Avrupa Bilim ve Teknoloji Dergisi
Sayı 54, S. 144-151, Aralık 2024

Araştırma Makalesi

www.ejosat.com ISSN:2148-2683

European Journal of Science and Technology
No. 54, pp. 144-151, December 2024

Research Article

Spectroscopic, Thermodynamic, Electronic, HOMO-LUMO, MEP and NLO Analyses of 3-(Benzyl)-4-(3-Acetoxy-4-methoxybenzylideneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

Songül Boy[1], Gül Kotan[2*], Haydar Yüksek[3]

[1]Kafkas University, Atatürk Vocational School of Health Services, Kars, Turkey, ORCID: 0000-0002-6508-8600, Songulboy36@hotmail.com
[*2]Kafkas University, Kars Vocational School, Kars, Turkey, ORCID: 0000-0002-4507-9029, gulkemer@hotmail.com
[3]Kafkas University, Faculty of Sciences and Letter, Department of Chem, Kars,Turkey, ORCID: 0000-0003-1289-1800, hhigh61@gmail.com

(İlk Geliş Tarihi 29 Şubat 2024 ve Kabul Tarihi 24 Nisan 2024)

(**DOI:** 10.5281/zenodo.14202328)

ATIF/REFERENCE: Boy, S., Kotan, G. & Yüksek, H. (2024). Spectroscopic, Thermodynamic, Electronic, HOMO-LUMO, MEP and NLO Analyses of 3-(Benzyl)-4-(3-Acetoxy-4-methoxybenzylideneamino)-4,5-dihydro-1H-1,2,4-triazol-5-one. *European Journal of Science and Technology*, (54), 144-151.

Abstract
In this work, a triazole derivative that is commonly employed in industry, healthcare, particularly the pharmaceutical sector, was theoretically analyzed. The spectroscopic, electronic, thermodynamic, HOMO-LUMO, MEP and NLO properties of molecule were calculated. The molecule optimized with 6-311G(d,p) basis set and $DFT_{(B3LYP)}$ method. The structural properties such as dipole moment (μ), the total energy, electronic properties (electron affinity, molecular softness, ionization potential, molecular hardness and electronegativity), thermodynamic of molecule were determined. The infrared (FT-IR) vibrational data of molecule were determined with Veda 4 software set. The ^{1}H and ^{13}C NMR calculations spectral data were obtained using the GIAO approach in the same basis set and than chemical shift values were compared with experimental data in literature. Also, the surface map such as MEP were obtained and thus, the electrophilic and nucleophilic moieties were shown on the compound. The nonlinear optical properties (NLO) were investigated and the results were evaluated according to the urea reference. Finally, the spectral and structural data of 1,2,4-triazole derivative compound were obtained and assessed in this theoretical study.

Keywords: B3LYP, DFT, MEP, NLO.

3-(Benzil)-4-(3-Asetoksi-4-metoksibenzilidenamino)-4,5-dihidro-1*H*-1,2,4-triazol-5'in Spektroskopik, Termodinamik, Elektronik, HOMO-LUMO, MEP ve NLO Analizleri

Özet
Bu çalışmada endüstride, sağlık sektöründe ve özellikle ilaç sektöründe yaygın olarak kullanılan bir triazol türevinin teorik analizi yapılmıştır. Molekülün spektroskopik, elektronik, termodinamik, HOMO-LUMO, MEP ve NLO özellikleri hesaplanmıştır. Molekül 6-311G(d,p) temel seti ve DFT(B3LYP) yöntemi ile optimize edilmiştir. Molekülün dipol momenti (μ), toplam enerjisi, elektronik özellikleri (elektron ilgisi, moleküler yumuşaklık, iyonlaşma potansiyeli, moleküler sertlik ve elektronegatiflik), termodinamik gibi yapısal özellikleri belirlenmiştir. Molekülün kızılötesi (FT-IR) titreşim verileri Veda 4 yazılım seti ile belirlenmiştir. ^{1}H ve ^{13}C NMR hesaplamalarının spektral verileri aynı temel sette GIAO yaklaşımı kullanılarak elde edildi ve ardından kimyasal kayma değerleri literatürdeki deneysel verilerle karşılaştırılmıştır. Ayrıca MEP gibi yüzey haritası elde edilmiş ve böylece bileşiğin elektrofilik ve nükleofilik kısımları gösterilmiştir. Doğrusal olmayan optik özellikler (NLO) araştırıldı ve sonuçlar üre referansına göre değerlendirilmiştir. Bu teorik çalışmada son olarak 1,2,4-triazol türevi bileşiğinin spektral ve yapısal verileri elde edilmiş ve değerlendirilmiştir.

