2-2’Dihydroxye-azobenzene Dye Sensitizer Solar Cell DFT calculations

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***Abstract*—The geometries, electronic structures, Polarizability, and hyperpolarizability of organic dye sensitizer 2-2 Dihydroxye azobenzene were find out, based on ab initio HF and Density Functional Theory (DFT) using the hybrid functional B3LYP. Ultraviolet-visible (UV-Vis) spectrum was analysed by Time Dependent DFT (TDDFT). The intermolecular contacts have been studied using natural bond orbital and natural localized molecular orbital analysis. The main non-liner properties such as electric dipole moment and Polarizability and hyperpolarizability of 2-2 Dihydroxye azobenzene have been determined using B3LP quantum chemical calculations. Finally, the HOMO-LUMO energy gap and Mulliken population analysis on atomic charges and Global local reactivity descriptors of the title compound have been deliberated.**

***Index Terms*—Dye sensitizer, Density functional theory, electronic structure, Absorption spectrum, Natural localized molecular orbital.**

I. INTRODUCTION

Dye Sensitized Solar Cells (DSSCs) have merged as a potential low-cost alternative energy solution, related to the silicon-based p-n junction solar cell [1-2]. In the particular case, there are four factors that can affect the production of the DSSCs; there are photosensitive dyes, electrodes (anode and cathode) and electrolyte. Two general classes of dyes exist: metal-based and metal-free. Metal-free dyes are powerful because of their high molar extinction coefficients, in this case of developed and engineering; lower cost and environmental impact, and increased presentation in DSSC [3-4]. The thing, metal-free sensitizers belong to a class of dyes frequently used to as 2,2 Dihydroye azobenzene, and consist of the 2,2 Dihydroye azobenzene which also serves to chemically bind the dye to the surface of the TiO2. [5-8] The molecule 2,2 Dihydroye azobenzene dye exhibit several comforts over the coordination complex: high molar coefficient, low cost making and an extraordinary multiplicity. The metal-free organic dye sensitizers, such as cyanines, hemicyanines triphenylamine [9-10] propylene’s, Comorians, phorphyrins and idolize-based dyes have been expanded and acceptable performance. Hence, the current study we have chosen the effective of 2,2 Dihydroye azobenzene dye shown Fig. 1, Based on the theoretical calculate geometric, electronic structure and absorption properties of the molecule systems.

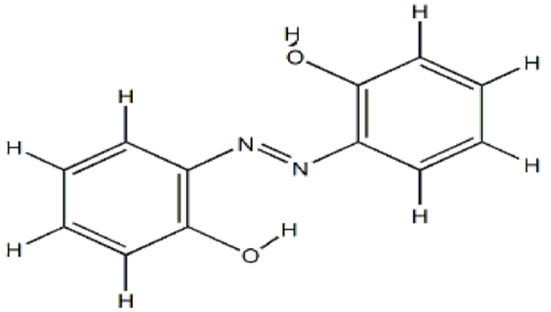


Fig.1. Chemical structure of the 2,2 Dihydroye azobenzene

II. COMPUTATIONAL METHODS

The Geometries, Electronic structure, Dipole moments, Polarizability, Hyperpolarizability and Electronic absorption spectra for description of the organic (accepter changes) dyes properties were find out theoretically by using Density functional theory with Gaussian09w package [11]. The DFT calculations were established on hybrid functions Becke’s three parameter the Lee-Yang-Parr (B3LYP).

The electronic absorption spectrum need calculation of the allow excitations and oscillator strengths. These calculations were done using Time Dependent-Density Functional Theory with the same basis sets and exchange – correlation functional in vacuum and solution and the non-equilibrium version of the polarisable continuum model (PCM) was adopted for determined the solvent effects.

III. RESULT AND DISCUSSION

3.1. Molecular structure geometry

The optimized molecular structure of 2,2 Dihydroye azobenzene of secured from Gaussian03 is shown in Fig.2.The title compound parameters like bond lengths, bond angles, and dihedral angels of 2,2 Dihydroye azobenzene are given Table 1,using both the methods namely B3LYP/6-311+G(d,p) and HF/6-311+G(d,p)[12-14].All bond lengths ranges from 1.7211 to 0.9646 A' and the calculated bond length of C_4-016 in both the DFT values in 1.34A' and HF values is 1.35 A' as listed in Table 1.

