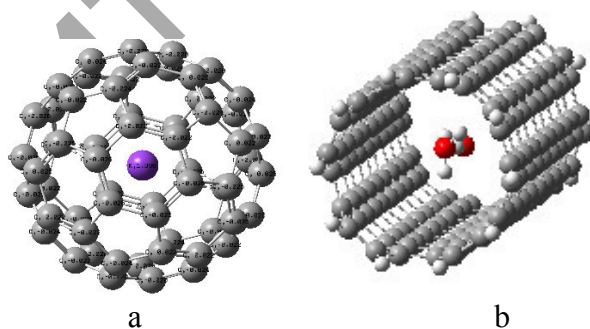
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Ab-initio investigations of the several known nanoclusters, for example fullerenes, show that their ionization potentials and electron affinity values more than analogous parameters for organic oxidized molecules.

The values of adiabatic ionization potentials (IP-a) and electron affinity (EA) molecules, obtained by ROHF 3-21G method of quantum-chemical program package “Gaussian-2016” [1].

Molecules	IP-a, eV	EA, eV
Benzene	-8.027353971	-3.005932115
Naphtalene	-7.330990079	-2.120812238
Anthracene	-7.055584196	-2.284038300
Phenanthrene	-7.057676768	-2.052421324
Pyrene	-6.960387135	-1.703008053
Benzopyrene	-6.257701988	-0.881764686
Coronene	-6.075547538	-0.746210101
Fullerene-60	-7.859888342	0.938329439
Fullerene-70	-7.760024491	1.136029877

From calculated data presented in table it can be seen that one-electron adding to fullerenes molecules are the exothermic process.



Pictures: a – complex C-60 with potassium atom; b – complex nanotube (5.5) with linear waters dimer, calculated by ab-initio ROHF 3-21G method.

Quantum-chemical investigation of complex fullerene-60 with potassium atom located in center of nanocluster has shown that molecule spherical electric field polarize alkali metal to value $qK = +1.395$.

Distribution of bimolecular linear waters complex, with quantum-chemical optimized hydrogen bonds structure, inside of nanotube (5.5) gave the monomolecular dissociation of dimer in cylinder electric carbon-tubes field.

References

1. Foresman J.B., Frisch A.E., Exploring Chemistry with Electronic Structure Methods, Gaussian, Inc., 3d Edition, Wallingford, CT USA, 2015, p. 87.