Study of Electronic Structure, Optoelectronics, Linear and Nonlinear Optical Properties and chemical descriptors of 4, 5-dibromo-2, 7dinitro- fluorescein and 2,7-dibromo-4,7-dinitro- fluorescein in Gas Phase and Solvent media Using Ab Initio and DFT Methods

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Abstract

In this work, we have studied the electronic structure, optoelectronics, linear and nonlinear optical properties of 4, 5-dibromo-2, 7dinitro- fluorescein and 2,7-dibromo-4,7-dinitro- fluorescein *in the gas phase and some solvents media using RHF and B3LYP levels of theory with a cc-pVDZ basis set. Our results suggest that solvent media have an effect on certain properties while some are unaffected. We have also determined the energy band gap and some other parameters like ionization potential, electron affinity, and molar refractivity. Finally, we have calculated the reactivity descriptors through some parameters including chemical hardness (*η*), chemical potential* (μ)*, electrophilicity index*(ω)*, softness* (ϑ)*, electronegativity (EN), Fermi energy (E_F), Electro accepting power* (ω^+)*, electron-donating power* (ω^-) *and net electrophilicity* $\Delta\omega^{+}_{-}$ *, the reflectivity* (R)*, optical frequency* ω_{op}*, Max of Electron charge* (ΔE_{MAX})*, Energy change* (ΔE) *and total Energy minimum* (ΔE_{MIN}) *of the compounds. Due to the large* $\langle\alpha\rangle$, β, γ, *E, P,* χ, $\mathcal{E}$, *n, and D of these molecules, we think that these molecules have potential applications in the field of optoelectronics, such as optical communication, optical computing, optical switching, and dynamic image processing.*

Keywords: *electronic structure; chemical reactivity; optoelectronic properties; optical limiting applications*.