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Quantum Chemical Calculations of 3-Benzyl-4-(3-Ethoxy-2-(4-Toluenesulfonlyoxy)-Benzlyideneamino]-4,5-Dihydro-1*H*-1,2,4-Triazol-5-One

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Absract: In this study, 3-Benzyl-4-(3-ethoxy-2-(4-toluenesulfonlyoxy)-benzlyideneamino]-4,5-dihydro-1H-1,2,4-triazol-5-one was theoretically investigated. Initialy, the molecule was optimized by using DFT(B3LYP)/6-31G(d, p) basis set. The molecule's structural parameters (dihedral angles, bond lengths and bond angles), HOMO (the highest occupied molecular orbital) and LUMO (the lowest unoccupied molecular orbital) energies, vibrational frequencies, thermodynamic and electronic properties (thermal capacity , rotation constants, entropy , total energy, electronegativity, electron affinity, chemical softness and hardness), the energy gap (ΔEgap = E_{LUMO}-E_{HOMO}), mulliken atomic charges, the surface maps were calculated by using Gaussian09W program. ^{13}C- NMR and ^{1}H-NMR chemical shift values of molecule also were calculated by GIAO. In additon, theoretical infrared (IR) vibration frequencies values which were scaled with certain scala factor were obtained using the veda4f program. Infrared spectra of molecul were formed according to obtained these values. The all spectroscopic and structural data of compounds were calculated by using 6-31G(d, p) basis set with density functional method (DFT/B3LYP) and compared with experimental values.

Keywords: 4,5-Dihydro-1*H*-1,2,4-triazol-5-one, Gaussian 09W, 6-31G(d,p), DFT.

Introduction

Many diseases caused by pathogens as bacteria, viruse fungal have affected negatively human life and have caused the death of many people from the history of humanity to the present. In order to protect of human healty, many experimental studies have been conducted against pathogens and many drugs have been developed. However, both the emergence of new patogens and the development of resistance of pathogens to drugs necessitated new drug studies (Shalini et al.,2011; Chowdhary et al.2013). Aromatic compounds containings heteroatoms such as N, O, S in their structure are important core structures used in these studies. Triazol compounds are also heteroaromatic compounds consisting of three nitro atoms and two carbon atoms. Thanks to the nitrogen atoms and acidic hydrogen in its structure, triazoles can give a wide variety of reactions and provides the synthesis of new bioactive compounds (Saag et al., 1998). When studies with triazole compounds were examined it was seen that triazole compounds especially ıts Schiff Base derivatives and ıts methal have shown wide biological and theoretical properties (Kardaş et al, 2016, Bahçeci et al., 2017; Çiftçi et al., 2018; Beytur et al., 2019; Gürsoy Kol et al.,2020; Koç et al., 2020; Kotan et al., 2020; Beytur, 2020; Uğurlu

& Beytur, 2020; Boy et al, 2021 Kotan et al., 2021) anti-fungal (Zafar et. al.,2021), anti-bacterial (Chohan et al.,2010, Hanif et al.,2013), anti-tuberculosis (Zhang et al., 2017), anti-cancer (Mareddy et al.2013; Xia et al., 2019) anti-HIV (Feng et al.,2021). In addition, triazole derivatives are also used in the fields of polymer , agriculture (Satapute et al.,2019) and metal science (Struthers et al.,2010; Struthers et al.,2014).

In this study, Gaussian09W program package which frequently used in teoreical studies, was used (Frisch et al., 2003, 2009). The optimized molecular structure, vibrational frequencies, atomic charges and frontier molecule orbitals (HOMO and LUMO) of the Schiff Base compound have been calculated by using B3LYP method with 6-31G basis set. Also, Infrared spectrum data of schiff base were obtained by using same method (Wolinski et al., 1990). Then, teoretical IR data were compared with experimental data in literature. The basis of total energy distribution (TED) analysis of schiff base compound were performed by using veda4f program. Thermodynamic properties of analyzed molecule were calculated by the same basis set.

