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The study of the effect of changing the substituted on electron and orbital properties of the drug 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol on nano structure fullerene using Hartree- fock method

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Abstract

In this research work at The first compounds [C60- 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65-2X]$^{+}$ (X=F,Cl,Br) were optimized. Then the calculation of natural bond orbitals was performed with the NBO technique. All calculations using Hartree- fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results showed that the energy levels of molecular orbital (HOMO & LUMO) in the RF has the lowest value. C65-X has a length of the shortest bond and the bond has most power. Comparison of the dipole moments of compounds shows this trend: RF> R-Cl> R-Br. Both ratio Core / charge and the valence / charge for carbon atoms 31, 55, 65 and 63 in the RF has the highest value.

Keywords: Bond lenhgt , Dipole moment , fullerene , 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol