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Experimental (FT-IR, $^{13}C/^{1}H$-NMR) and DFT (B3LYP, B3PW91) Studies of 3-*n*-Propyl-4-[2-(4-Methoxybenzoxy)-3-Methoxy] Benzylidenamino-4,5-Dihydro-1*h*-1,2,4-Triazol-5-Ones Molecule

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Abstract: All theoretical calculations of 3-*n*-propyl-4-[2-(4-methoxybenzoxy)-3-methoxy] benzylidenamino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones has been performed with B3LYP/B3PW91 functions of DFT method using the 6-311G(d,p) basis set (Frisch et al., 2009; Wolinski et. al., 1990). Firstly, optimized to achieve the most stable form of the molecule. Then, the veda4f program was used in defining Infrared (IR) data (Jamróz, 2004). The standard error values were found via the Sigma plot with regression coefficient of a and b constants. The vibrational frequency values of this molecule have been calculated by using 6-311G(d,p) basis set with DFT (B3LYP/ B3PW91) methods. Then, these values are scaled with appropriate scala factors (Merrick et al., 2007). ^{1}H-NMR and ^{13}C-NMR spectral values according to GIAO method (Wolinski et al., 1990) was calculated using Gaussian G09W program package in DMSO solvent and in gas phase. Theoretical spectral values of molecule were compared with experimental values. Experimental data obtained from the literature (Alkan et al., 2014). In addition, electronic properties (electronegativity (χ), global hardness (η), electron affinity (A), ionization potential (I), softness (σ), thermodynamics properties (heat capacity CV^0, entropy S^0 and enthalpy H^0), HOMO-LUMO energy, E_{LUMO}-E_{HOMO} energy gap (ΔEg), geometric properties (bond angles, bond lengths), dipole moments, Mulliken atomic charges, total energy of the molecule were calculated. Finally, the molecular surfaces such as the electron density, molecular electrostatic potential (MEP), contour and the total density maps were designated.

Keywords: B3LYP, B3PW91, DFT, HOMO-LUMO, MEP.

Introduction

The 1,2,4-triazole and its derivatives are important heterocyclic compounds. They are also present in the structure of Schiff bases, which contain a (-C=N-) azomethine group in their structure and, are generally synthesized by the condensation of primary amines with an aldehyde or ketone. The Schiff bases containing 1,2,4-triazole are very active in terms of showing biological activity. In particular, they show antitubercular (Amim, et al., 2017), antibacterial (Kotan, 2021) , antitumor (Demirbaş, et al., 2002), antioxidant (Yüksek, et al., 2011; Manap, et al., 2020), analgesic (Rana, et al., 2012), antifungal (Dharmaraj, et al., 2001), anti-inflammatory (Shukla, et al., 2014) and anticancer properties (Uddin, et al., 2020). The Schiff bases are important molecules in the pharmaceutical and medicinal fields. In recent years, many theoretical studies for Schiff bases containing 1,2,4-triazole have been carried out (Kotan, et al., 2020; Yüksek, et al., 2017; Kotan, et

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al., 2021; Beytur, et al., 2021). Gaussian 09W program was used for quantum chemical calculations. First, the optimization process was carried out to reach the most stable state of the molecule, then the atoms of the molecule were numbered. From this optimized structure, all electronic, thermodynamic, spectroscopic and geometric theoretical values of the molecule were calculated (Frisch et al., 2009). IR vibration frequency values were calculated with the Veda 4f program (Jamróz., 2004) and the vibration frequency data were multipled with definite scala factor (Merrich, et al., 2007) The ^{1}H-^{13}C/ NMR isotropic shift values were calculated by the GIAO method using the Gaussian G09 package program (Wolinski et al., 1990). These values were compared with the experimental values (Alkan, et al., 2002) and the difference values were found, and these values were δ exp=a+b. δ calc. plotted according to the equation. The bond length, HOMO-LUMO energy, total energy, bond angle, mulliken atomic charges, dipole moment of the molecule were calculated. In addition, MEP surface maps were determined.

