First-principles calculations study of electronic structure, optoelectronic, vibrational analysis, linear and nonlinear optical properties of eosin b (4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate)

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A. A. Waheed and P. D. Gupta used eosin b dye to do the Estimation of Protein. Eosin B (4',5'-dibromo-2',7'-dinitrofluorescein is a red dye which is unconditionally soluble in water with green fluorescence (λmax 514 nm). This biological stain is used as a counterstain for collagen following Mayer's Hemalum or with azure A to stain cell granules, nuclei, and microorganisms and for differential staining of cells of the anterior pituitary [1]. W. C. HOLMES, C. G. MELIN and A. R. PETERSO have prepared it in a fairly pure state and have determined absorption spectra of the two known isomeric dibromodinitrofluoresceins to obtain criteria for the identification of the dye, to secure further information on the character of market supplies, and to determine the relative reliability of different methods for evaluating dye content [2]. The aims of this research are to investigate the electronic structure, thermodynamics, linear and nonlinear optical and optoelectronic properties of the title molecule and to compare the performance of the RHF and different DFT methods in the predicted properties above.

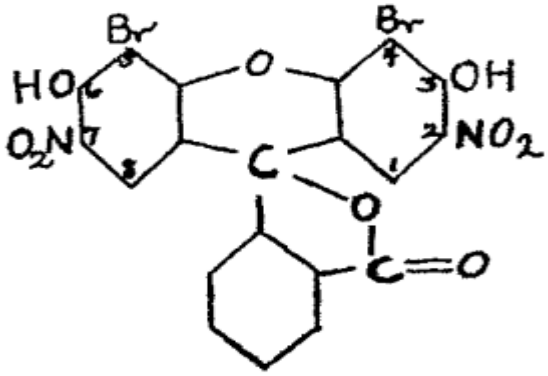

Fig1: 4', 5'-dibromo-2', 7'-dinitrofluorescein

The properties above were done using ab initio Hartree Fock method at the RHF level and different DFT Methods such as PBE1PBE, mPW1PW91, B3PW91 and B3LYP with the cc-pVDZ basis set with the help of Gaussian 09 [3] suit of program, which is one of the most used

computational chemistry software. We have firstly modeled and optimized the geometry of the structure and further, we have computed the frequencies analysis to show the value of dipole moment (μ), Zero-point vibrational energy (ZPVE), total electronic energy (Eelec), Gibbs free energy(G), Enthalpy(H), molar heat capacity at constant volume (Cv) and Entropy(S) and calculated the value of average polarizability (<α>), polarizability anisotropy (Δα), hyperpolarizability (βmol), electric susceptibility (χ), linear refractive index (η), dielectric constant (ε). As far as this analysis are concerned, we have also been able to come out successfully with a well calculated chemical reactivity and stability of the molecule through the frontier molecular orbitals defined by the higher occupied and lower unoccupied molecular orbitals (E_{HOMO} and E_{LUMO}).

Our results insinuate that this molecule has a potential application in linear and nonlinear optical materials, and optoelectronic devices due to his large hyperpolarizability and can be a promising compound for optical limiting applications.

Presently, no experimental values in literature were obtained for the above properties that we have calculated and theoretical values are not available, we are hopeful that our final results will provide significant information for further studies of this compound for application as NLO materials and optoelectronic devices.

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