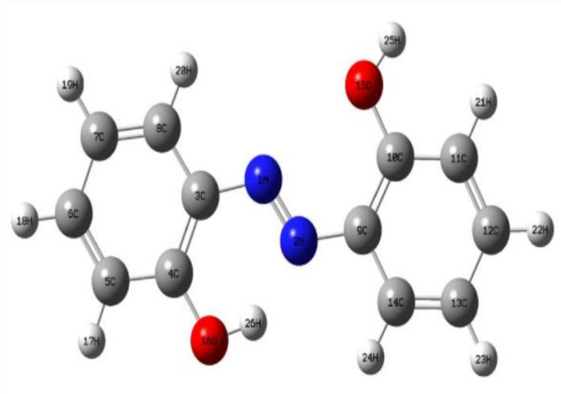


Fig .2 The geometrical structure of 2,2 Dihydroye azobenzene

Table 1. Bond lengths (in Angstrom), Bond angles (in degree) and Dihedral angles (in degree) of the 2,2 Dihydroye azobenzene.

S.No	Bond lengths(Å) Bond angles (in degree) and Dihedral angles (in degree)	B3LYP/6-311+G(d,p)	HF/6-311+G(d,p)
Bon d Lengths (Å)			
1	N1-N2	1.2663	1.2396
2	N1-C3	1.3967	1.4126
3	N2-C9	1.4067	1.4211
4	N2-26	1.7211	1.9163
5	C3-C4	1.4238	1.3981
6	C3-C8	1.4077	1.3935
7	C4-C5	1.3996	1.3884
8	C4-O16	1.3418	1.3582
9	C5-C6	1.3873	1.3802
10	C5-H17	1.0835	1.0685
11	C6-C7	1.4021	1.3937
12	C6-H18	1.0845	1.0707
13	C7-C8	1.3828	1.3776
14	C7-H19	1.083	1.0692
15	C8-H20	1.0836	1.0692
16	C9-C10	1.4185	1.3934
17	C9-C14	1.4056	1.3875
18	C10-C11	1.3983	1.386
19	C10-O15	1.3572	1.3705
20	C11-C12	1.3898	1.385

21	C11-H21	1.0868	1.072
22	C12-C13	1.3946	1.3856
23	C12-H22	1.0838	1.0702
24	C13-C14	1.3859	1.3839
25	C13-H23	1.0829	1.0693
26	C14-H24	1.0837	1.0697
27	O15-H25	0.9646	0.9458
28	O16-H26	0.9921	0.9534
Bond a ngles (in degree)			
1	N2-N1-C3	115.9875	118.5229
2	N1-N2-C9	118.7443	118.2048
3	N1-C3-C4	125.5077	125.5802
4	N1-C3-C8	115.3715	114.92
5	C4-C3-C8	119.1208	119.4998
6	C3-C4-C5	119.1272	119.4375
7	C3-C4-O16	122.0135	123.2353
8	C5-C4-O16	118.8593	117.3272
9	C4-C5-C6	120.4114	120.2843
10	C4-C5-H17	118.0989	117.8761
11	C6-C5-H17	121.4897	121.8396
12	C5-C6-C7	120.9789	120.7509
13	C5-C6-H18	119.2165	119.3586
14	C7-C6-H18	119.8046	119.8905
15	C6-C7-C8	119.1661	118.9608
16	C6-C7-H19	120.3774	120.5467
17	C8-C7-H19	120.4565	120.4924
18	C3-C8-C7	121.1956	121.0665
19	C3-C8-H20	117.119	117.2915
20	C7-C8-H20	121.6854	121.6418
21	N2-C9-C10	127.7377	124.8048
22	N2-C9-C14	114.0825	116.0126
23	C10-C9-C14	118.1798	119.1057
24	C9-C10-C11	119.0204	119.6188
25	C9-C10-O15	120.2967	119.0746
26	C11-C10-O15	120.6829	121.2721
27	C10-C11-C12	121.5176	120.6737
28	C10-C11-H21	118.5871	119.1963
29	C12-C11-H21	119.8953	120.1294
30	C11-C12-C13	119.9672	120.047
31	C11-C12-H22	119.5149	119.554
32	C13-C12-H22	120.5179	120.3966

