## عنوان مقاله:

Theoretical study of chemical properties of Fulleromethyldopa and derivatives

## محل انتشار:

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## خلاصه مقاله:

In recent years, many studies have been done on structure of fullerene derivatives asmedicine nano-carrier compounds. In this work mechanical quantum calculations in theorylevel of B3lyp/6-31g* and HF/6-31G in the gas phase were performed on structural ofmethyl dopa (MD) and fulleromethyle dopa (FMD) with different halogen substitutions. Inthe other hand some different properties such as HOMO and LUMO levels, Chemicalhardness, Energy gap, Conductivity, ΔNmax and Dipole moment value were studied. Alsothe activity of chemical sites such as acid and base site and the hydrogens of benzene ringwere investigated. The result showed that the value of energy gap and chemical hardnessdecreased by linking structure of methyl dopa to fullerene (C60) and the value of Chemicalpotential, ΔNmax and Dipole moment were increased in fullerene methyl dopa (FMD).However, after binding of methyldopa to fullerene, acidic sites, it is more acidic than beforelink. And the activities of the alkali site are reduced. These structures showed that change insubstitution (X=F, Cl, Br and H) changed values of these parameters. These changes showdependency of the results on power of electro negativity and atomic radius of .substitution X.Finally, the data were compared and discussed

## کلمات کلیدی:

,DFT, Electrophilicity, Chemical hardness; Chemical potential