

Computational Studies of Quantum Chemical Descriptors of Sudan Orange G (SOG) dye derivatives by using Density Functional Theory (DFT) methods

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Abstract: Quantum chemical descriptors of Sudan Orange G (SOG) dye derivatives were computed, using Density functional theory (DFT) in the gas phase. All the dye derivatives structures were optimized by a method of DFT at B3LYP level with 6-31G(d) basis set. All the dye derivatives structures were optimized at DFT/B3LYP method with 6-31G(d) basis set. HOMO and LUMO orbital energies utilize to determine, the quantum chemical descriptors like, chemical potential (μ), softness (S), chemical hardness (η), electrophilicity index (ω), electrofugality (ΔE_e), and nucleofugality (ΔE_n). These values are to prediction of the reactivity of derivatives. All quantum chemical parameters, in general, are dependent on the molecular structure, and are clearly influenced the substitution of different groups and different position of SOG dye.

Key words: Sudan Orange G (SOG), Density functional theory (DFT) quantum chemical descriptors and HOMO-LUMO energies.

1. INTRODUCTION

For the most part colorants are added into nourishment to improve its visual appearance, and to advance deals [1]. In spite of the fact that the admissible measure of manufactured colorants is decreased for customer wellbeing reasons as of late, numerous sorts of engineered sustenance colors are still generally utilized everywhere throughout the world because of their low value, high viability, and astounding soundness [2]. Azo compounds are broadly utilized as manufactured natural colorants. For the most part, manufactured dye may be classified water-solvent or fat-soluble dye in view of their solvability. Around half of the aggregate world colorant creation has a place with the alleged azo dye compounds [3]. The principle highlight of sudan dye group is the nearness of the azo gathering (N=N-) which gives the likelihood of giving a more broadened electronic conjugation of π electrons, and thusly taking into consideration a solid light retention in the noticeable area of the electromagnetic range.

Sudan Dyes are synthesized from azo-dyes which are broadly used to produce color in plastics, leather, fabrics, oil, waxes, and so on. They are classified as Group 3 cancer-causing agents by the International Agency for Research on Cancer (IARC) and are restricted as sustenance added substances overall [4]. However, in a few nations these dyes are still every so often utilized keeping in mind the end goal to increase the shading in items. The SOG is a yellowish red lysochrome azo color and it resembles an unscented rosy orange powder with melting point 225 °C. It is soluble in fats and utilized for coloring of fats, oils, and waxes, incorporating the waxes utilized in turpentine-based shines. Sudan Orange G (SOG) [4(Phenylazo) resorcinol] is valuable for recoloring triglycerides in creature tissues (solidified areas) [5]. To the best of our insight an orderly theoretical investigation of such compounds has not been accounted for. Key comprehension of auxiliary and optical and electronic properties of this sort of materials could be valuable so as design new molecules.

Theoretical analysis of the electronic structure of conjugated frameworks can set up the connections between molecular structure and quantum chemical descriptors. Theoretical investigations on the electronic structures of π -conjugated compounds have given extraordinary commitments to the legitimization of the properties of known materials and to the forecast of the yet obscure ones.

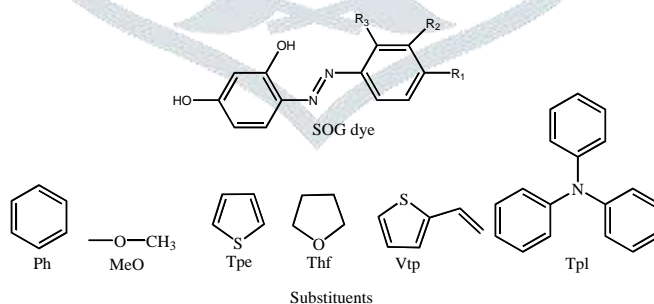
Quantitative structure-activity structure-property relationship (QSAR/QSPR) thinks about are un-tentatively to incredible significance in advanced chemistry and biochemistry. The actual idea of QSAR/QSPR will be change looks to materials with wanted properties utilizing instinct that is synthetic knowledge straight into a scientifically evaluated as well as modernized shape. As soon as a relationship amongst structure and activit /property is discovered, any group of compounds, including them not still incorporated, is often promptly screened on the computer in order to choose structures with the properties wanted. It is subsequently conceivable for choose the majority compounds that are encouraging integrate and experiment in the investigation center. The QSAR/QSPR approach preserves assets and quickens the procedure of improvement of new molecules for use as drugs, materials, additives, or for any other purpose in this manner.