Table 1. The calculated bond lengths of the titled compound

Bond lengths (A^o)	B3LYP	Bond lengths (A^o)	B3LYP	Bond lengths (A^o)	B3LYP
C(1)-N(50)	1.30	C(11)-H(33)	1.38	C(16)-C(17)	1.39
C(1)-N(52)	1.38	C(11)-H(34)	1.08	C(17)-H(39)	1.08
C(1)-C(19)	1.49	C(11)-H(35)	1.39	C(18)-H(40)	1.50
N(50)-N(51)	1.38	C(8)-C(9)	1.08	C(18)-H(41)	1.09
N(51)-H(26)	1.00	C(9)-C(4)	1.39	C(18)-H(42)	1.09
N(51)-C(2)	1.36	C(11)-H(33)	1.35	C(19)-H(43)	1.09
C(2)-O(54)	1.22	C(11)-H(34)	1.43	C(19)-H(44)	1.09
C(2)-N(52)	1.41	C(11)-H(35)	1.09	C(20)-C(21)	1.52
N(52)-N(53)	1.37	C(8)-C(9)	1.09	C(21)-H(45)	1.08
N(53)-C(3)	1.28	C(9)-C(4)	1.52	C(21)-C(22)	1.39
C(3)-H(27)	1.08	C(9)-O(56)	1.39	C(22)-H(46)	1.08
C(3)-C(4)	1.46	O(56)-S(59)	1.69	C(22)-C(23)	1.39
C(4)-C(5)	1.40	S(59)-O(57)	1.46	C(23)-H(47)	1.08
C(4)-C(9)	1.40	S(59)-O(58)	1.45	C(23)-C(24)	1.39
C(5)-H(28)	1.08	S(59)-C(12)	1.77	C(24)-H(48)	1.08
C(5)-C(6)	1.38	C(12)-C(13)	1.39	C(24)-C(25)	1.39
C(6)-H(29)	1.08	C(12)-C(17)	1.39	C(25)-H(49)	1.08
C(6)-C(7)	1.39	C(13)-C(14)	1.39	C(20)-C(25)	1.40
C(7)-H(30)	1.08	C(13)-H(36)	1.08		
C(7)-C(8)	1.39	C(14)-H(37)	1.08		
C(8)-O(55)	1.35	C(14)-C(15)	1.40		
O(55)-C(10)	1.43	C(15)-C(18)	1.50		
C(10)-H(31)	1.09	C(16)-H(38)	1.08		

Materials and Methods

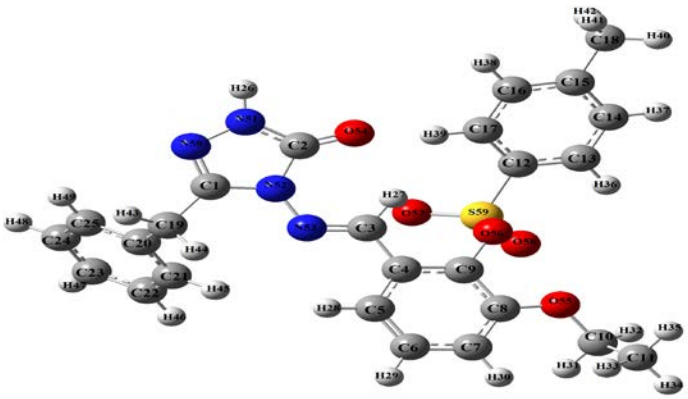

Figure 1. The optimized molecular structure

The geometry optimizations of the 3-benzyl-4-(3-ethoxy-2-(4-toluenesulfonlyoxy)-benzlyideneamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one was performed by using B3LYP method with 6-31G (d,p) basis set. ^{1}H and ^{13}C NMR data and chemical shift values in DMSO of title compound were were calculated by the same basis set. The standard error rate was calculated according to obtained data. The teoretical IR data of the titled compound were carried out with the veda4f program. The geometrical properties of the optimized compoun (bond lengths, dihedral angles, bond angles), the atomic charges, dipole moments, energy, fundamental vibrational frequencies and thermodynamical parameters were obtained.

Result and Discussions

Molecular Structure

The optimized molecular bond lengths of the molecule by using B3LYP/6-31G basis set are listed in Table 1.

Vibrational frequencies

According to Veda4 basis set obtained IR graphic, vibrational frequencies of optimized of 3-Benzyl-4-(3-ethoxy-2-(4-toluenesulfonlyoxy)-benzlyideneamino-4,5-dihydro-1*H*-1,2,4-triazo-5-one summarized in Table 2 and Figure 2.

