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In Silico Calculations of 2-Methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] Phenyl Benzoate

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Abstract: Schiff's bases are significant compound for organic chemistry. In the last year, computational properties of Schiff bases were examined on a computer. In this study, we investigated theoretical features of 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate with B3LYP/6-311G(d) basis set. All quantum chemical calculations were carried out using the Gaussian09W program package and the Gauss View molecular visualization program. The IR vibrational frequency values of the titled compound were calculated using B3LYP/6-311G(d) basis set. The vibrational spectral analysis was carried out using infrared spectroscopy in the range 4000-400 cm^{-1} for titled compound. The IR vibrational frequency values were defined using the veda4f software. The ^{1}H-NMR and ^{13}C-NMR spectral values of the titled compound were calculated utilizing the B3LYP/6-311G(d) basis set. To determine the ^{1}H-NMR and ^{13}C-NMR isotropic shift values, the gauge independent atomic orbital (GIAO) methodology was used. The UV-vis spectral calculations in the ethanol solvent of the titled compound were performed via the same basis set. TD-DFT computations in ethanol solvent were used to identify the UV-Vis spectral analyses. In addition, dipole moments, LUMO-HOMO, total energy, and electronic properties; E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), thermodynamics properties; (thermal energies (E), thermal capacity (CV), entropy (S) were calculated.

Keywords: Schiff base, Gaussian09W, GIAO, UV-vis, HOMO-LUMO

Introduction

Heterocyclic organic compound having three nitrogen atoms in the five-membered ring have been extensively studied for their applicability in various areas such as biological, chemical and pharmaceutical applications (Alkan et al., 2007; Aytac et al., 2009; Aktaş-Yokuş et al., 2017; Boy et al., 2021; Çiftçi et al., 2018; Gürsoy-Kol et. al., 2010; Turhan-Irak et. al., 2019). There has recently been an increase in studies on heterocyclic organic compound in relation to corrosion inhibitors, optical sensors, theoretical, highly selective polymer membrane electrodes, highly thermal stability, modern technology (nonlinear optical materials), various coordination complexes, homogenous catalysis and biological probes (Bahçeci et al., 2016; Bahçeci et al., 2017; Beytur et al., 2019; Koç et al., 2019; Beytur et. al., 2021; Beytur, 2020; Uğurlu et. al., 2020). Also, several articles reporting the synthesis of some *N*-arylidenamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one compounds and derivatives have been published (Yüksek et al., 2004; Turhan-Irak, 2017).

In this paper, the optimized molecular structure, vibrational frequencies, spectroscopic parameters, atomic charges and frontier molecule orbitals (HOMO and LUMO) of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate have been calculated by using DFT/B3LYP method with 6-311G(d) basis set. All quantum chemical calculations were carried out by using Gaussian 09W (Frisch et al.,

2009; Wolinski et. al., 1990) program package and the GaussView molecular visualization program (Frisch, Nielson & Holder, 2003) (Figure 1). The molecular structure and vibrational calculations of the molecule were computed by using Becke-3-Lee Yang Parr (B3LYP) (Becke, 1993; Lee et al.,1998) density functional method with 6-311G(d) basis set in ground state. IR absorption frequencies of analyzed molecule were calculated by two methods. Then, they were compared with experimental data (Gürbüz et al., 2021), which are shown to be accurate. The assignments of fundamental vibrational modes of the title molecule were performed on the basis of total energy distribution (TED) analysis by using VEDA 4f program (Jamróz, 2004). Furthermore, molecular structure, HOMO and LUMO energy analysis, total energy, and electronic properties; E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), thermodynamics properties; (thermal energies (E), thermal capacity (CV), entropy (S) were calculated.

