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Research note

The chemical shielding and magnetizability relationship in potassium-doped (5,0) zigzag SWCNT nanotube

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Abstract

In this study, the relationship between daimagnetic shielding (σ_d), paramagnetic shielding ($\sigma_p+\sigma'_p$) and ^{13}C isotropic shielding tensors $^{13}C(\sigma_{iso})$ with Mulliken, NBO and QTAIM atomic charges and also, the relationship between chemical shielding and magnetizability in the (5,0) zigzag Single Walled Carbon Nanotube (SWCNT) as doped by potassium and without it are investigated using the Density Functional Theory (DFT), based on Periodic Boundary Condition (PBC) approach, at the PBEPBE/6-31G(d) level of calculation. The doped (5,0) zigzag SWCNT with potassium is converted to the n-type more stable carbon nanotube.There are linear relationships between mulliken, NBO and QTAIM atomic charges and ^{13}C isotropic chemical shielding (σ_{iso}), as well as with dia-magnetic shielding (σ_d) in the SWCNT with and without potassium doping. The relationships are nonlinear between the total para-magnetic shielding ($\sigma_p+\sigma'_p$) and all charges in the potassium doped SWCNT. In both potassium doped and without potassium SWCNT structures, there are strong linear correlations between the total-atomic magnetizability (χ (Ω)) and ^{13}C isotropic chemical shielding (σ_{iso}).

Keywords: (5,0) zigzag single walled carbon nanotube, potassium doping, magnetic shielding, mulliken, nbo, qtaim charge, magnetizability

For full article, refer to the Persian section