Anahtar Kelimeler: B3LYP, DFT, MEP, NLO.

1. Introduction

Triazoles including three nitro atoms are five-membered heteroaromatic compounds. This properties of allows easy synthesis of new triazole derivatives. The triazole derivatives have wide usage areas in organic chemistry, pharmacology especially drug designe. Many studies on the evaluation of the biological of the triazoles have shown that the triazole compounds exhibit anti-fungal (Peyton et al, 2015; Shalini et al., 2011; Koltin & Hitchcock, 1997), anti-oksidant (Yüksek et al., 2006; Kotan, 2021), anti-bacterial (Boy et al., 202; Al-Radadi et al., 2020), anti-cancer (Kamal et al., 2008), anti-tuberculos (Zhang et al., 2017), anti-HIV (Li et al., 2013) properties. The compound whose theoritical properties were investigated in this study is a triazole Schiff Base. The Schiff Baze compounds containe azomethine grup (-C=N-) and generaly obtaine by the reaction of aldehyde or ketone with primary amine (Berhanu et al., 2019). The Schiff Bases which have important uses fields as organic chemistry, analitycal chemistry, metal chemistry have played effective role in coordination chemistry and bioinorganic chemistry (Uddin et al., 2020). Many study deal with the Schiff Bazes ligands and their complexes have reported that these compounds show anti-cancer (Zafar et al., 2021), anti-fungal (Chohan et al., 2010), anti-microbiyal (Manap, 2020) properties. In addition , these compounds are inclued in the structure of drugs used in the treatment of many diseases in medicine (Uddin et al., 2020). The Gaussian 09W software was used to do all theoretical calculations for the focus on chemical. (Frisch et al., 2009). The DFT approach was used to optimize the molecule (Wolinski et al 1990; Frisch et al., 2009). The theoretical calculations were performed by using optimized molecule with DFT(B3LYP)/6-311G(d,p) (Boy et al., 2022). The experimental results were acquired from the literature (Bahçeci et al., 2017). Tables and graphs were used to compare and illustrate these results.

2. Result And Discussion

2.1. Computational details

The Gaussian 09W packet software (Frisch et al.,2009) was used to compute all quantum chemical calculations. The GaussView application was used to sketch the molecule Figure 1 depicts the geometric structure and formula that has been optimized. It is the molecule's most stable three-dimensional structure.

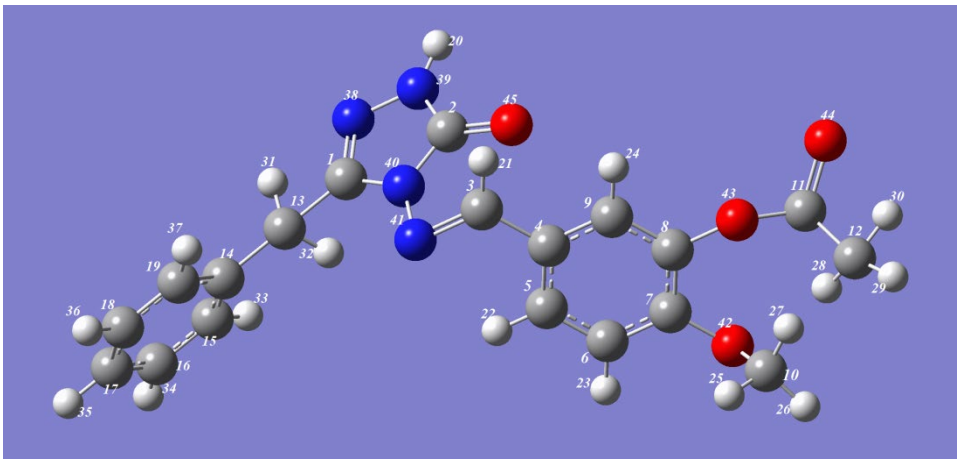

Figure 1. The Gaussview structure of the molecule.