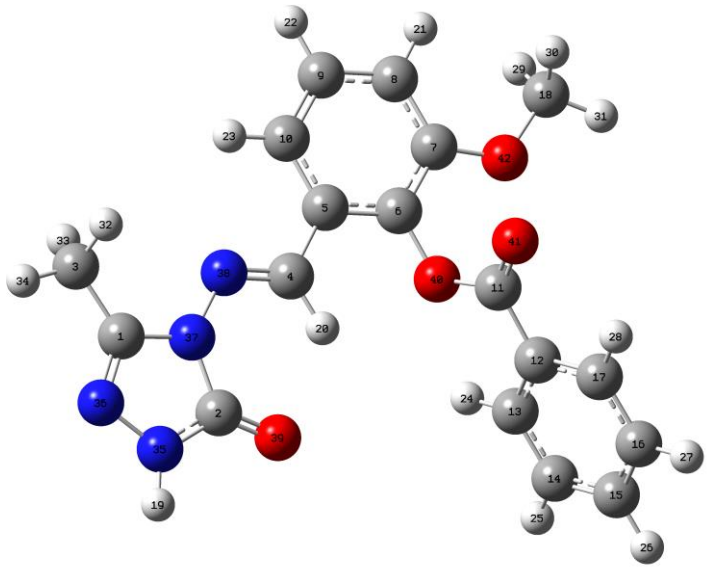


Figure 1. The optimized molecular structure (Gaussview Appearance) of 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl]phenyl benzoate with DFT/B3LYP 6-311G(d) level.

Method

The molecular structure of the title compound in the ground state is computed by performing both the density functional theory (DFT) (Becke, 1993; Lee, 1998) at 6-311G(d) level. Density functionals for all studies reported in this paper have been in the following form

$$E_{XC} = (1-a_0)E_X^{LSDA} + a_0 E_X^{HF} + a_X \Delta E_X^{B88} + a_C E_C^{LYP} + (1-a_C)E_C^{VWN}$$

where the energy terms are the Slater exchange, the Hartree-Fock exchange, Becke's exchange functional correction, the gradient corrected correlation functional of Lee, Yang and Parr, and the local correlation functional of Vosko, Wilk and Nusair (Vosko et al., 1980). The theoretical geometric structure of the title compound is given in Figure 1. Molecular geometry is restricted and the optimized geometrical parameters of the title compound in this study are carried out by using Gaussian 09W program package (Frisch et al., 2009) and the visualization parts were done with GaussView program (Dennington et al., 2009) on personal computer employing 6-311G(d) basis set. Additionally, harmonic vibrational frequencies for the title compound are calculated with these selected methods and then scaled by 0.9516 and 0.9905, respectively (Avcı et. al., 2008) and these results were compared with the experimental data (Gürbüz et al., 2021).

Results and Discussion

Analysis of Vibrational Modes

The number of potentially active fundamentals of non-linear molecule which have N atoms is equal to (3N-6) apart from three translational and three rotational degrees of freedom. The title molecule contains 42 atoms and

Table 1. The calculated frequencies values of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate.

Selected Vibrational Types	Experimental	Scaled DFT
τ HNNC (50)		442
τ HCCC (10), τ CCOC (23)		522
δ OCN (12), δ CCO (12), δ COC (20)		563
τ OCCC (35), τ CCCC (22)		592
δ OCN (16), δ CCC (12)		639
τ HCCC (14), τ ONNC (24)		688
τ HCCN (21), τ ONNC (41)	712	719
ν NC (16), CC (10), δ CNN (36)		762
τ HCCC (30), τ ONNC (36), τ CCCC (11)	783	776
δ OCO (15), δ COC (12), τ CCOC (11)		837
ν OC (26), δ HCC (11), δ CCC (22)		1025
ν NC (13), ν NN (52)		1060
ν CC (17), ν OC (15), δ HCC (19)		1069
δ HCC (11), τ HCCN (49), τ HCCC (14)		1073
ν NC (34), NN (17), δ OCN (12)		1182
ν NN (10), δ NCN (14), δ CNN (11), τ HCCN (19)		1217
ν CC (10), ν OC (17)	1259	1257
ν NN (12), τ HCCN (21)		1301
δ HCC (72), τ HCCN (13)		1333
ν NC (15), δ HCN (14), τ HCCN (33)		1355
δ HNN (64), τ HCCN (12)		1377
ν NC (14), δ HCN (11), τ HCCN (16)		1441
τ HCOC (12), τ CCCC (12)		1458
ν NC (47), ν CC (13)	1592	1588
ν NC (58)	1608	1600
ν OC (75), ν NC (11)	1700	1739
ν OC (87)	1744	1742
ν CH (95)		2899
ν CH (90)		2958
ν CH (100)		3066
ν CH (94)		3085
ν CH (96)		3096
ν NH (100)	3190	3549