The majority of efforts utilizing quantum chemical descriptors continue done in the discipline of QSAR as opposed to QSPR, i.e. the descriptors being connected to chemical, for example, enzyme inhibition activity, hallucinogenic activity, and so forth [6-9]. Partially this has been on account of, proven, the scan for the quantitative associations with concoction structure began with the improvement of theoretical drug designing methods. Quantum- chemical descriptors have additionally been accounted for to connect the reactivity of natural mixes, octanol/water segment coefficients, chromatographic maintenance lists, and also different physical properties of molecules [10-14].

In this article, a comprehensive quantum chemical study has been carried out for the Sudan Orange G (SOG) dye derivatives for quantum chemical descriptors using the, DFT method. The highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO} (ΔE_g), dipole moments (μ), global hardness (η), softness(S), chemical potential (μ), electronegativity (χ), electrophilicity index (ω), fractions of electrons transferred (ΔN_{max}), electron affinity (EA), ionization potential (IP) have been calculated.

2. COMPUTATIONAL DETAILS

The optimized structures of all studied SOG dye s have been calculated by DFT with the hybrid B3LYP functional theory coupled with Becke's three parameter gradient-corrected exchange potential and the Lee-Yang-Parr gradient-corrected correlation potential (B3LYP) [15-17] with 6- 31G(d) basis set. All calculations have been carried out performed using the GAUSSIAN-09W [18] software package and GaussView, Rev 5.0.9 [19] molecular visualization programs. The quantum chemical investigation has been performed to the optical and quantum chemical parameters| of a series of compounds based on sudan dye derivatives. Different side groups were introduced to investigate their impacts on the electronic structure. The structures of the studied sudan dye derivatives are shown in Fig.1.



D1	R ₁ = Ph,	R ₂ = H,	R ₃ = H	D11	R ₁ = Ph,	R ₂ = H,	R ₃ = Thf
D2	R ₁ = H,	R ₂ = Ph,	R ₃ = H	D12	R ₁ = Vtp,	R ₂ = H,	R ₃ = H
D3	R ₁ = MeO,	R ₂ = H,	R ₃ = H	D13	R ₁ = Ph,	R ₂ = Vtp,	R ₃ = H
D4	R ₁ = Ph,	R ₂ = MeO,	R ₃ = H	D14	R ₁ = Ph,	R ₂ = H,	R ₃ = Vtp
D5	R ₁ = Ph,	R ₂ = H,	R ₃ = MeO	D15	R ₁ = Ph,	R ₂ = Tpl,	R ₃ = H
D6	R ₁ = Tpe,	R ₂ = H,	R ₃ = H	D16	R ₁ = Ph,	R ₂ = H,	R ₃ = Tpl
D7	R ₁ = Ph,	R ₂ = Tpe,	R ₃ = H	D17	R ₁ = Ph,	R ₂ = MeO,	R ₃ = Tpe
D8	R ₁ = Ph,	R ₂ = H,	R ₃ = Tpe	D18	R ₁ = Ph,	R ₂ = Thf,	R ₃ = Tpl
D9	R ₁ = Thf,	R ₂ = H,	R ₃ = H	D19	R ₁ = MeO,	R ₂ = Tpe,	R ₃ = Vtp
D10	R ₁ = Ph,	R ₂ = Thf,	R ₃ = H	D20	R ₁ = H,	R ₂ = H,	R ₃ = Ph

Ph = Phenyl; MeO = Methoxy; Tpe = Thiophene; Thf = tetrahydrofuran; Vtp = 2 vinylthiophene; Tpl = triphenylamine