2.2. ^{1}H-NMR calculations

In comparison to experimental values, the theoretical ^{1}H-Nükleer magnetic rezonans chemical shift values were computed in gaseous and solvent (DMSO) environments and are displayed in Table 1. The "GIAO" method (Wolinski, 1990) was used to calculate the proton NMR chemical shift values. The regression analyses were performed, and graphs were created.

Table 1. *^{1}H/ ^{13}C-NMR(DMSO) isotropic chemical shifts (δ/ppm)*

Atoms	Experimental	DFT	Differ/6-311G(d.p)
H20	11.9	7.46	4.44
H21	9.58	9.98	-0.40
H22	7.65	8.28	-0.63
H23	7.55	7.43	0.12
H24	7.17	7.18	-0.01
H25	3.85	3.40	0.45
H26	3.85	3.96	-0.11
H27	3.85	4.04	-0.19

H28	2.3	2.48	-0.18
H29	2.3	2.38	-0.08
H30	2.3	1.75	0.55
H31	4.05	4.05	0.00
H32	4.05	3.89	0.16
H33	7.3	7.73	-0.43
H34	7.2	7.58	-0.38
H35	7.27	7.44	-0.17
H36	7.2	7.52	-0.32
H37	7.3	7.62	-0.32

2.3. Regression Analysis

There is such a link between the compound's R^2-values. B3LYP/6-311G(d,p) (DMSO): 1H: 0.8303, as shown in Figure 2. Theoretical and experimental proton chemical shifts ratios between R2 lineer correlations were observed.

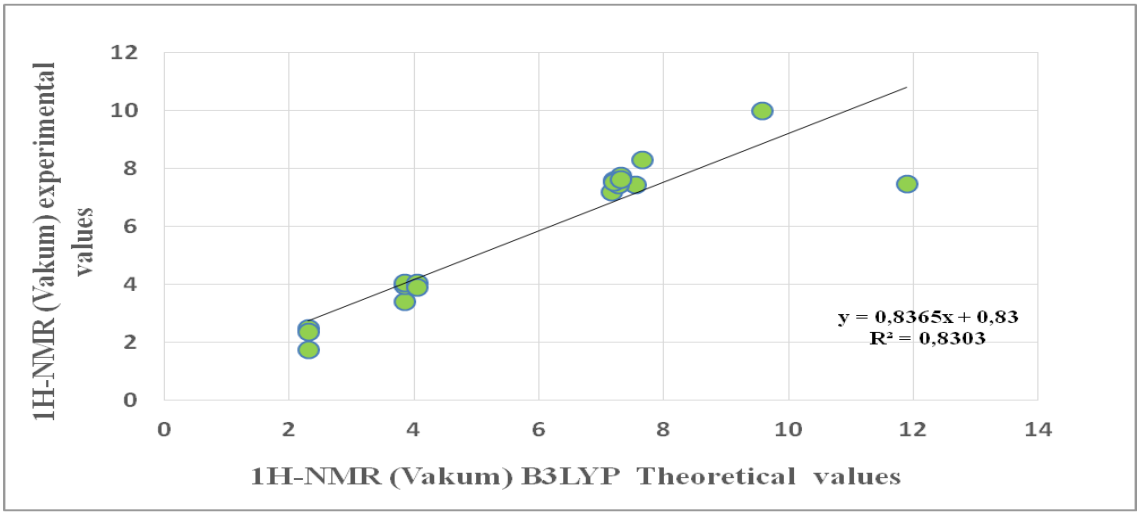

Figure 2. *The ^{1}H-NMR correlation graph*

2.4. The IR Analysis

The theoretical scala values and IR values were calculated using the Veda 4F software (Jamroz et al., 2004). The harmonic vibrational frequency readings were scaled for the B3LYP level using 0.9688. (Merrich et al., 2007). In the data, a positive frequency was discovered. In accordance with DFT method, IR spectrums were drawn using the measured data. Theoretical and empirically acquired IR values were compared, and their values coincided.