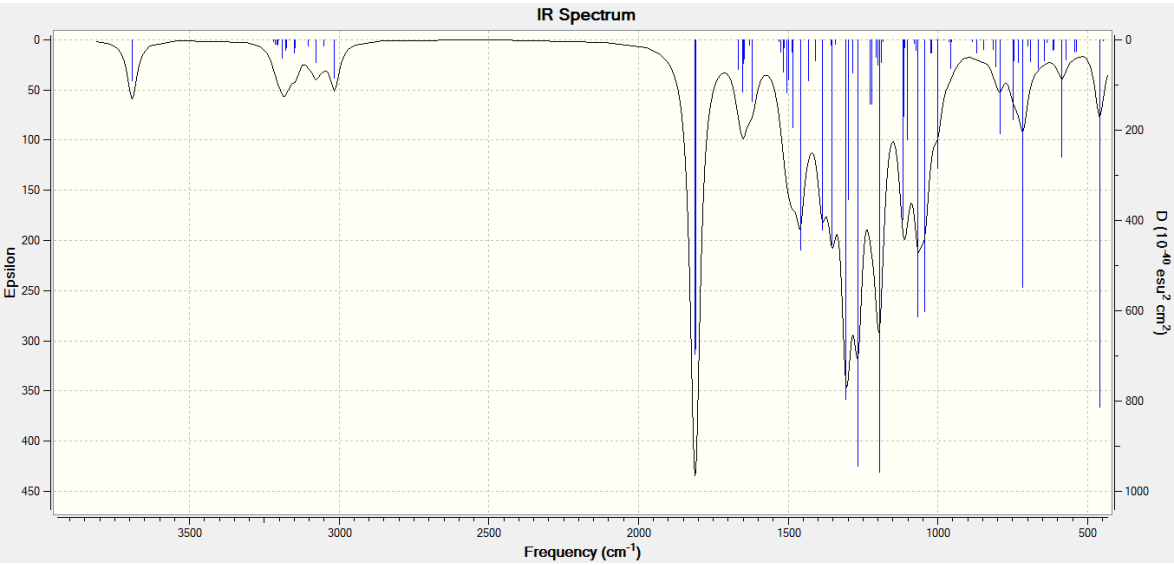


Figure 2. IR spectra simulated with DFT/B3LYP/6-311G(d) level of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl]phenyl benzoate

120 normal vibration modes have C1 symmetry (Table 1). Experimentally (Gürbüz et al., 2021), the investigated 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate, as expected the IR spectra data, the N-H stretching vibration at 3190 cm^{-1} and two C=O peak at 1744 and 1700 cm^{-1} range was observed. In addition, C=N stretching vibration at 1608 and 1592 cm^{-1} and COO stretching vibrations at 1259 cm^{-1} are occurred. Theoretically and experimentally (Gürbüz et al., 2021), the calculated vibrational frequencies for the compound are summarized in Table 1. Furthermore, the experimental IR (Gürbüz et al., 2021) and simulated spectra by using B3LYP/6-311G(d) levels of the titled compound under investigation are given in Figure 2.

NMR Spectral Analysis

The isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties in nuclear magnetic resonance (NMR) spectroscopy which provide the accurate predictions of molecular geometries (Wade, 2006; Rani, et al., 2010; Subramanian et al., 2010). For this purpose, the optimized molecular geometry of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate was obtained by using B3LYP method with 6-311G(d) basis level in DMSO solvent. By considering the optimized molecular geometry of the titled compound, the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital method (Table 2). Theoretically and experimentally values (Gürbüz et al., 2021) 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 SigmaPlot program. The correlation graphics are given Figure 3 and the linear correlation data of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate by considering the results are given in Table 2. Therefore, the (R^2) values (DFT) for ^{1}H NMR (DMSO) and ^{13}C NMR (DMSO) chemical shifts in different solvents has been found as 0.8252 and 0.9971 for the compound (Figure 3). In our study, the ^{1}H-NMR spectrum of the titled compound was observed belong to H19 proton peak at 11.76 ppm because acidic show feature (Yüksek, 1992; Yüksek et al., 2005; Yüksek et al., 2006, Gürbüz et al., 2021). H20 protons were observed at 9.90 ppm. Theoretically, DMSO solvent these values for the mentioned proton atoms were found as 6.61 and 9.73 ppm, respectively. In Table 2, the biggest ^{13}C chemical shift value of the molecule are observed at 164.28 ppm for the C11 carbon atom double bounded to the oxygen in carbonyl group (Anderson et al., 2004). DMSO solvent the calculated ppm values (DFT) for C11 carbon atom were theoretically found as 168.64 ppm. Additionally, due to the electronegative property of nitrogen atoms in molecule, the experimental NMR chemical shift values for C1 and C2 carbon atom the bounded to nitrogen atoms in 1,2,4-triazol ring and C3 carbon atom with sp^2 hybrid are observed at 148.84, 152.03, and 144.62 ppm, respectively.