Table 2. The calculated and observed frequencies values of the titled compound

Vibrational frequencies	Experimental IR	Scaled B3LYP
ν (NH)	3173	3555
ν (C=O)	1696	1739
ν (C=N)	1591	1611
ν (SO2)	1350 and 1149	1291 and 1105
1,4-Disübstitüe-benzen	814	786
monosübstitüe-benzen	748-715	746-706

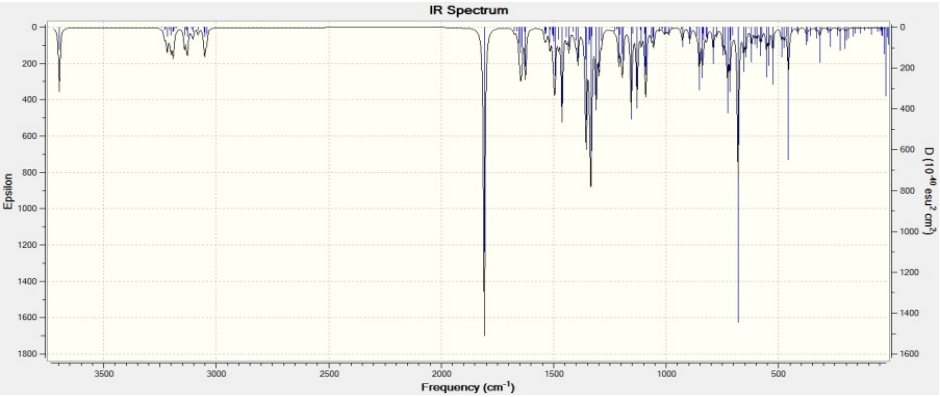

Figure 2. The experimental IR spectrum of the titled compound

NMR spectral analysis

In this study, the ^{1}H and ^{13}C NMR spectral data of Schiff base calculated B3LYP method with 6-31G basis level in DMSO solvent and then compared experimental data in literature. In addition, the calculated isotropic chemical shift analysis for compound allows us to identify relative ionic species and to calculate reliable magnetic properties which provide the accurate predictions of molecular geometries (Jamróz, 2005; Rani et al., 2010; Subramanian et al., 2010). ^{1}H and ^{13}C NMR chemical shift values of the optimized titled compound were calculated at the same level by using Gauge-Independent Atomic Orbital (GIAO) method (Wolinski et al., 1990). Theoretically and experimentally values were plotted according to δ exp=a. δ calc.+ b, Eq. a and b constants regression coefficients with a standard error values were found using the Sigma Plot program (Table 3 and Figure 3).

Table 3. The calculated and experimental ^{13}C and ^{1}H NMR isotropic chemical shifts of the titled compound

No	Experimental	DFT/6-31G(d.p) /DMSO	Shifts /DMSO
C1	146.10	135.92	10.18
C2	151.86	135.54	16.32
C3	147.40	134.93	12.47
C4	128.45	119.66	8.79
C5	117.17	102.07	15.10
C6	128.09	114.52	13.57
C7	116.59	101.58	15.01
C8	150.74	139.51	11.23
C9	135.71	125.47	10.24
C10	64.33	54.29	10.04
C11	14.08	4.98	9.10
C12	132.28	124.01	8.27
C13	128.32	113.98	14.34
C14	129.86	115.15	14.71
C15	145.60	134.07	11.53
C16	129.86	116.31	13.55
C17	128.32	114.71	13.61
C18	20.98	13.07	7.91
C19	30.99	24.00	6.99
C20	128.72	123.12	5.60
C21	129.70	115.11	14.59
C22	128.91	113.17	15.74
C23	128.09	112.51	15.58
C24	128.91	114.13	14.78
C25	129.70	114.77	14.93
H26	11.97	8.66	3.31
H27	9.51	11.36	-1.85
H28	7.44	9.00	-1.56
H29	7.35	8.48	-1.13
H30	7.30	8.12	-0.82
H31	3.93	5.34	-1.41
H32	3.93	5.43	-1.50
H33	1.15	2.50	-1.35
H34	1.15	1.96	-0.81
H35	1.15	2.15	-1.00
H36	7.64	8.90	-1.26
H37	7.38	8.45	-1.07
H38	7.38	8.59	-1.21
H39	7.64	9.61	-1.97
H40	2.29	3.06	-0.77
H41	2.29	3.31	-1.02
H42	2.29	3.51	-1.22
H43	4.02	4.60	-0.58
H44	4.02	5.19	-1.17
H45	7.35	8.69	-1.34
H46	7.31	8.28	-0.97
H47	7.27	8.26	-0.99
H48	7.31	8.39	-1.08
H49	7.35	8.52	-1.17