Table 3. *Same IR vibrational frequencies (cm^{-1})*

vibrational frequencies	Experimental IR	Scaled B3LYP
ν (NH)	3186	3565
ν (C=O)	1765, 1705	1806-1750
ν (C=N)	1604-1590	1613, 1593
ν (COO)	1276	1279

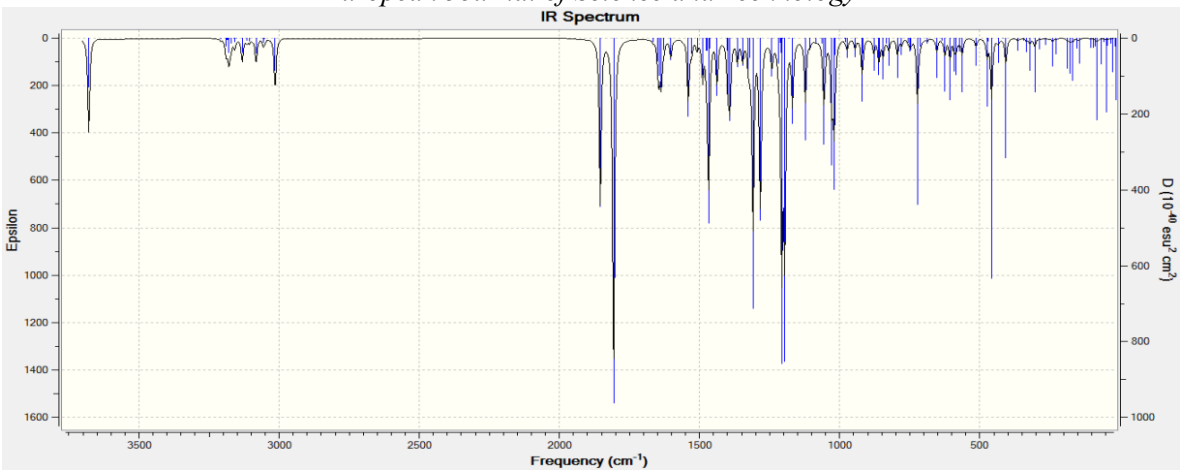

Figure 3. *Experimental Theoretical IR spectrum*

2.5. The mulliken charge calculation

With the use of the 6-311G(d,p) basis set and the "B3LYP" approach, the molecule's mulliken charge values were computed. The mulliken atomic charges (Mulliken, 1955) of the electronegative N38-N41 atoms in the molecule were estimated as negative, while the mulliken charges of all protons in the molecule were computed as positive, according to the findings of the calculations with 6-311G(d,p). In addition, it was discovered that "C1, C2, C3, C7 and C8" atoms had positive mulliken charge values whereas other carbon atoms had negative values. This is due to the presence of one electronegative oxygen atom and two electronegative nitrogen atoms next to the C1, C2, and C3 atoms, respectively.

Table 6. *The calculated all atomic charges*

	B3LYP		B3LYP
C1	0.357	**H24**	0.099
C2	3.535	**H25**	0.101
C3	0.128	**H26**	0.120
C4	-0.168	**H27**	0.115
C5	-0.001	**H28**	0.138
C6	-0.086	**H29**	0.136
C7	0.168	**H30**	0.141
C8	0.161	**H31**	0.152
C9	-0.004	**H32**	0.138
C10	-0.114	**H33**	0.086
C11	0.307	**H34**	0.093
C12	-0.296	**H35**	0.095
C13	-0.161	**H36**	0.096
C14	-0.122	**H37**	0.100
C15	-0.059	**N38**	-0.216
C16	-0.097	**N39**	-0.312
C17	-0.087	**N40**	-0.383
C18	-0.091	**N41**	-0.205
C19	-0.038	**O42**	-0.388
H20	0.251	**O43**	-0.367
H21	0.142	**O44**	-0.371
H22	0.112	**O45**	-0.304
H23	0.102		