Table 2. The calculated and experimental ^{1}H and ^{13}C NMR isotropic chemical shifts of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate

No	Experim.	DFT/6311(d) DMSO	Diff./ DMSO	No	Experim.	DFT/6311(d) DMSO	Diff./ DMSO
1C	148.84	150.27	-1.43	19H	11.76	6.61	5.15
2C	152.03	153.29	-1.26	20H	9.90	9.73	0.17
3C	11.32	12.43	-1.11	21H	7.36	6.63	0.73
4C	144.62	147.85	-3.23	22H	7.43	7.15	0.28
5C	128.65	132.85	-4.20	23H	7.65	7.52	0.13
6C	139.49	146.77	-7.28	24H	8.17	8.10	0.07
7C	151.63	157.65	-6.02	25H	7.57	7.40	0.17
8C	115.84	115.76	0.08	26H	7.79	7.56	0.23
9C	127.64	130.06	-2.42	27H	7.6	7.4	0.20
10C	118.74	118.08	0.66	28H	8.17	7.88	0.29
11C	164.28	168.64	-4.36	29H	3.81	3.44	0.37
12C	127.67	131.79	-4.12	30H	3.81	3.29	0.52
13C	130.42	134.05	-3.63	31H	3.81	3.66	0.15
14C	129.56	131.98	-2.42	32H	2.11	2.05	0.06
15C	134.76	138.43	-3.67	33H	2.11	2.1	0.01
16C	129.56	131.70	-2.14	34H	2.11	1.7	0.41
17C	130.42	134.52	-4.10				
18C	56.71	54.02	2.69				

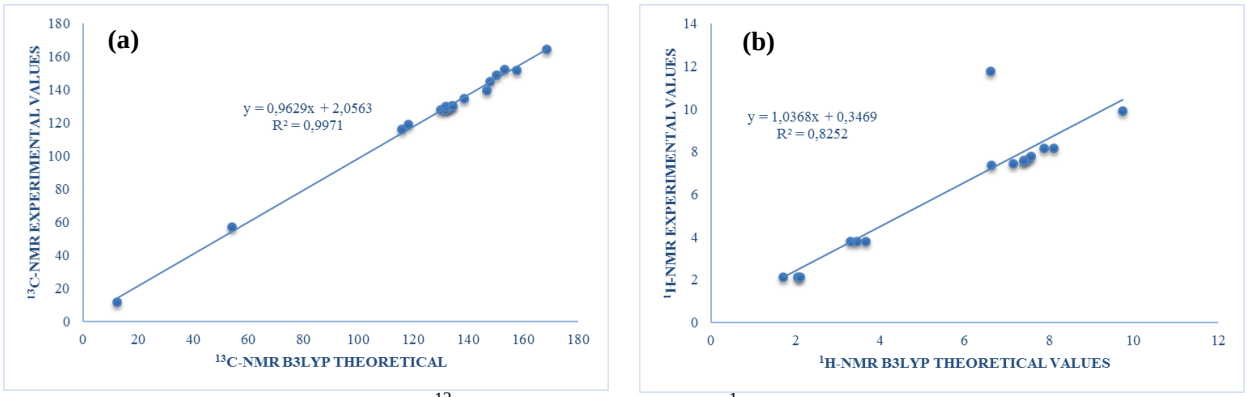


Figure 3. The correlation graphics for ^{13}C-NMR (DMSO) (a) and ^{1}H-NMR (DMSO) (b), chemical shifts of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl]phenyl benzoate.