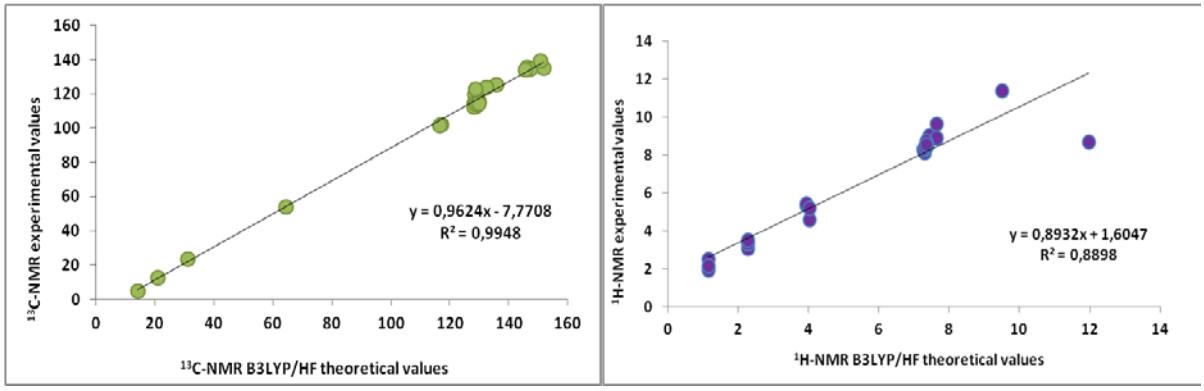

Figure 3. The correlation graphics for ^{13}C-NMR (DMSO), ^{1}H-NMR (DMSO), chemical shifts of the titled compound.

Mulliken Atomic Charge Evaluation

One of the simplest and most understandable ways to describe how charges are distributed in chemical systems is through atomic charge. Both in terms of theory and actual applications, it is quite important (Lu & Chen, 2012). In the molecule, some of the carbon atoms and all of the H atoms are in a positive mulliken charge. Electronegative atoms such as nitrogen, oxygen and sulfur are negative.Mulliken atomic charges of the titled compound have been shown in Table/Figure 4.

Table 4. Mulliken atomic charges of the titled compound

Atoms	B3LYP	Atoms	B3LYP
C1	0,552	H30	0,095
C2	0,825	H31	0,106
C3	0,154	H32	0,125
C4	0,089	H33	0,118
C5	-0,124	H34	0,11
C6	-0,091	H35	0,12
C7	-0,133	H36	0,134
C8	0,369	H37	0,091
C9	0,211	H38	0,098
C10	0,044	H39	0,162
C11	-0,335	H40	0,117
C12	-0,203	H41	0,125
C13	-0,072	H42	0,135
C14	-0,12	H43	0,135
C15	0,132	H44	0,135
C16	-0,126	H45	0,098
C17	-0,066	H46	0,098
C18	-0,382	H47	0,089
C19	-0,305	H48	0,085
C20	0,112	H49	0,085
C21	-0,115	N50	0,089
C22	-0,084	N51	-0,338
C23	-0,084	N52	-0,432
C24	-0,084	N53	-0,417
C25	-0,112	O54	-0,329
H26	0,288	O55	-0,548
H27	0,167	O56	-0,511
H28	0,105	O57	-0,631
H29	0,092	O58	-0,501
		S59	-0,528