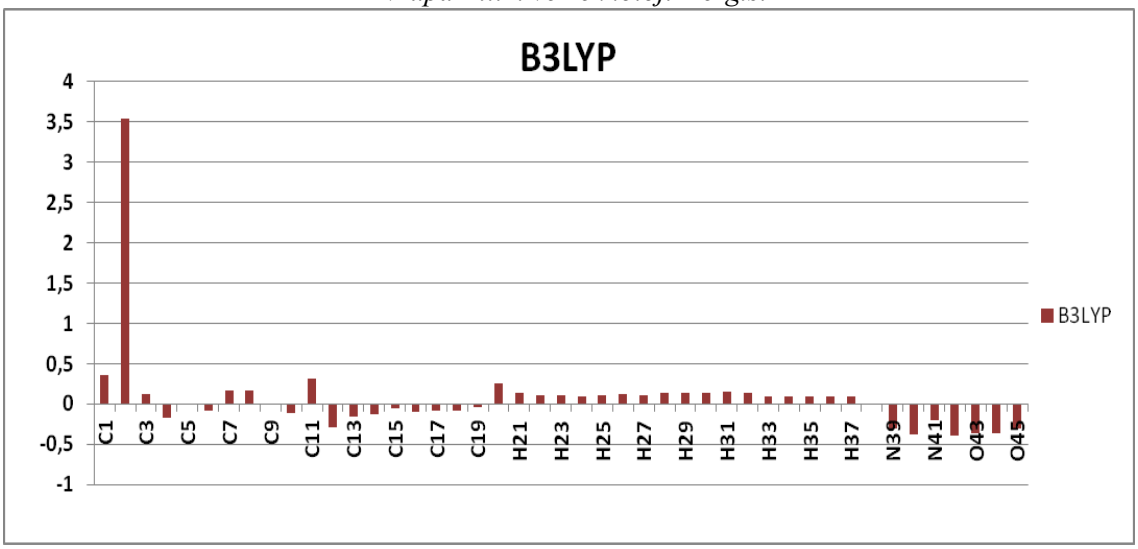

Figure 4.*The calculated mulliken charges*

2.6. FMO's Calculations

Quantum chemical characteristics, for example, E_{HOMO}, E_{LUMO}, and ΔE are useful indicators of a chemical's reactivity. The zone of reactivity at a molecule's border is indicated by the electron density of the molecule. Using DFT/6-311G(d,p), the frontier electron density was determined (Fukui et al., 1952) The excitation energy is calculated as the difference between the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO). The stability of molecules is represented by this energy gap. In a molecule, LUMO stands for an electron acceptor and HOMO for an electron donor (Amudha et al., 2022)