UV–visible Spectroscopy

The title molecule allow strong $\pi \rightarrow \pi^*$ and $\sigma \rightarrow \sigma^*$ transitions in UV–vis region with high extinction coefficients (Silverstein, et al., 1991). The absorption wavelengths (λ) excitation energies, and oscillator strengths (*f*) of UV–vis absorption spectroscopy of the titled compound has been calculated in ethanol solvents by using TD–DFT/B3LYP method (Figure 4 and Table 3).

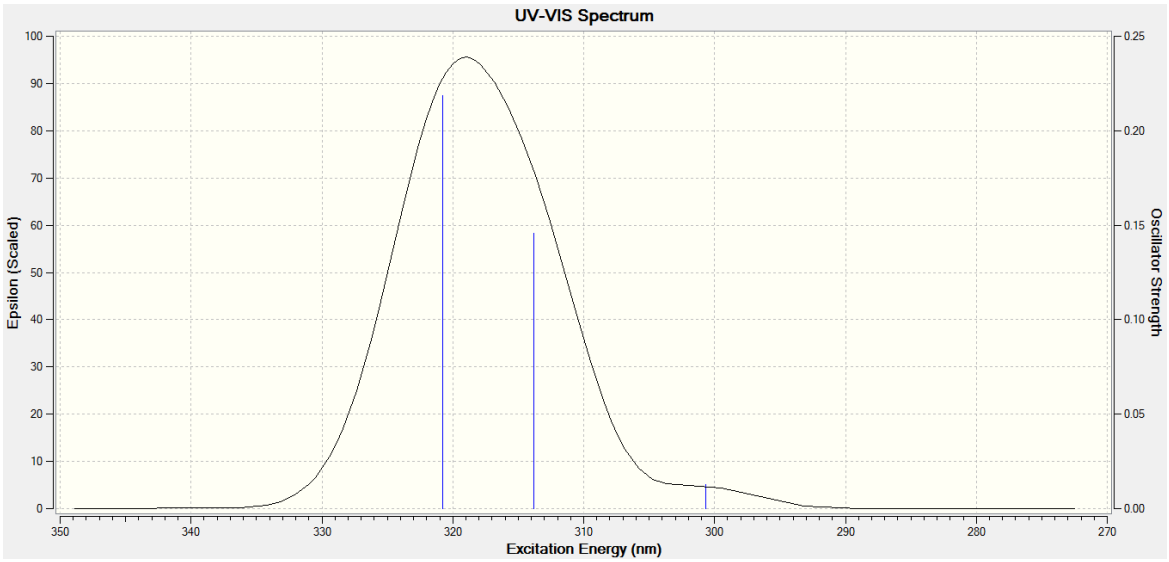


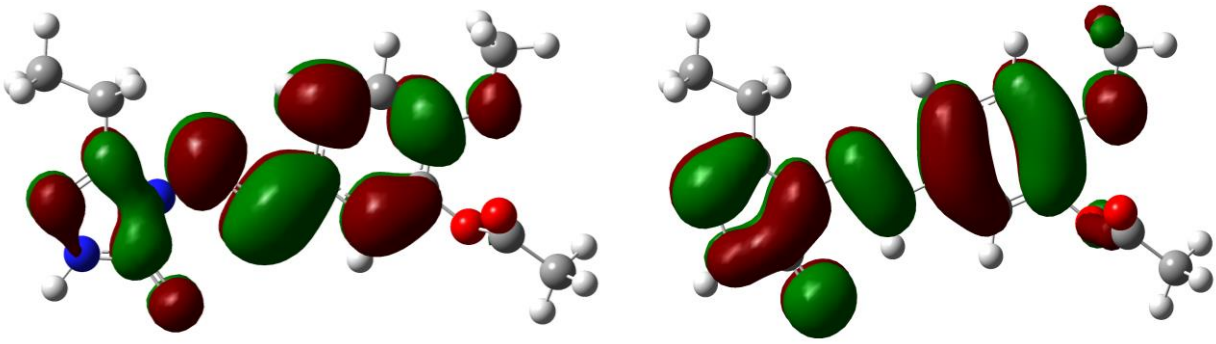
Figure 4. Simulated UV-Visible spectra with DFT/B3LYP/6-311G(d) level of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl]phenyl benzoate.