33	C12-C13-C14	118.9985	119.1694
34	C12-C13-H23	120.6869	120.6337
35	C14-C13-H23	120.3146	120.1957
36	C9-C14-C13	122.3166	121.347
37	C9-C14-H24	117.1385	117.914
38	C13-C14-H24	120.5449	120.7373
39	C10-O15-H25	108.7338	114.0972
40	C4-O16-H26	106.1538	112.4442
Dihedral angles (in degree)			
1	C3-N1-N2-C9	-180.008	179.954
2	N2-N1-C3-C4	0.0075	-0.9172
3	C2-N1-C3-C8	-179.993	179.0896
4	N1-N2-C9-10	0.0288	-41.178
5	N1-N2-C9-C14	-179.976	142.0526
6	N1-C3-C4-C5	180.0002	179.9121
7	N1-C3-C4-O16	0.0015	-0.1619
8	C8-C3-C4-C5	0.0006	-0.095
9	C8-C3-C4-O16	180.0019	179.8311
10	N1-C3-C8-C7	-180	-179.852
11	N1-C3-C8-20	0.0001	0.2783
12	C4-C3-C8-C7	-0.0007	0.1542
13	C4-C3-C8-H20	179.9997	-179.715
14	C3-C4-C5-C6	-0.0002	-0.0254
15	C3-C4-C5-H17	-180	179.9681
16	O16-C4-C5-C6	-180.001	-179.956
17	O16-C4-C5-H17	-0.0011	0.0378
18	C3-C4-O16-H26	0.0013	-0.5144
19	C5-C4-O16-H26	180.0026	179.413
20	C4-C5-C6-C7	-0.0002	0.0905
21	C4-C5-C6-H18	180	-179.972
22	H17-C5-C6-C7	-180.001	-179.903
23	H17-C5-C6-H18	-0.0002	0.035
24	C5-C6-C7-C8	0.0002	-0.0329
25	C5-C6-C7-H19	180	179.8911
26	H18-C6-C7-C8	179.9999	-179.97
27	H18-C6-C7-H19	-0.0002	-0.0464
28	C6-C7-C8-C3	0.0003	-0.0901
29	C6-C7-C8-H20	-180	179.7738
30	H19-C7-C8-C3	-180	179.9859
31	H19-C7-C8-H20	0	-0.1502
32	N2-C9-C10-C11	179.9968	-178.521

33	N2-C9-C10-O15	-0.0004	-0.6304
34	C14-C9-C10-C11	0.0015	-1.8437
35	C14-C9-C10-O15	-179.996	176.0466
36	N2-C9-C14-C13	-179.998	179.3192
37	N2-C9-C14-H24	0.0024	-1.1365
38	C10-C9-C14-C13	-0.0023	2.355
39	C10-C9-C14-H24	179.9984	-178.101
40	C9-C10-C11-C12	0.0001	0.3049
41	C9-C10-C11-H21	-180	-179.954
42	O15-C10-C11-C12	179.9972	-177.538
43	O15-C10-C11-H21	-0.0025	2.2031
44	C9-C10-O15-H25	179.9896	-174.24
45	C11-C10-O15-H25	-0.0076	3.6146
46	C10-C11-C12-C13	-0.0009	0.7839
47	C10-C11-C12-H22	179.9997	-179.786
48	H21-C11-C12-C13	179.9989	-178.955
49	H21-C11-C12-H22	-0.0006	0.4754
50	C11-C12-C13-C14	0.0001	-0.3049
51	C11-C12-C13-H23	-179.999	179.2897
52	H22-C12-C13-C14	179.9995	-179.73
53	H22-C12-C13-23	0	-0.1354
54	C12-C13-C14-C9	0.0015	-1.2794
55	C12-C13-C14-H24	-179.999	179.1891
56	H23-C13-C14-C9	-179.999	179.1242
57	H23-C13-C14-H24	0.0003	-0.4073