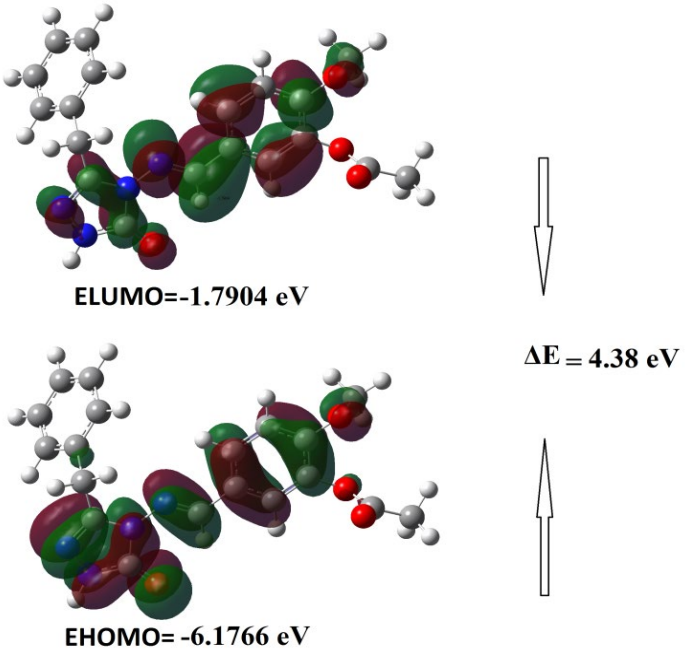

Figure 4. *HOMO-LUMO energy and ΔE*

Table 7. *The calculated electronic data*

		Hatree	ev	kcal/mol	KJ/mol
	LUMO	-0,0658	-1,79046	-41,2897	-172,758
	HOMO	-0,227	-6,17683	-142,443	-595,989
A	Electron Affinity	0,0658	1,79046	41,2897	172,758
I	Ionization Potential	0,227	6,17683	142,443	595,989
ΔE	Energy gap	0,1612	4,38636	101,153	423,231
χ	electronegativity	0,1464	3,98365	91,8664	384,373
Pi	chemical potential	-0,1464	-3,98365	-91,8664	-384,373

ω	electrophilic index	0,000863748	0,0235	0,542	2,26777
IP	Nucleophilic index	-0,01179984	-0,32108	-7,40443	-30,9805
S	molecular softness	12,4069	337,602	7785,4	32574,4
η	molecular hardness	0,0806	2,19318	50,5767	211,615

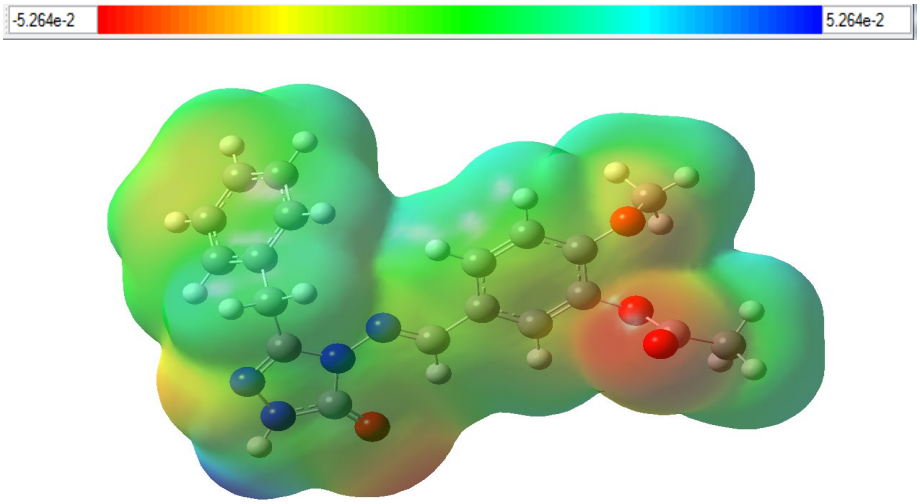

Figure 5. *The MEP*

2.7. Non-Linear Optic Analysis (NLO)

Numerous technologies, including optical computers, dynamic image processing, optical switches, dye lasers, telecommunication devices, and optical disks, have benefited greatly from the development of nonlinear optical (NLO) materials. As a result, efforts are being made to mimic several NLO-phores, including inorganic and organic semiconductors, naturally occurring and artificial nanomaterials, polymers and dyes (Fonseca et al., 2018; Halasyamani et al., 2017; Hussain et al., 2020; Deb et al., 2020; Guo et al., 2018). NLO parameters such as anisotropy of polarizability ($\Delta\alpha$), , average linear polarizability (α), first hyperpolarizability (β_{total}), the total static dipole moment (μ) were determined with DFT_{B3LYP}.

