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DFT Comparative Studies of Substituted Quinoxaline

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ABSTRACT

Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) were treated according to Becke's three Lee–Yang–Parr (B3LYP) correlation potential due to its less error value than other functionals. This molecule has biological studies are useful for fields, due to its thermal stability and less energy bang gap of probe has luminescence applications.

1. Introduction

Both DFT and TDDFT theories are used in analyzing the energies, electronic structure in excited state with excited and emission wavelength, also useful in the analyzing of atomic charge distribution, optical spectral determinations and photochemical properties [1-6]. The structural, optical and charge distribution can be helpful for knowing the nature of the probe. Besides biological activities quinoxaline derivatives were helpful in industrial applications due to its thermal stability and less energy bang gap of molecule indicates good luminescence behavior and it can be consider for display applications like photovoltaics. Quinoxaline based molecules containing polymers used in optical components and used in quantum dot light emitting diodes (QLEDs) as transport layers. Quinoxalines shows good results against fungal infection and various chronic and metabolic disease treatments [7-9].

2. Methods

The molecule was drawn with the help of Gauss view 5.0 and calculations were done using density functional theory (DFT), time dependent density functional theory (TDDFT) with a basis set of 6-311G(d,p) with a functional of B3LYP, using Gaussian 09 software.

3. Results and Discussion

The optimized structure of 2Cl5,6Dm3MsQ molecule is shown in Figure 1. The bond length between the carbon and sulfur atoms shows higher value than carbon-carbon (C-C) and carbon-hydrogen (C-H), the lesser bond length between 7H-5C shows 1.0827Å and higher value of bond length 1.8338 Å between carbon and sulphur (15C-13S). The bond angle at 9C-4C-3C (90.178^0) and higher angle at 14Cl-9C-4C (148.075^0) between atom [10]. Mulliken charge on each atom of molecule in which the atoms, the lesser charge in 15C (-0.453) in vacuum, 15C (-0.452) in hexane and 15C (-0.451) in octanol are observed. Theses computational charges are higher in 16H in vacuum and solvents. The atomic charge of sulfur atom (13S) also increases with solvent polarity like carbon, hydrogen, nitrogen and chlorine atoms but in the case of nitrogen atoms its vice versa [10-12]. These variations are indicates the nature of the molecule in the different conditions. Energy band gap (E_g) between HOMO and LUMO in vacuum medium is 6.273 eV, energy gap between HOMO-1 to LUMO+1 and HOMO+2 to LUMO-2 in vacuum are varies [13], these orbitals are indicates π-bonding symmetry and the π* antibonding symmetry. FMO used to identify the donor and acceptor group and the charge transfer between them by π-conjugate. HOMO is the electron-donating group which associated with ionization potential and LUMO is electron-accepting group associated with electron affinity of the molecule.

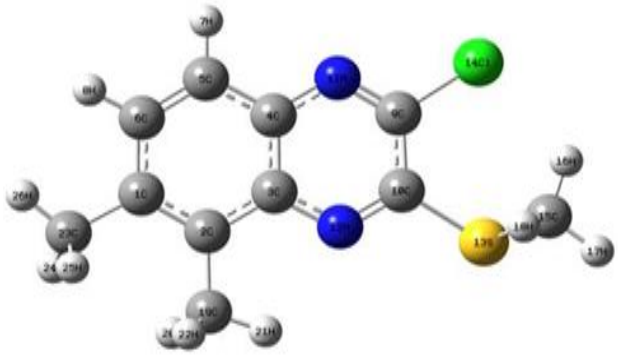

Figure 1. Optimized molecular structure of 2Cl5, 6Dm3MsQ

4. Conclusions

The energy band gap of molecule increases with solvent polarity. The optoelectronic developments may directly depends on polarity of the medium. These studies helps in recognizing of other molecular factors and nucliophilic

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atomic positions with the help of color code and stability of the probe, hence the molecule useful in optoelectronic fields.

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