3.2. Polarizability and Hyperpolarizability

Polarizability and Hyperpolarizability collection are notable parameters to recognize about the sensitizing property of the designed dye sensitizer in the external field. These parameters contribute in the non-linearity of the denoted dye architecture unit [15-17]. The optimized molecule with highest Polarizability and Hyperpolarizability exhibits good sensitizing characteristic upon photo excitation because it trends to decrease the total formation on the surface of TiO_2 leads to better conversion efficiency [18-20]. The Polarizability and Hyperpolarizability of the selected dyes sensitizer can be obtained by using the following mathematical formula.

$$\alpha = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right)$$

$$\Delta\alpha = \frac{1}{\sqrt{2}}\left[\left(\alpha_{xx} - \alpha_{yy}\right)^2 + \left(\alpha_{yy} - \alpha_{zz}\right)^2 + \left(\alpha_{zz} - \alpha_{xx}\right)^2 + 6\alpha_{xz}^2 + 6\alpha_{xy}^2 + 6\alpha_{yz}^2\right]^{1/2}$$

The average Hyperpolarizability is calculated by using following mathematical derivation.

$$\beta = \left(\beta_x + \beta_y + \beta_z\right)^{1/2}$$

$$\beta_x = \left(\beta_{xxx} + \beta_{xyy} + \beta_{xzz}\right)^2$$

$$\beta_y = \left(\beta_{yyy} + \beta_{xxy} + \beta_{yzz}\right)^2$$

$$\beta_z = \left(\beta_{zzz} + \beta_{xxz} + \beta_{yyz}\right)^2$$

Where, α_{XX}, α_{YY}, and α_{ZZ} are tensor components of Polarizability; β_{iiZ}, β_{iZi}, and β_{Zii} (i from X to Z) are tensor components of Hyperpolarizability.

Table 2 and 3 the Polarizability and Hyperpolarizability of choose organic dyes was studied by using DFT calculations [21]. The highest molecular Polarizability shows to increase the NLO property of the system results good photoelectric conversion efficiency according to Z.

Table2. Polarizability (α) of the 2,2 Dihydroye azobenzene (in a.u).

*	α_{xx}	α_{xy}	α_{yy}	α_{xz}	α_{yz}	α_{zz}	α (esu)	Δα (esu)
DFT/6-311G++(d,p)	70.754	1.6720	85.473	0.0007	0.0014	98.561	$1.258\text{X}10^{-23}$	$3.571\text{X}10^{-24}$

Table3. Hyperpolarizability (β) of the 2,2 Dihydroye azobenzene (in a.u)

*	β_{xxx}	β_{xxy}	β_{xyy}	β_{yyy}	β_{xxz}	β_{xyz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}	β_{ii} (esu)
DFT/6-311G++(d,p)	19.698	21.532	31.86	34.61	-0.00	0.0115	-0.003	0.691	0.781	0.009	$6.671\text{X}10^{-31}$

3.3 Absorptions spectra of organic sensitizers

The electronic absorption spectrum performed in vacuum and solvent (using TD-DFT (B3LYP)/6-311++G (d,p) calculations. The major absorption bands are noted in solvent are 410,426,492,564 and 575 nm whereas in vacuum in is slightly blue sifted to lower wavelength [22-24]. This is attributed to the fact that the polar solvents normally stabilize or destabilize the molecular orbital of the sensitizer either in the ground state or excited state [25]. The usually absorption band n-n transition of cis-stilbene molecule is noted around 410,426,492,564 and 575 nm. The absorption in the UV-Visible zone is one of the most important zones for photocurrent conversion region.

Figure3.Calculated electronic absorption spectra of the 2,2 Dihydroye azobenzene in solvent

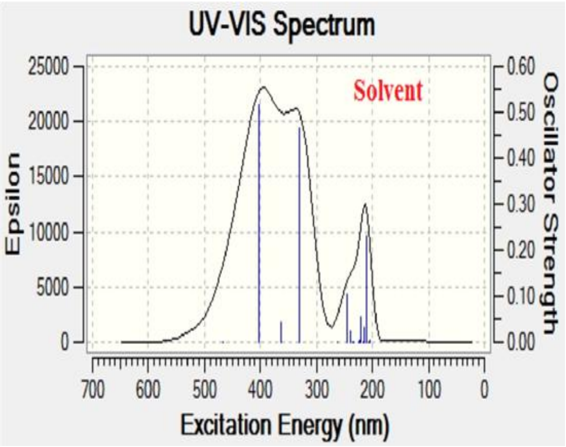


Figure4.Calculated electronic absorption spectra of the 2,2 Dihydroye azobenzene in Vaccum.