Scheme 1. The structures of studied SOG dyes derivatives

3. THEORETICAL BACKGROUND

3.1 Quantum-Chemical Descriptors

The quantum chemical descriptors may be classified into four totally different electronic classes including: local charges, dipole moments, orbital energies and also relative descriptors. According to, the Koopmans' theorem [20] for closed-shell molecules, ionization potential (I) and electron affinity (A) may be expressed as follows in terms of the highest occupied molecular orbital energy (E_{HOMO}) and the lowest unoccupied molecular orbital energy (E_{LUMO}), respectively,

$$I = -E_{HOMO} ; A = -E_{LUMO} \quad (1)$$

From the values of I and A, to calculate the following descriptors such as; the electron negativity (χ), the hardness (η), the chemical potential (μ) and the softness S [21]:

$$\chi = \frac{I+A}{2} ; \quad \eta = \frac{I-A}{2} ; \quad \mu = \frac{I+A}{2} ; \quad S = \frac{1}{\eta} \quad (2)$$

The electrophilicity is a reactivity descriptor which allows a quantitative characterization of the electrophilic idea of a particle inside a relative scale. Parr have proposed electrophilicity descriptor as a proportion of energy bringing due down to maximal electron stream among benefactor and acceptor and characterized electrophilicity index (ω) as follows[22].

$$\omega = \frac{\mu^2}{2\eta} \quad (3)$$

As indicated by the definition, electrophilicity descriptor estimates the penchant of concoction species to acknowledge electrons. A decent, more responsive, nucleophile is portrayed by lower estimation of μ , ω , and on the other hand a decent electrophile is described by a high estimation of μ , ω . This new reactivity index estimates the adjustment in energy when the framework procures an extra electronic charge ΔN_{max} from the earth [23].

$$\Delta N_{max} = -\frac{\mu}{\eta} \quad (4)$$

The maximum charge transfer ΔN_{max} in the direction of the electrophile was examined utilizing Eq. (4). Hence the quantity represents the tendency of the system to gain extra electronic charge from the environment. Recent years, Ayers and co-workers [24, 25] have suggested two new reactivity indices to measure nucleophilic and electrophilic possibilities of a leaving group, nucleofugality (ΔE_n) and electrofugality (ΔE_e), defined as follows,

$$\Delta E_n = -A + \omega = \frac{(\mu + \eta)^2}{2\eta} ; \quad \Delta E_e = I + \omega = \frac{(\mu - \eta)^2}{2\eta} \quad (5)$$

4. RESULTS AND DISCUSSION

4.1 Optimization and energies

The optimized structures of all studied SOG dye derivatives dyes are shown in figure 2. All the molecular geometries have been calculated by DFT with hybrid B3LYP functional theory combined with 6-31G(d) basis sets using Gaussian 09 program. The optimization of structures of the all dye derivatives of SOG were calculated according to atom numbering system specified in figure.1, in gas phase.