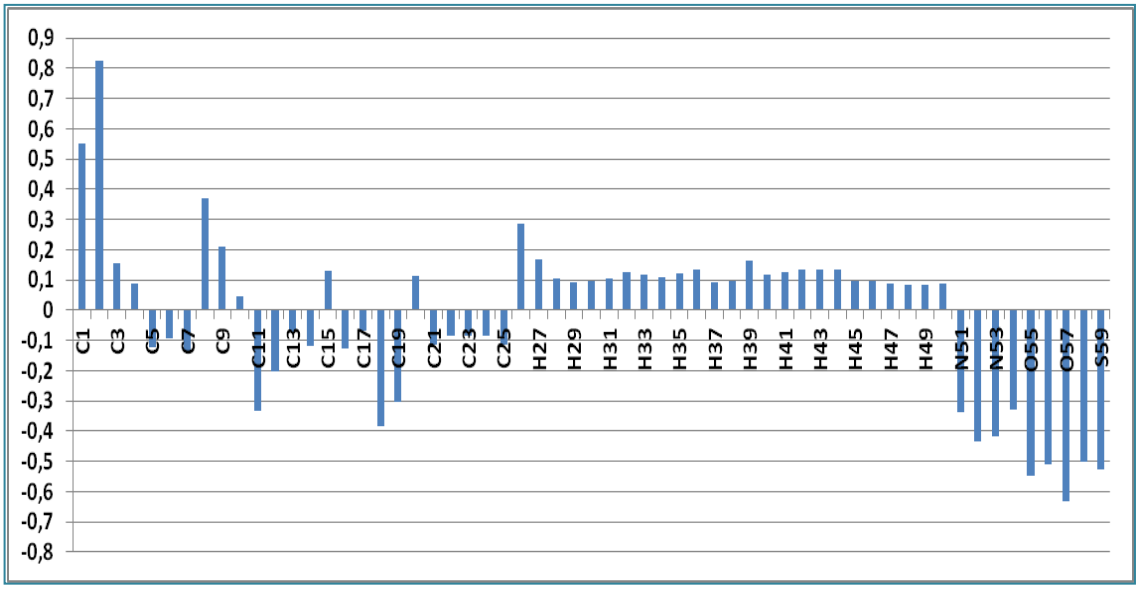

Figure 4**.** The Mulliken atomic charges of the titled compound

NLO Analysis

Understanding the electronic polarization underlying the molecular Non Lineer Optic processes and establishing structure-property connections have greatly benefited from quantum-chemical computations. The response of a system to an applied electric field is defined by the polarizabilities and hyperpolarizabilities(Christiansen et al., 1999). The polarizabilities and hyperpolarizabilities abilities also determine whether the system is a linear optic (Prasad & Williams, 1991). With calculated NLO values using B3LYP/6-31G(d,p) levels, The total energy $\mathbf{E_{total}}$ (Hatree), the electric dipole moment **μ** (Debye), the average polarizability $\boldsymbol{\alpha_{total}}$ (10^{-24} esu) and first hyperpolarizability $\boldsymbol{\beta_{total}}$ (10^{-30} esu) of the title compound were obtained. These data were compared with urea used as a reference substance in NLO. The published data for ure, the NLO parameters are: $\boldsymbol{\alpha_{total}}$: 5.07643717x$10^{-24}$ esu, $\boldsymbol{\Delta\alpha}$: 2.13568262x$10^{-24}$ esu, and $\boldsymbol{\beta^0}$: 7.2228469891x10^{-31} esu (Beytur et al., 2020). The calculated data for title structure $\boldsymbol{\alpha_{total}}$**:** 49.270x$10^{-24}$ esu, $\boldsymbol{\Delta\alpha}$: 26.801x$10^{-24}$ esu, $\boldsymbol{\beta^0}$: 38.08x10^{-30} esu and summarized in Table 5. The NLO values were approximative 10, 13, and 5.5 times more than urea as compared to the reference material.

Table 5. The total energy $\mathbf{E_{total}}$ (Hatree), the electric dipole moment **μ** (Debye), the average polarizability $\boldsymbol{\alpha_{total}}$ (10^{-24} esu) and first hyperpolarizability $\boldsymbol{\beta_{total}}$ (10^{-30} esu) of molecule

	B3LYP		B3LYP
E_{total}	-1960.366867	βxxx	218.405797
μx	-2.8125	βxxy	180.7235769
μy	3.4904	βxyy	-69.898884
μz	3.1052	βyyy	264.387726
$\mu Toplam$	5.4530	βxxz	24.8767922
αxx	400,8282	βxyz	0.348737
αxy	-27.1755257	βyyz	-98.1437388
αyy	384.2602892	βxzz	3.7051325
αxz	8.2447225	βyzz	-23.5130535
αyz	28.2142439	βzzz	-5.1364997
αzz	212.272956	β_{total}	38.08x10^{-30}
α_{total}	49.270x10^{-24}		
$\Delta\alpha$ *(esu)*	26.801x10^{-24}		

