COMPUTATIONAL SYNTHESIS OF THE FULLERENE C_{60} STAR-LIKE ADDUCTS WITH A PRIMARY AMINE

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The reaction of fullerene C_{60} with a primary amine NH_2-$(CH_2)_2$-CH(*pyrr*)-CH_3 (here *pyrr* is pyrrolydone heterocycle) (**I**) has been studied using HF SCF semi-empirical calculations (UHF versions of the AM1 technique of the CLUSTER-Z1 codes). The calculations are focused on a sequential addition of the amine to the C_{60} molecule. The preferred binding sites for sequential steps are selected by the largest value of the released electron density (RED) generated by partial exclusion of the molecule odd electrons from covalent bonding [1]. The relevant RED values are determined by using the broken symmetry approach [2] as suggested in [3].

Monoadduct C_{60}-$\mathbf{I}_1$ is formed in due course of a donor-acceptor reaction between molecular ions C_{60}^- and $\mathbf{I}^+$. The preferred binding site on the fullerene ion has been selected by the largest RED value for the ion in the doublet ground state. The $\mathbf{I}^+$ addition to C_{60}^- occurs dissociatively via two chemical bonds C_f-N and C_f-H. Due to lowering the formed adduct ionization potential with respect to that of amine, the adduct losses a possibility to form a charge-transfer complex with **I**. The next adduct C_{60}-$\mathbf{I}_2$ is formed by interaction of neutral molecules C_{60}-$\mathbf{I}_1$ and **I**. As previously, **I** attaches the adduct core dissociatively at the core site, which characterized by the RED largest values related to C_{60}-$\mathbf{I}_1$. Further addition leads to adducts C_{60}-$\mathbf{I}_3$ and C_{60}-$\mathbf{I}_4$, which are subordinated to similar rules. Addition in the other two adducts C_{60}-$\mathbf{I}_5$ and C_{60}-$\mathbf{I}_6$ occurs associatively via a single chemical bond C_f-N. As occurred, central C_f - C_f bonds of six naphthalene-core fragments C_{10}, which form the fullerene structure $C_{60}\equiv 6^*$ C_{10}, are the binding sites for the above six addends in turn that forms a pseudo-octahedral configuration of the obtained C_{60}-**I** star [4].

Литература

1. *Noodleman L.* J.Chem.Phys. 1981. V. 74. P.5737- 5743.
2. *Sheka E.F.* CEJP, 2004, V. 2. P,160-182.
3. *E.F.Sheka.* This School, Paper 976.
4. *Hirsh A., Vostrowski O.,* Eur. J.Org.Chem. 2001. P. 829-848.