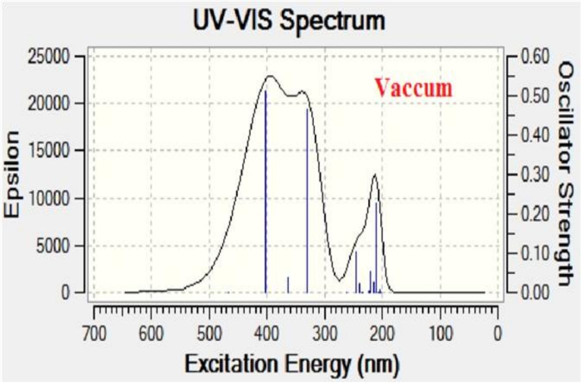
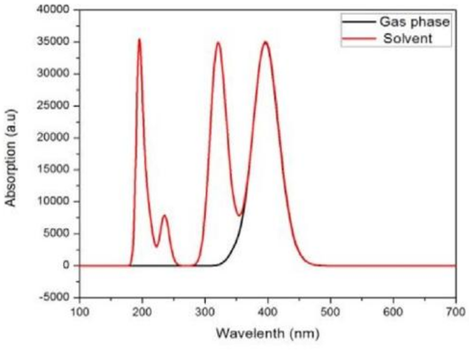


Figure5.Calculated electronic absorption spectra of the 2,2 Dihydroye azobenzene in Gas Phase



The electronic transitions on take place from donor methanol group through stilbene mood to fullerene acceptor group involve 20 singlet-singlet transitions and the electronic transitions. Here the cis-stilbence group launch the electron from its LUMO to the conduction band of the TiO_2 [26-28]. This electron injection produced charge divided states in the interface results photo induced charge transfer processes take place from the dye sensitizer to TiO_2 semiconductor surfaced [29].

Table 4. The computed excitation energies, electronic transition, configuration and oscillator strengths (f) for the optical transitions with f>0.01 of the absorption bands in visible and near-UV region for the 2,2 Dihydroye azobenzene.

Excited state	Configurations composition (Corresponding transition orbital's)	Wavelength λ (nm)	Excitation energy(eV)	Oscillator strength(f)	Major contributions
S1	55 -> 57	21458.53	466.0152	0.0001	H-1->L (99%)
S2	53 -> 57 56 -> 57	24808.98	403.0799	0.5142	H->L (95%)
S3	54 -> 57	27544.02	363.0552	0.0419	H-2->L (96%)
S4	53 -> 57 56 -> 57	30334.72	329.6552	0.4644	H-3->L (92%)
S5	52 -> 57 56 -> 58 56 -> 59	38230.94	261.5682	0.0001	H-4->L (74%), H->L+1 (13%)
S6	52 -> 57 53 -> 60 54 -> 60 56 -> 58 56 -> 59	40817.58	244.9925	0.102	H->L+1 (65%), H->L+2 (17%)
S7	52 -> 57 53 -> 60 54 -> 60 54 -> 65 56 -> 58 56 -> 59	41658.02	240.0498	0.0245	H-4->L (13%), H->L+1 (10%), H->L+2 (60%)
S8	55 -> 58	42393.6	235.8847	0.0003	H-1->L+1 (98%)
S9	55 -> 59	42776.72	233.772	0.0007	H-1->L+2 (99%)
S10	54 -> 61 56 -> 61	44289.82	225.7855	0.0019	H->L+4 (92%)
S11	53-> 58 53 -> 59 54-> 58 54 -> 59 56 -> 60	44662.45	223.9017	0.0033	H-2->L+1 (35%), H->L+3 (49%)
S12	55 -> 60	44997.18	222.2362	0	H-1->L+3 (97%)
S13	53-> 58 53 -> 60 54-> 58 54 -> 59 56 -> 60	45281.89	220.8388	0.0539	H-2->L+1 (48%), H->L+3 (25%)
S14	54 -> 61 56 -> 62 56 -> 63	46109.42	216.8754	0.0007	H-2->L+4 (13%), H->L+5 (58%), H->L+6 (25%)
S15	56 -> 62 56 -> 63	46533.67	214.8981	0.0001	H->L+5 (30%), H->L+6 (64%)
S16	51 -> 57 53 -> 58 53 -> 60 54 -> 59 56 -> 60 56 -> 65	46542.54	214.8572	0.0291	H-2->L+2 (74%)
S17	51 -> 57 53 -> 58 53 -> 59 54 -> 60 56 -> 59 56 -> 65	47373.3	211.0894	0.2302	H-5->L (20%), H-3->L+1 (32%), H-3->L+2 (19%), H-2->L+3 (18%)