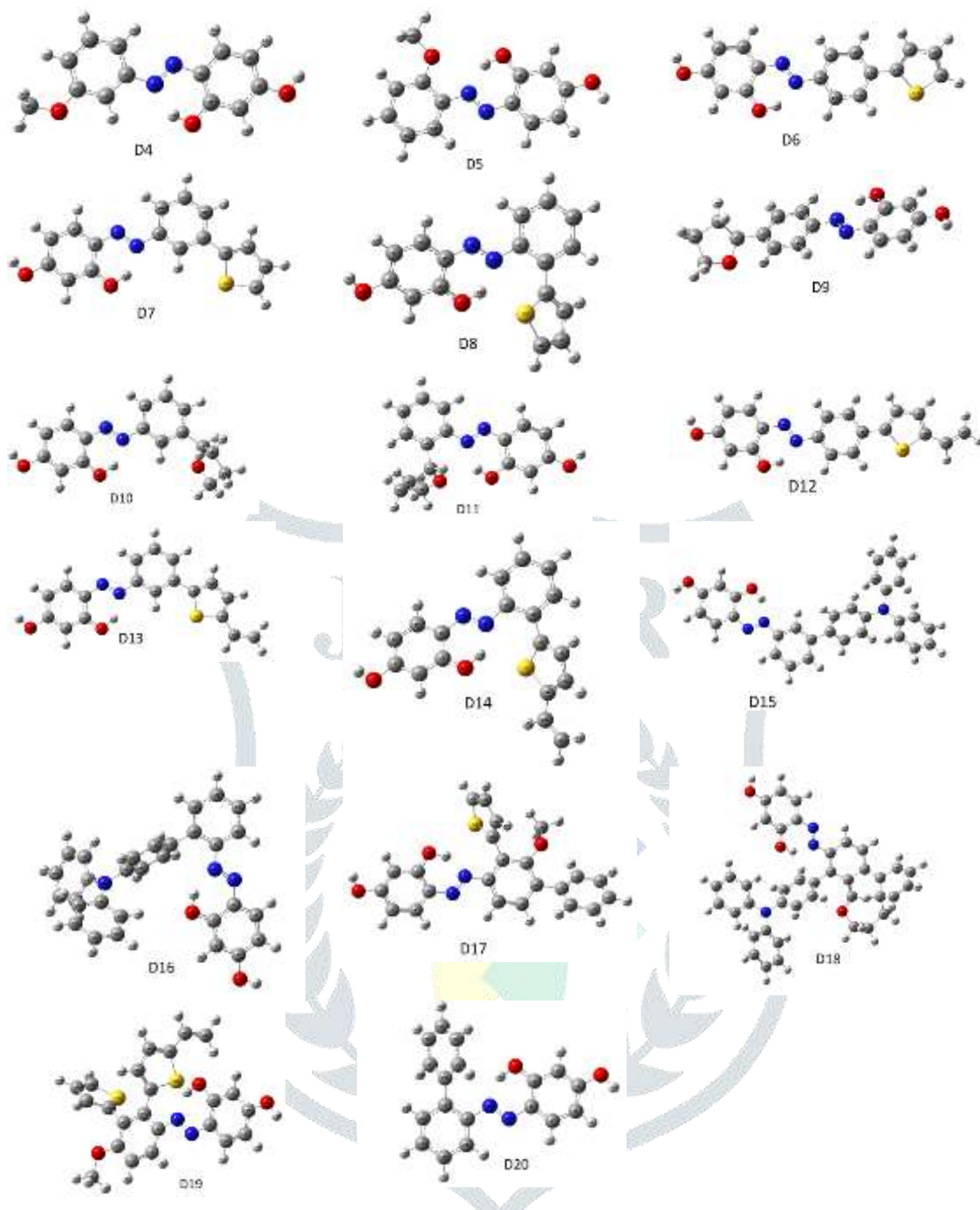


Fig.1. Optimized geometrical structures of SOG dye derivatives in gas phase.

The energies of the SOG dye derivatives are listed in table 1. The D19 dye is more stable than others because of all the substitutions are electron donating groups. The energies are responsible for the different substitutions groups and different positions. The dipole moments are also change with different substitutions and different positions with respective groups.

Table 1. Energies (a.u) of dye derivatives at DFT/B3LYP level with 6-31G in gas.

dye	Energy a.u	Dipole moments (Debye)	HOMO (ev)	LUMO (ev)	dye	Energy a.u	Dipole moments (Debye)	HOMO (ev)	LUMO (ev)
D1	-954.17845694	2.3285	-5.6091	-1.8316	D11	-954.45928411	1.9522	-5.5977	-2.0591
D2	-954.26761278	3.9413	-5.7490	-2.2055	D12	-1352.4253852	3.0216	-5.3326	-2.3500
D3	-873.73408984	3.9413	-5.4379	-2.0158	D13	-1352.4237664	2.6469	-5.4834	-2.2512
D4	-837.73266686	2.9238	-5.6997	-2.1211	D14	-1352.4192410	1.9219	-5.4069	-2.2270
D5	-837.73089812	1.6788	-5.4668	-2.0409	D15	-1471.7168712	1.7429	-4.9628	-2.1696
D6	-1275.0242639	3.0211	-5.4910	-2.3032	D16	-1471.7115687	2.4922	-4.8956	-2.1777
D7	-1275.0228400	2.5523	-5.7141	-2.2373	D17	-1620.5861665	1.2556	-5.5582	-2.2169