Method

The 1,2,4-triazole and its derivatives are important heterocyclic compounds. They are also present in the structure of Schiff bases, which contain a (-C=N-) azomethine group in their structure and, are generally synthesized by the condensation of primary amines with an aldehyde or ketone. The Schiff bases containing 1,2,4-triazole are very active in terms of showing biological activity. In particular, they show antitubercular (Amim, et al., 2017), antibacterial (Kotan, 2021) , antitumor (Demirbaş, et al., 2002), antioxidant (Yüksek, et al., 2011; Manap, et al., 2020), analgesic (Rana, et al., 2012), antifungal (Dharmaraj, et al., 2001), anti-inflammatory (Shukla, et al., 2014) and anticancer properties (Uddin, et al., 2020). The Schiff bases are important molecules in the pharmaceutical and medicinal fields. In recent years, many theoretical studies for Schiff bases containing 1,2,4-triazole have been carried out (Kotan, et al., 2020; Yüksek, et al., 2017; Kotan, et al., 2021; Beytur, et al., 2021). Gaussian G09W program was used for quantum chemical calculations. First, the optimization process was carried out to reach the most stable state of the molecule, then the atoms of the molecule were numbered. From this optimized structure, all electronic, thermodynamic, spectroscopic and geometric theoretical values of the molecule were calculated (Frisch et al., 2009). IR vibration frequency values were calculated with the Veda 4f program (Jamróz., 2004) and the vibration frequency data were multipled with definite scala factor (Merrich, et al., 2007) The ^{1}H-^{13}C/ NMR isotropic shift values were calculated by the GIAO method using the Gaussian G09 package program (Wolinski et al., 1990). These values were compared with the experimental values (Alkan, et al., 2014) and the difference values were found, and these values were δ exp=a+b. δ calc. plotted according to the equation. The bond length, HOMO-LUMO energy, total energy, bond angle, Mulliken atomic charges, dipole moment of the molecule was calculated. In addition, MEP surface maps were determined.

Results and Discussion

Theoretical Study

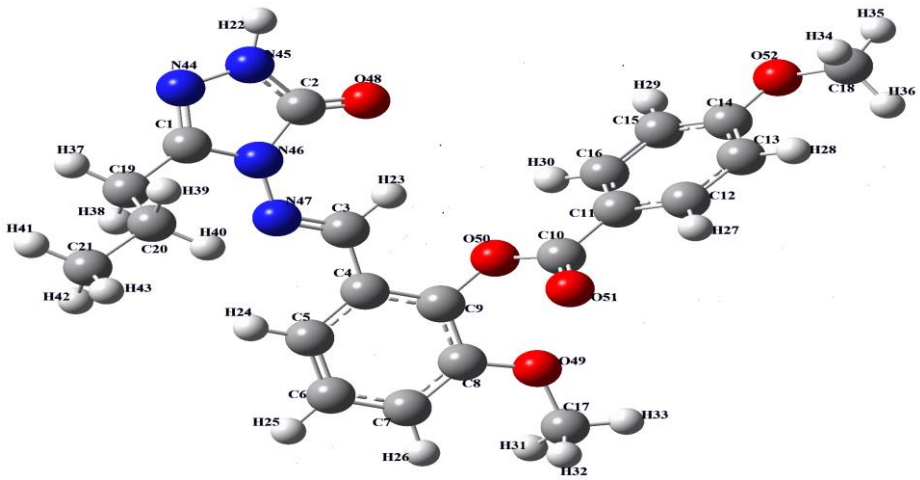


Figure 1. The minimized energy optimized structure of the molecule.

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

No	Experimental	B3LYP/Vacuum	Difference	B3PW91/Vacuum	Difference
C1	147.28	152.53	-5.25	146.91	0.37
C2	152.13	152.32	-0.19	147.29	4.84
C3	148.89	149.45	-0.56	145.22	3.67
C4	127.82	133.94	-6.12	129.05	-1.23
C5	118.58	118.90	-0.32	114.92	3.66
C6	127.42	128.80	-1.38	124.76	2.66
C7	115.65	113.57	2.08	109.72	5.93
C8	151.74	157.90	-6.16	152.42	-0.68
C9	139.71	148.41	-8.7	142.98	-3.27
C10	164.42	166.49	-2.07	161.58	2.84
C11	120.7	125.40	-4.7	120.48	0.22
C12	132.67	138.09	-5.42	134.19	-1.52
C13	114.82	109.64	5.18	105.91	8.91
C14	163.93	169.31	-5.38	163.6	0.33
C15	114.82	120.49	-5.67	116.52	-1.7
C16	132.67	136.93	-4.26	132.79	-0.12
C17	56.6	54.25	2.35	50.36	6.24
C18	56.1	54.25	1.85	50.69	5.41
C19	26.97	31.53	-4.56	27	-0.03
C20	19.17	25.35	-6.18	20.66	-1.49
C21	13.8	14.62	-0.82	11.18	2.62
H22	11.8	7.41	4.39	7.5	4.3
H23	9.9	11.19	-1.29	11.38	-1.48
H24	7.55	8.57	-1.02	8.76	-1.21
H25	7.39	7.92	-0.53	8.09	-0.7
H26	7.31	7.36	-0.05	7.54	-0.23
H27	8.1	9.00	-0.9	9.18	-1.08
H28	7.13	7.33	-0.2	7.52	-0.39
H29	7.13	7.76	-0.63	7.92	-0.79
H30	8.1	9.11	-1.01	9.28	-1.18
H31	3.8	4.58	-0.78	4.3	-0.5
H32	3.8	4.24	-0.44	4.21	-0.41
H33	3.8	4.14	-0.34	4.66	-0.86
H34	3.88	4.28	-0.4	4.35	-0.47
H35	3.88	4.26	-0.38	4.77	-0.89
H36	3.88	4.69	-0.81	4.33	-0.45
H37	2.48	2.95	-0.47	3.07	-0.59
H38	2.48	3.47	-0.99	3.57	-1.09
H39	1.6	2.03	-0.43	2.12	-0.52
H40	1.6	2.68	-1.08	2.77	-1.17
H41	0.88	1.59	-0.71	1.66	-0.78
H42	0.88	1.68	-0.8	1.76	-0.88
H43	0.88	1.87	-0.99	1.94	-1.06