S18	50 -> 57 53 -> 58 53 -> 60 55 -> 61 55 -> 64	48250.84	207.2503	0.0005	H-1->L+4 (71%)
S19	53 -> 61 53 -> 62 54 -> 61 54 -> 62 56 -> 62 56 -> 63 56 -> 64	48518.62	206.1065	0.0012	H-3->L+4 (10%), H-2->L+4 (59%)
S20	51 -> 57 53 -> 58 53 -> 59 54 -> 60 55 -> 61 56 -> 65	48738	205.1787	0.0024	H-5->L (21%), H-2->L+3 (14%), H->L+8 (45%)

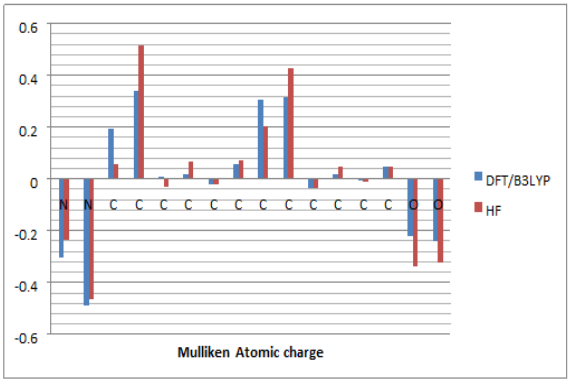
3.4 Natural atomic charges

The calculated values of the reactive atomic charges play a major role in the implementation of quantum mechanical calculations for the molecular system [30]. Mulliken population analysis issued a separate of either a total charge density or an orbital density order to directed the electron population of each atom of the title molecule, natural atomic charges of 2,2 Dihydroye azobenzene calculated by Becke's three parameter gradient-Corrected exchange potential and the Lee-Yang-Parr Gradient-Corrected correlation potential (B3LYP)/6311++G(d,p) basis set [31]. The picture of atomic charges plotted graphically and structurally are shown in figure 6 and 7. For Mulliken charge distribution, the Gauss View adopts the follow colours scheme: Bright red for more positive charge and bright green for more positive charge [32-33]. The red hues figure negative charges while green hues opened positive charge. The Mulliken charge studied different level and at same basis set values have been calculated and also shown in Table 5.

Table 5 The calculated Mulliken atomic charge distribution of the 2,2 Dihydroye azobenzene.

Atoms	DFT/B3LYP	HF
N	-0.300550	-0.236182
N	-0.487305	-0.465552
C	0.192517	0.059221
C	0.338744	0.517438
C	0.008922	-0.027273
C	0.016721	0.066766
C	-0.020573	-0.020668
C	0.059255	0.073768
C	0.306941	0.205300
C	0.315583	0.430925
C	-0.034996	-0.033046
C	0.018633	0.048164
C	-0.005960	-0.008983
C	0.047182	0.048379
O	-0.217716	-0.336719
O	-0.237397	-0.321537

Figure 6. Calculated Mulliken atomic charges of 2,2 Dihydroye azobenzene. (graph)



The charge depending on basis set and are changed due to Polarizability. The C_4 atom has more positive charge both HF/ B3LYP)/6-311++G(d,p), and also N_2 atom has more negative charge compare other atoms as shown in Table 5.

