INFLUENSES OF ADDENDS ON ELECTRONIC AND MOLECULAR STRUCTURE OF THE FULLERENES

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X-ray data substituted fullerenes reveal significant diversity of bond lengths with the structure of fullerene core and the bonds of the same type included in the same molecule. Thus it is not clear in what degree the distinction of bonds lengths are caused by effects of crystal field, by presence of solvated molecules, by intrinsic error of an method or caused by addend's electronic properties. In the present study the conformations and molecular structure of the fullerene C®, pyrrolidmofullerenes $C6_2H_4NR$ and mcthanofullerenes GnXY containing symmetric and asymmetric addends were investigated by the density functional theory with the program PRIRODA and Perdew-Burke-Ernzerhof exchange-correlation functional (DFT/PBE/TZ2P).

We studied the compounds $C6]H_2$, G51H (COOMe), Cei $(COOMe)_2$, C«i **(COOEO2,** Cei (COOMe) [P (O) $(OMe)_2$], C_6iH [P (S) $(OMe)_2$], Cei [P (S) $(OMe)_2$]i, CsiH [P (0) $(OMe)_2$], $C_{6]}$[P(0)(0Me) $_2]_2$, C_6i(H)CN, C« (COOMe)CN, C_6, $(CN)_2$and $C_{62}H_4NR$ and found the next conclusion.

Electronic effects of the substitutes, what are not forming short contacts and are not overlapping with atoms of fullerene's core,

do not derivate the geometrical non-equivalence of fragments and are mainly mediated through bonds. The asymmetry of fullerene cores of compounds C61HX and **C6iCN**(C00Me) is small. Average values of bond lengths investigated compounds also are determined by interactions through bonds. Length of double bonds for separate fragments and average values of lengths of the same type double bonds of methanofullerenes C61XY are changing monotonously and alternate in two conjugated branches. Alternation and attenuation of change of bond lengths of in the connected branches cisl-**cis2**-eq2-

tr3 and cisl-cis3-tr4-tr2-trl is established. The lengths of 1,2 bonds have the greatest changes. It is maximal for X = H (1,6469 A^D) and minimal for X = CN (1,5669 A°). Calculations at level HF/6-31G gives similar results 1,5952 A° and 1,5445 A^0, accordingly.

Asymmetric addends C_6iXY (X, Y = COOMe, COOEt, P(0)(0Me):, P(S)(OMe); polarize and divide fullerene core on two or four nonequivalent fragments. The most stable conformations of pyrrolidine and methano fullerenes are characterized by through space interaction of nitrogen lone pairs, phosphory 1, carbony 1 or ester oxygen atoms of with one of carbon atoms of fullerene core and polarization of the appropriate fragment. It creates asymmetry of lengths of bonds and charges on carbon atoms of fullerene core. Asymmetry of lengths of bonds and atomic charges is a consequence of interaction of addend atoms with fullerene core through space and has conformational pecularities.

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