D8	-1275.0183704	1.7944	-5.6061	-2.1973	D18	-1933.9110802	3.2221	-4.4714	-2.1051
D9	-954.46661994	2.8281	-5.6262	-2.1138	D19	-2018.7452702	3.6562	-5.3685	-2.0455
D10	-954.46624901	2.5978	-5.6730	-2.1070	D20	-954.26373190	1.9617	-5.6548	-2.1524

4.2 CALCULATION OF THE HOMO, LUMO ENERGIES

HOMO and LUMO energies are famous quantum mechanical descriptors. The highest occupied molecular orbital (HOMO), which speaks to the appropriation and vitality of the base immovably held electrons in the molecule. The lowest unoccupied molecular orbital (LUMO) is portrays the least tightly kept electrons in the molecule. For detail, the energy of the HOMO is a decent estimation to the ionization capability that is least of the particle however the energy of the LUMO for the most part is a poor estimate to the molecule proclivity. A particle whose HOMO isn't doubly included or that does not have a huge HOMO - LUMO energy gap is artificially responsive. High value of HOMO energy is likely to indicate a tendency of the molecule to donate electrons to relevant acceptor molecule of low empty molecular orbital energy. The low value of LUMO energy illustrates higher probability to acknowledge electrons. The idea of hard and delicate nucleophiles and electrophiles has been likewise straightforwardly identified with the relative energies of the HOMO and LUMO orbital's. Hard nucleophiles have a low energy HOMO, delicate nucleophiles have a high energy HOMO, hard electrophiles have a high energy LUMO and sensitive electrophiles have a low energy LUMO [26]. HOMO-LUMO hole is a critical strength record [27]. Figure 2 exhibits that the HOMO and LUMO diagrams of SOG dye derivatives at DFT/B3LYP level of theory in gas phase.

The computed HOMO and LUMO energy level and HOMO-LUMO energy gap (ΔE_g) are given in Table 2 in the gas phase. The HOMO and LUMO energy gap (ΔE_g) has significance that is extraordinary understanding the molecular reactivity and describes the compound reactivity and kinetic stability of the molecule. A molecule with a little energy gap is more polarizable and is for the part that is most connected with a high chemical reactivity, low kinetic stability and is likewise named as soft molecule. The energy gap (ΔE_g) between HOMO and LUMO and reactive descriptors ionization potential (IP), electron proclivity (EA), electronegativity (χ), hardness (η), delicate quality (s), synthetic potential (μ), non-abrasiveness (S), electrophilicity record (ω), charge exchange (ΔN_{max}), nucleofugality (ΔE_n) and electrofugality (ΔE_e) of SOG dye derivatives computed by DFT/6-31G(d) basis set in gas phase were provided in Table.3.

Ionization energy is a central descriptor of the chemical reactivity of atoms and particles. High ionization energy shows high stability and chemical inactivity and low ionization energy demonstrates high reactivity of the atoms and molecules [28]. The low ionization energy of D18 dye (4.4714 eV) shows that is less stability. Absolute hardness and softness are vital properties to quantify the molecular stability and reactivity. It is clear that the chemical hardness on a very basic level means the obstruction towards the deformation or polarization of the electron billow of the atoms, molecules or molecules under small perturbation of chemical reaction. A hard molecule has a high hardness value and a soft molecule has a hardness value [29]. In our present investigation D18 dye have with low hardness value of 1.1832 (eV) compared with other dyes respective substitutions. Therefore, D18 isomer is stable and less reactivity.

The electrophilicity file (ω) has been utilized as auxiliary depicter for the investigation of the chemical reactivity of molecules [30, 31]. That it quantifies the inclination of chemical reactivity of molecules. A decent, more responsive, nucleophile is portrayed by a low estimation of (ω), in inverse a decent electrophile is described by a high value of (ω). The electrophilicity index values were calculated by equation (3) and are presented in the table 2. The D1 dye is a decent electrophile and D12 is good nucleophile in gas phase.