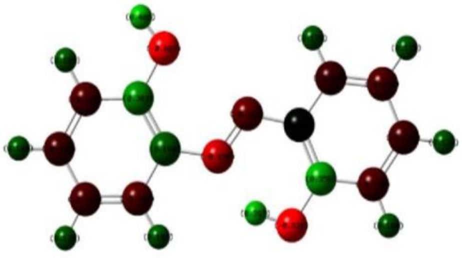


Figure 7. Structural charge distribution of the 2,2 Dihydroye azobenzene

3.5 Global and local reactivity descriptors

The highest occupied molecular orbital's (HOMOs) and Lowest Unoccupied Molecular Orbital's (LUMOs) are identified As Frontier Molecular orbital's (FMOs). The Energy gap between the HOMOs and LUMOs is the critical parameters in manage molecular electrical convey properties assisted in the studied the electron conductivity [25-26]. To note the bonding feature of the title molecule, the plat the Frontier orbital's, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) shown in Figure 8 [34]. The DOS (Figure 9) spectrum was produced by involved the molecular orbital information with GAUSSIAN curves of the unit height.

By using HOMO and LUMO energy values for a molecule, the global chemical reactivity, such as Chemical hardness(Ƞ), Softness(S), Electro negativity(χ), Electrophilicity index(ω), EHOMO (eV), E_{LUMO} (eV) and Ionisation potential(I)eV are described as followed following mathematical formulas.

$$Ƞ = 1/2\ (\delta^2 E/ \delta^2 N^2)\ V(r)=1/2(\delta\mu/ \delta N)V(r)$$

$$\mu = (\delta E / \delta N)\ V(r)$$

$$\chi = - \mu = - (\delta E / \delta N)\ V(r)$$

Where E and V(r) are electronic energy and surface potential of an N-electron system, respectively. Softness is a characteristic of a molecule that analysed the range of chemical responsiveness. It is the reciprocal of hardness:

$S = 1/ Ƞ$

Using Koopmans theorem for the closed shell molecules, Ƞ, μ, and χ can be noted as:

$Ƞ = (I-A)/2$

$\mu = - (I+A)/2$

$\chi = (I-A)/2$

Where A and I are the ionization potential and electron affinity of the molecules. The ionization energy and electron affinity can be expressed through HOMO and LUMO and LUMO orbital energies as I = - EHOMO and A = - E LUMO. Electron affinity refers to the ability of a legend to accept precisely one electron from a donor [27]. The ionization potential calculated B3LYP/6-311++G (d,p) method for 2,2 Dihydroye azobenzene is -4.291 eV. Considering the chemical hardness, large HOMO-LUMO gap means a hard molecule and small HOMO-LUMO gap means a soft molecule [35]. One can also relate the strength of the molecule to hardness, which means that the molecule with least HOMO-LUMO gap means it, is more reactive. It has noted a new descriptor to quantify the international electrophilic power of the molecule as an electrophilicity index (ω), which defines a quantitative ranking of the global electrophilic nature of a molecule.

They defined electrophilicity index (ω)

$\omega = \mu^2/2$

Using the above mathematical equations the chemical potential, hardness and electrophilicity index have been calculated for 2,2 Dihydroye azobenzene and their values are shown in Table 6. The usefulness of this new reactivity quantity has been recently designed with understanding the toxicity of different pollutants in terms of their reactivity and site selectivity. The calculated value of electrophilicity index reported the biological activity of 2,2 Dihydroye azobenzene as follows.

Table 6 Molecular Properties of 2,2 Dihydroye azobenzene.