Surface Map and MEP Study

The potential surface map electrostatic (MESP) (Reed et al., 1985) which provides a visual method to determine the relative polarity of the compounds, identifies the nucleophilic and electrophilic sites that, along with the molecule's dipole moment, can be used to predict the types of intermolecular interactions as well as the most

advantageous sites for the formation of interactions between biological molecules and receptors and is also a crucial tool in the study of molecular interactions (Politzer & Murray, 2002; Yearley et al., 2008)

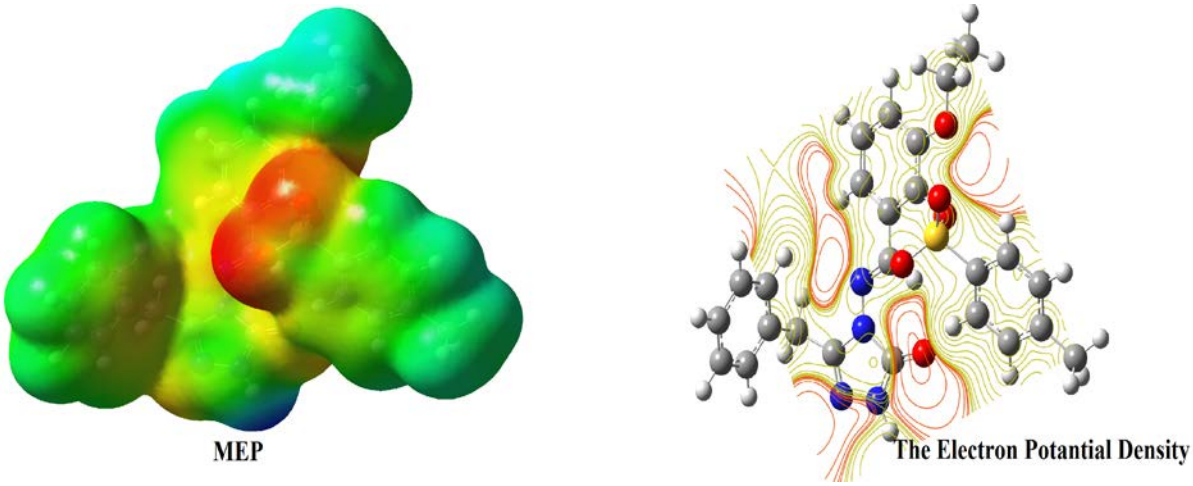

Figure 6. The MEP and electron potantial density of molecule

Table 6. The thermodynamic properties of the titled compound.

Rotational temperatures (Kelvin)	DFT (B3LYP)
A	0.00637
B	0.00350
C	0.00263
Rotational constants (GHZ)	
A	0.13270
B	0.07284
C	0.05470
Thermal Energies E(kcal/mol)	
Translational	0.889
Rotational	0.889
Vibrational	306.892
Total	308.670
Thermal Capacity CV(cal/mol-K)	
Translational	2.981
Rotational	2.981
Vibrational	115.361
Total	121.322
Entropy S(cal/mol-K)	
Translational	44.468
Rotational	37.650
Vibrational	132.069
Total	158.506
Zero-point correction (Hartree/Particle)	0.459669
Thermal correction to Energy	0.491778
Thermal correction to Enthalpy	0.492722
Thermal correction to Gibbs Free Energy	0.390954
Sum of electronic and zero-point Energies	-1959.907199
Sum of electronic and thermal Energies	-1959.875090
Sum of electronic and thermal Enthalpies	-1959.874146
Sum of electronic and thermal Free Energies	-1959.975913

HOMO-LUMO Calculations

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy values and HOMO-LUMO energy gap were calculated. According to Eqs. (1.1) and (1.2), the HOMO and LUMO energy levels are correlated with the ionization potential (IP) and electron affinities (EA), respectively.

The HOMO-LUMO energy gap is determined by the difference between the LUMO and HOMO energy values. The E_{LUMO}-E_{HOMO} is associated with kinetic stability and the chemical reactivity (Dennington, 2009). Important electronic features including global hardness (η), global softness (σ), electronegativity (ω), chemical potential (μ), and electrophilicity index (ω) were estimated using these HOMO-LUMO energy values (Beytur, 2021) .

$$IP = -E_{HOMO} \quad (2.1)$$
$$EA = -E_{LUMO} \quad (2.2)$$

The HOMO and LUMO isosurfaces in both pictures are green and dark red, signifying positive and negative values, respectively (Kotan et al., 2020).