Polarizability "*αxx, αxy, αyy, αxz ,αyz, αzz*"= 347.2495516; 34.860844; 263.7561871; 1.4105161; 7.1858105; 165.1231724 and HyperPolar "*βxxx, βxxy, βxyy, βyyy, βxxz, βxyz, βyyz, βxzz, βyzz, βzzz*" = -139.2929225; 1.2451982; 33.584864; 175.4535599; 42.7543767; -36.4465889; -32.4295204; 15.8601426; 54.6213466; -29.2101699 values, respectively were obtained. These values using assigned theoretical results are $\boldsymbol{\alpha_{total}}$: 38.341x$10^{-24}$ esu, $\boldsymbol{\Delta\alpha}$: 23.402 x$10^{-24}$ esu and $\boldsymbol{\beta^0}$: 20.83 x10^{-31} esu. The primary reference material for NLO qualities is the urea molecule. The NLO parameters for urea refereans according to literature 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 (Kotan et al., 2022). The NLO values were 7.6, 11, and 2.8 times more than urea as compared to the reference material.

Table 8. *The the average polarizability $\boldsymbol{\alpha_{total}}$ (10^{-24} esu), total energy $\boldsymbol{E_{total}}$ (Hatree), the electric dipole moment $\boldsymbol{\mu}$ (Debye) and first hyperpolarizability $\boldsymbol{\beta_{total}}$ (10^{-31} esu) of molecule*

	B3LYP
$\boldsymbol{E_{total}}$	-1255.05045284
μx	0.8805
μy	-2.3122
μz	2.0732
$\boldsymbol{\mu_{Total}}$	3.2280
αxx	347.2495516
αxy	34.860844
αyy	263.7561871
αxz	1.4105161
αyz	7.1858105
αzz	165.1231724
$\boldsymbol{\alpha_{total}}$	38.341x10^{-24} esu
$\boldsymbol{\Delta\alpha}$	23.402 x10^{-24} esu
βxxx	-139.2929225
βxxy	1.2451982
βxyy	33.584864

βyyy	175.4535599
βxxz	42.7543767
βxyz	-36.4465889
βyyz	-32.4295204
βxzz	15.8601426
βyzz	54.6213466
βzzz	-29.2101699
β_{total}	20.83 x10^{-31} esu

2.8. Thermodynamics parameters

Thermodynamic parameters were estimated using B3LYP functionals in the DFT technique at 298.150 K and 1 atm pressure using the 6-311G(d,p) basis.

Table 10. *The calculated thermodynamics parameters of the molecule*

Rotational temperatures (Kelvin)	DFT
A	0.01477
B	0.00423
C	0.00348
Rotational constants (GHZ)	
A	0.30786
B	0.08815
C	0.07245
Thermal Energies E(kcal/mol)	
Translational	0.889
Rotational	0.889
Vibrational	232.220
Total	233.997
Thermal Capacity CV(cal/mol-K)	
Translational	2.981
Rotational	2.981
Vibrational	85.947
Total	91.908
Entropy S(cal/mol-K)	
Translational	43.587
Rotational	36.345
Vibrational	99.280
Total	179.212
Zero-point correction (Hartree/Particle)	0.348073
Thermal correction to Energy	0.372898
Thermal correction to Enthalpy	0.373842
Thermal correction to Gibbs Free Energy	0.288693
Sum of electronic and zero-point Energies	-1254.702380
Sum of electronic and thermal Energies	-1254.677555
Sum of electronic and thermal Enthalpies	-1254.676610
Sum of electronic and thermal Free Energies	-1254.761760
Zero-point vibrational energy (Kcal/mol)	218.41889

3. Conclusion

Some theoretical calculations of the target molecule were made. By comparing the proton nmr data with the experimental one, regression graphs were created. As a result, it was seen that there was a deviation in the ^{1}H-NMR because of the acidic proton (N-H). In addition, the reactivity of the molecule was calculated from the HOMO-LUMO energy difference and many electronic parameters were calculated using this difference. MEP surface map was created and as a result electrophile and nucleophile atoms were determined. Mulliken load values were found. The estimated IR vibration frequency values were compared to the experimental results and their were in agreement with each other.

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