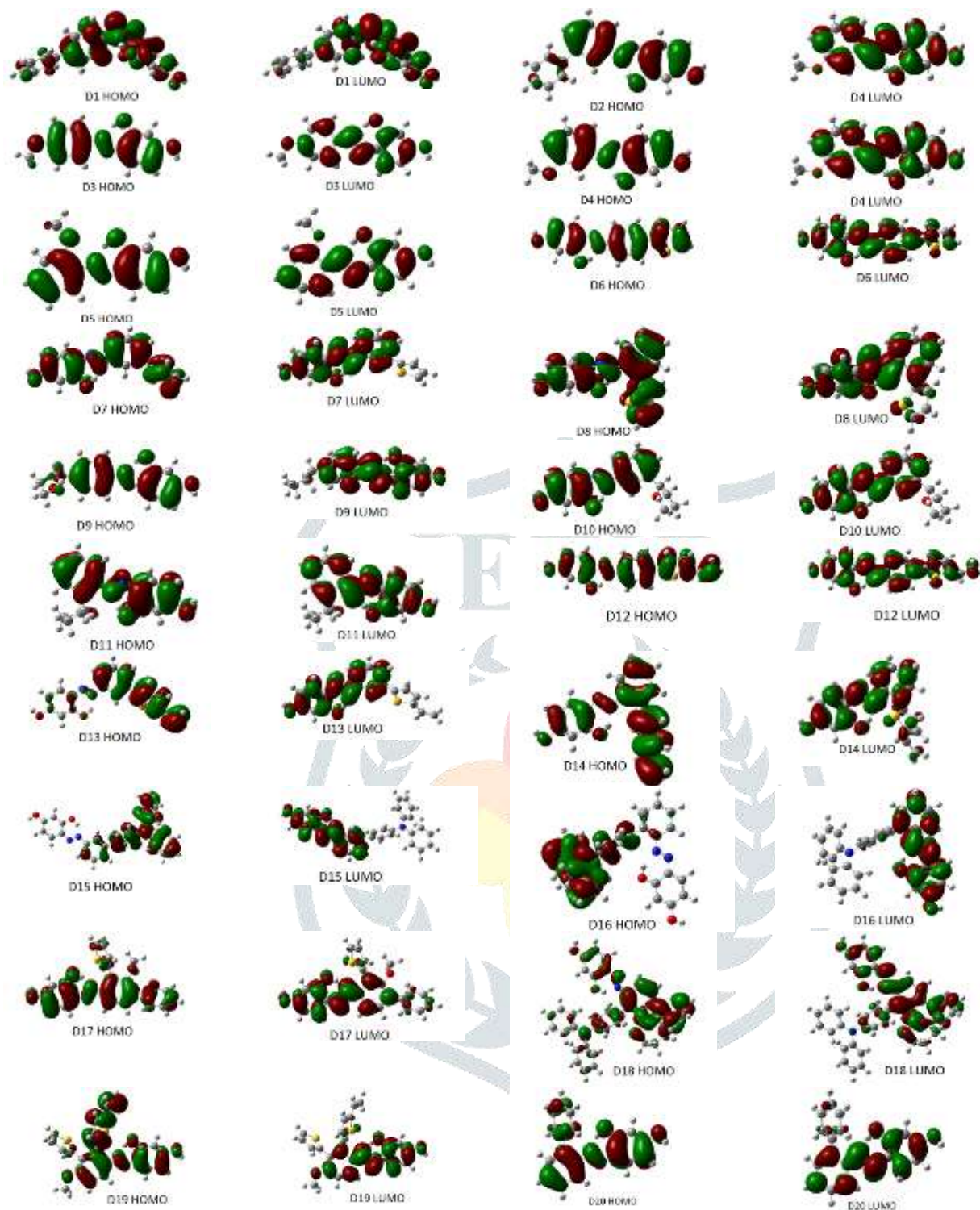


Fig. 2. 3D plots of HOMO and LUMO of studied molecules by B3LYP/6-311G with energies.

Physically, chemical potential (μ) designates the finding away propensity of electrons from an equilibrium system. The greater electronic chemical potential leads to the less stable and more reactive of the compound.