Table 3. The experimental and calculated absorption wavelength (λ), excitation energies and oscillator strengths (*f*) the -methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate.

λ (nm)Exp/B3LYP	Uyarma Enerjisi (eV) B3LYP	*f* (osilatör gücü) B3LYP
296/320.76	3.8653	0.2186
256/313.82	3.9208	0.1456
214/300.66	4.1237	0.0127

Frontier Molecular Orbital Analysis

The energies of two important molecular orbitals of the title molecule; the second highest and highest occupied MO's (HOMO), the lowest and the second lowest unoccupied MO's (LUMO) (Figure 5) were calculated by using DFT/B3LYP method with 6-311G(d) level and are presented in Table 4. The energy gap of the title molecule was calculated at DFT/B3LYP level, which reveals the chemical reactivity and proves the occurrence



E_{LUMO} (B3LYP): -2.1042 eV E_{LUMO} (B3LYP): -6.0168 eV

Figure 5. The calculated HOMO-LUMO energies of the molecule according to DFT/B3LYP/6-31G(d) level

Table 4. The calculated HOMO-LUMO energies of the 2-methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl]phenyl benzoate according to DFT/B3LYP/6-311G(d) levels

Electronic properties	B3LYP	Electronic properties	B3LYP
I; Ionization Potential (eV)	6.1159	χ; Electronegativity (eV)	3.9307
A; Electron Affinity (eV)	1.7456	Total Energy (a.u.)	-1215.7066
η; Chemical Hardness (eV)	4.3703	ΔE; Energy Gap (eV)	4.3703
S; Molecular Softness (eV)	2.1852	Pi; chemical potential	-3.9307

Table 5. The thermodynamic properties of the -methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate

Rotational temperatures (Kelvin)	B3LYP
A	0.0117
B	0.0067
C	0.0045
Rotational constants (GHZ)	
A	0.2435
B	0.1396
C	0.0937
Zero-point vibrational energy (Kcal/Mol)	201.6304
Thermal correction to Energy	0.3444
Thermal correction to Enthalpy	0.3453
Thermal correction to Gibbs Free Energy	0.2656
Sum of electronic and zero-point Energies	-1215.3853
Sum of electronic and thermal Energies	-1215.3622
Sum of electronic and thermal Enthalpies	-1215.3613
Sum of electronic and thermal Free Energies	-1215.4410
Thermal Energies E(Kcal/mol)	
Translational	0.889
Rotational	0.889
Vibrational	214.329
Total	216.106
Thermal Capacity CV(Cal/Mol-Kelvin	
Translational	2.981
Rotational	2.981
Vibrational	80.719
Total	86.680
Entropy S (Cal/Mol-Kelvin)	
Translational	43.470
Rotational	35.866
Vibrational	88.472
Total	167.808

of eventual charge transfer. The HOMO is located almost over the carbon atoms, oxygen atoms and also slightly delocalized in hydrogen atom and the LUMO is mainly delocalized in carbon atoms of benzene ring. The energy gap (energy difference between HOMO and LUMO orbital) is a critical parameter in determining molecular electrical transport properties (Fukui, 1982).

Conclusion

In this paper, the structure of the -methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate is characterized by using FT-IR, ^{1}H, ^{13}C NMR and Uv-Vis spectroscopic methods. The molecular structures, vibrational frequencies, ^{1}H and ^{13}C NMR chemicals shifts, UV–vis spectroscopies, HOMO and LUMO analyses and atomic charges of -methoxy-6-[(3-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)-iminomethyl] phenyl benzoate obtained have been calculated by using DFT/B3LYP method. By considering the results of experimental works it can be easily stated that the ^{1}H and ^{13}C NMR chemical shifts, and vibrational frequencies spectroscopic parameters obtained theoretically are in a very good agreement with the experimental data. Also, the electronic structure of titled compound is determined electronic structure identifiers such as the Energy of the Highest Occupied Molecular Orbital, Energy of the Lowest Unoccupied Molecular Orbital, molecular hardness, chemical softness, electronegativity, chemical potential, electrophilicity index, nucleophilicity index and dipole moment. Finally, in this study, the thermodynamic properties of the compound were calculated theoretically.

Scientific Ethics Declaration

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

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