Molecular Parameters	Energy in (eV)
EHOMO	-6.07
ELUMO	-2.52
Ionization potential (μ)	-4.291
Chemical hardness (η)	1.775
Softness (S)	0.887
Electronegativity (χ)	4.291
Electrophilicity index (ω)	2.417

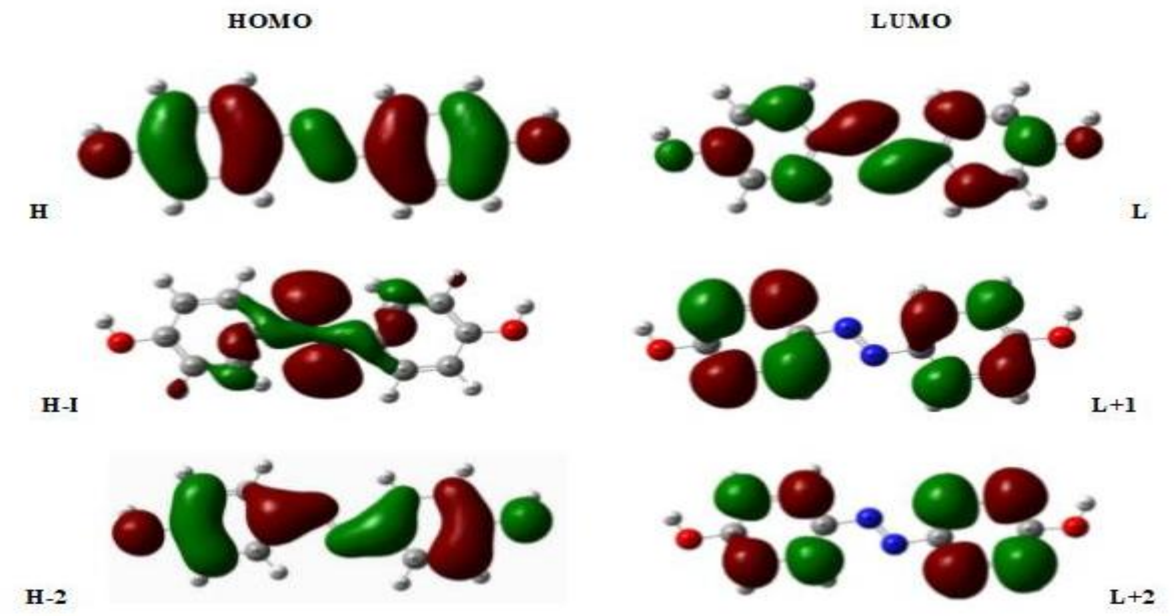


Figure 8. The Frontier molecular orbital of 2,2 Dihydroye azobenzene.

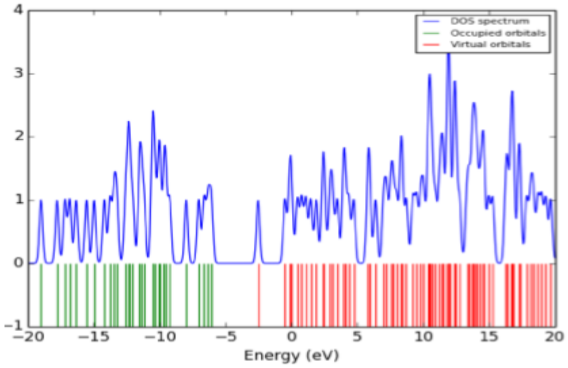


Figure 9. DOS spectrum of 2,2 Dihydroye azobenzene

IV. CONCLUSION

The geometric and electronic properties of the molecule 2,2 Dihydroye azobenzene organic dye molecule analysed by used DFT/B3LYP and HF methods. The molecule geometry was computed and bond angles, bond lengths, and also dihedral angles noted by HF and DFT methods. The studied Polarizability of 2,2 Dihydroye azobenzene is $3.571X10^{-24}$esu and hyperpolarizability of 2,2 Dihydroye azobenzene is $6.671X10^{-31}$esu respectively. The absorptions spectrum of organic sensitizers analysed by solvent and gas phase values is 410,426,492,564 and 575 nm respectively. The various intermolecular interactions that is responsible for the stabilization of the molecule was revealed by natural bond orbital analysis. The global chemical reactivity labelled of molecules such as Chemical hardness(Ƞ), Softness(S), Electro negativity(χ), Electrophilicity index(ω), EHOMO (eV), ELUMO (eV) and Ionisation potential(I)eV are described. The HOMO and LUMO orbital's which can be finding the conversion of solar cell applications of this compound.

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