The Relation between R Values of the Compound

There is such a relationship between R^2-values of the compound. B3LYP(vacuum): ^{1}H: 0.8749, ^{13}C: 0.9945; B3PW91(vacuum)6-311G(d,p) ^{1}H: 0.8722,^{13}C: 0.9955. These values for compound were seen in the table 2. Theoretical and experimental carbon/proton chemical shifts ratios between according to R^2 lineer a correlation was observed (Figure 2).

Table 2. The correlation data for chemical shifts

	^{13}C-NMR/ R^2	^{1}H-NMR /R^2
B3LYP/ Vakum	0.9945	0.8749
B3PW91/ Vakum	0.9955	0.8722

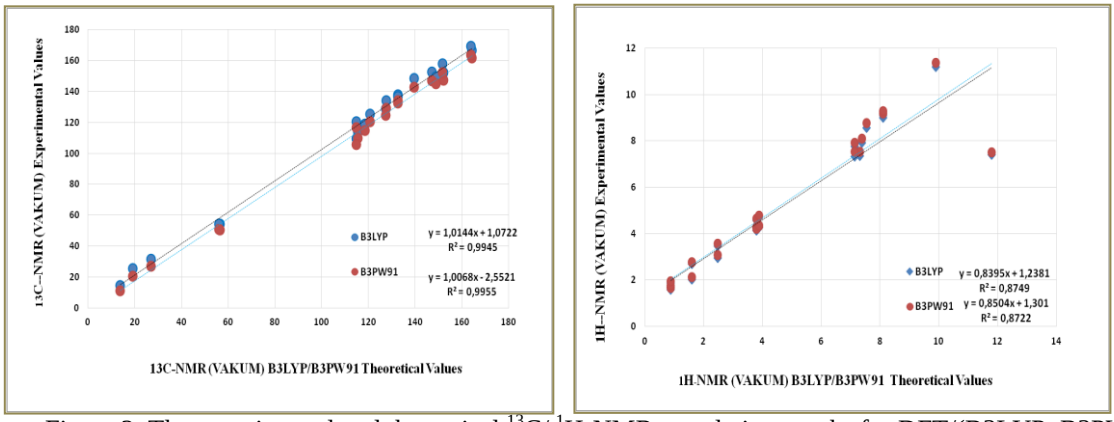


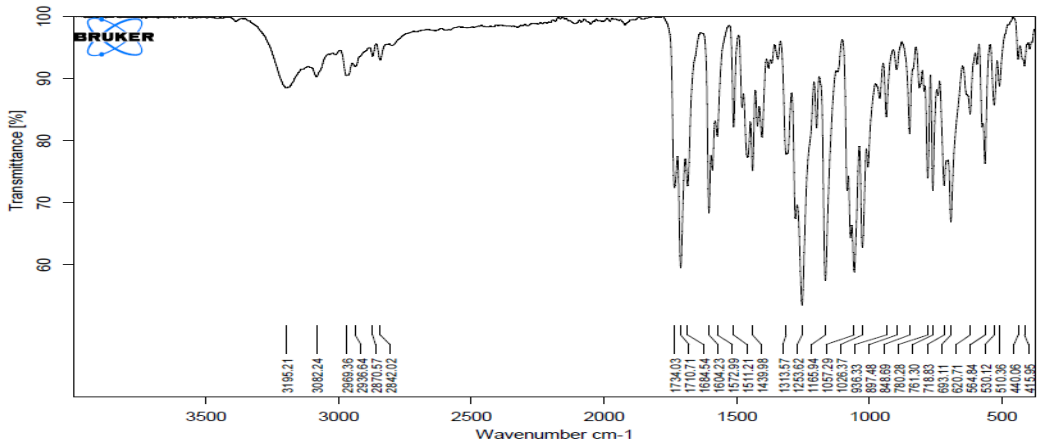
Figure 2. The experimental and theoretical ^{13}C/ ^{1}H-NMR correlation graphs for DFT/(B3LYP, B3PW91) methods chemical shifts