Table 2. The computed quantum chemical descriptors in eV at DFT/B3LYP method with 6-31G basis set.

Mol.	<i>I</i>	<i>A</i>	χ	η	<i>S</i>	μ	ω	ΔN_{max}	ΔE_n	ΔE_e	ΔE_c
D1	5.6091	1.8316	3.7203	1.8887	-3.7203	0.5295	3.6641	1.9697	1.8325	9.2731	-3.7775
D2	5.7490	2.2055	3.9772	1.7717	-3.9772	0.5644	4.4641	2.2448	2.2586	10.2130	-3.5435
D3	5.4379	2.0158	3.7269	1.7111	-3.7269	0.5844	4.0588	2.1781	2.0430	9.4967	-3.4221
D4	5.6997	2.1211	3.9104	1.7893	-3.9104	0.5589	4.2730	2.1855	2.1519	9.9727	-3.5786
D5	5.4668	2.0409	3.7538	1.7130	-3.7538	0.5838	4.1131	2.1914	2.0722	9.5799	-3.4259

D6	5.4910	2.3032	3.8971	1.5939	-3.8971	0.6274	4.7642	2.4450	2.4610	10.2551	-3.1878
D7	5.7141	2.2373	3.9757	1.7384	-3.9757	0.5752	4.5462	2.2870	2.3089	10.2604	-3.4768
D8	5.6061	2.1973	3.9017	1.7044	-3.9017	0.5867	4.4659	2.2892	2.2686	10.0720	-3.4088
D9	5.6262	2.1138	3.8700	1.7562	-3.8700	0.5694	4.2640	2.2036	2.1502	9.8902	-3.5124
D10	5.6730	2.1070	3.8900	1.7830	-3.8900	0.5608	4.2434	2.1817	2.1364	9.9164	-3.5661
D11	5.5977	2.0591	3.8284	1.7693	-3.8284	0.5652	4.1419	2.1638	2.0828	9.7396	-3.5386
D12	5.3326	2.3500	3.8413	1.4913	-3.8413	0.6705	4.9471	2.5758	2.5972	10.2798	-2.9826
D13	5.4834	2.2512	3.8673	1.6161	-3.8673	0.6188	4.6272	2.3930	2.3760	10.1106	-3.2322
D14	5.4069	2.2270	3.8169	1.5900	-3.8169	0.6289	4.5816	2.4007	2.3546	9.9885	-3.1799
D15	4.9628	2.1696	3.5662	1.3966	-3.5662	0.7160	4.5530	2.5534	2.3835	9.5158	-2.7933
D16	4.8956	2.1777	3.5367	1.3589	-3.5367	0.7359	4.6021	2.6025	2.4244	9.4977	-2.7179
D17	5.5582	2.2169	3.8876	1.6706	-3.8876	0.5986	4.5231	2.3270	2.3062	10.0813	-3.3413
D18	4.4714	2.1051	3.2882	1.1832	-3.2882	0.8452	4.5693	2.7792	2.4643	9.0407	-2.3663
D19	5.3685	2.0455	3.7070	1.6615	-3.7070	0.6019	4.1353	2.2311	2.0898	9.5039	-3.3231
D20	5.6548	2.1524	3.9036	1.7512	-3.9036	0.5710	4.3508	2.2291	2.1984	10.0056	-3.5024

5. CONCLUSION

Computational study of the quantum chemical descriptors was calculated at the density functional theory (DFT/B3LYP) level of theory with 6-311G (d) basis set for the SOG dye derivatives. The relative stabilities calculated for isomers in the gas phase with respect to SOG dye. The relative energies are change with the substitutions at different positions with respective groups. The HOMO and LUMO energies in order to identify, the utility of global reactivity descriptors such as, the chemical hardness (η), chemical potential (μ), electrophilicity index (ω), softness (S), nucleofugality (ΔE_n), and electrofugality (ΔE_e), values for the prediction of the reactivity of the tautomers. Quantum chemical descriptors to identify the stability of the dyes, with respective substitutions and different positions of SOG dye. This information leads to determine the optical and electronic properties of dyes in Dye sensitized solar cells (DSSC).

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