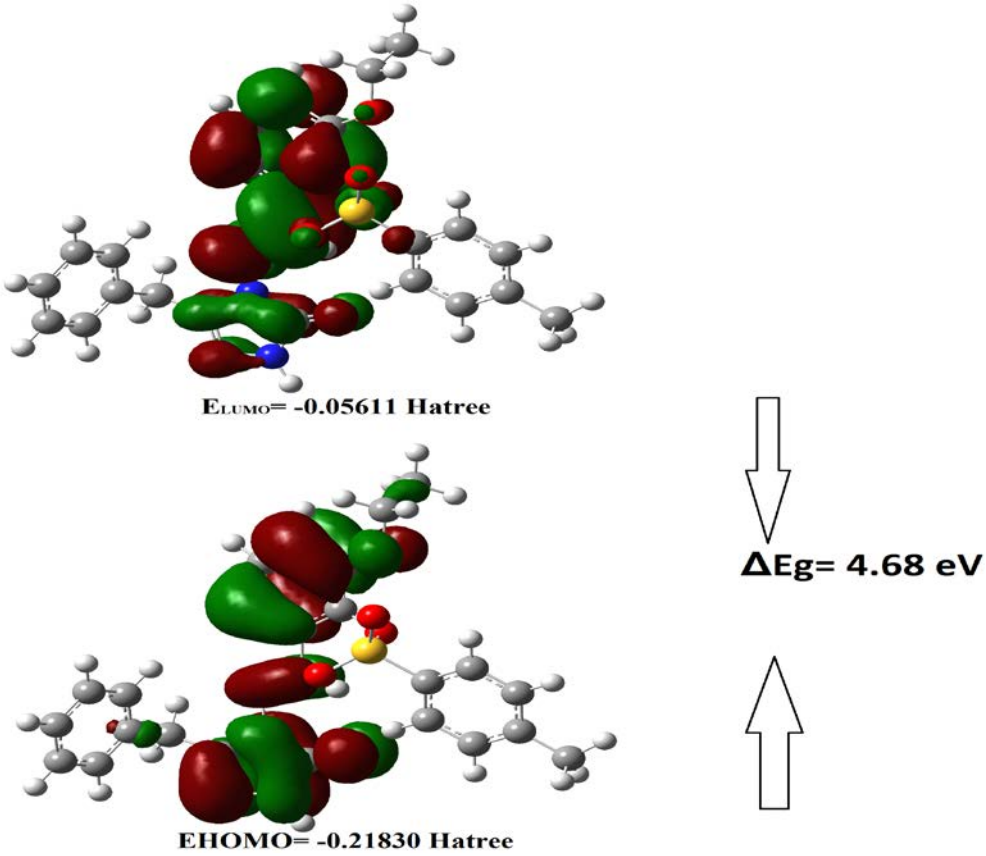

Figure 7. The LUMO-HOMO and ΔEg

Table 7. The electronic properties of the titled compound.

		Hatree	eV	kcal/mol	KJ/mol
	LUMO	-0.05611	-1.52679	-35.2092	-147.317
	HOMO	-0.2183	-5.9401	-136.984	-573.147
A	Electron affinity	0.05611	1.52679	35.2092	147.317
I	Ionization potential	0.2183	5.9401	136.984	573.147
ΔE	energy gap	0.16219	4.4133	101.775	425.83
χ	electronegativity	0.137205	3.73344	86.0965	360.232
Pi	chemical potential	-0.137205	-3.73344	-86.0965	-360.232
Ω	electrophilic index	0.000763315	0.02077	0.47898	2.00408
IP	Nucleophilic index	-0.01112664	-0.30276	-6.982	-29.213
S	molecular softness	12.3312	335.541	7737.88	32375.6
H	molecular hardness	0.081095	2.20665	50.8874	212.915

Conclusion

All of the molecule's theoretical properties were computed, and the spectroscopic calculation results were compared to the published experimental findings. Infrared results did not contain any negative frequency values,

and this is consistent with experiment. Additionally, regression analysis was carried out, visuals were produced, and the theoretical and experimental nmr values were compared. Although the regression analysis of the ^{13}C-NMR shows no divergence, the N-H acidic proton causes a deviation in the study of the ^{1}H-NMR. HOMO-LUMO analyses, MEP analyses, and picture creation were done. Numerous atomic charges, thermodynamic characteristics, and electrophilic and nucleophilic areas were identified.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Acknowledgements or Notes

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