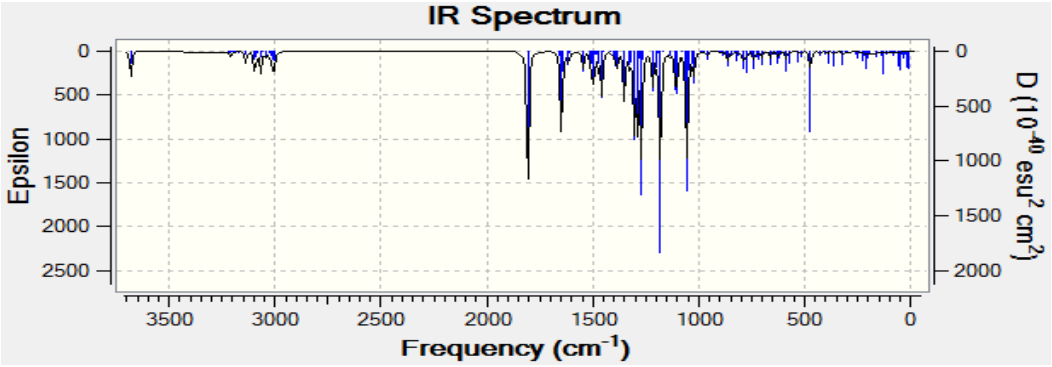
The Infrared Analysis

The IR vibration frequencies were calculated theoretically with the Veda 4f program and the scaled values were obtained by multiplying 0.915 for B3LYP/ 6-311G(d,p) and 0.9905 for B3PW91/ 6-311G(d,p).The using these values were created theoretical IR spectrum graphs and were listed in Table 3.

Table 3. Significant vibrational frequencies (cm^{-1})

vibrations	Scaled B3LYP	Scaled B3PW91	Experimental IR
ν (NH)	3503	3664	3198
ν (C=O)	1720,1718	1812, 1808	1735, 1708
ν (C=N)	1580	1611	1603
ν (COO)	1255	1245	1253





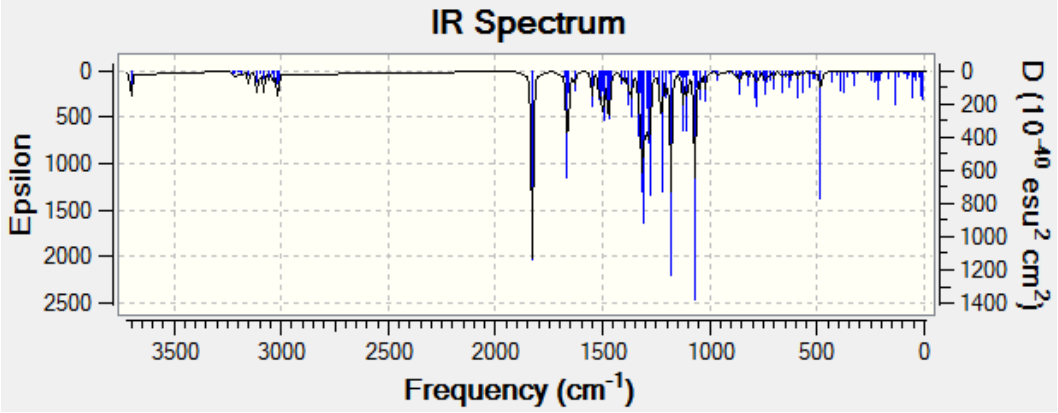


Figure 3. Experimental and theoretical IR spectrums simulated with DFT/(B3LYP, B3PW91)

Molecular Geometry

To calculate these two structure parameters, 6-311 G(d,p) basis set and B3LYP and B3PW91 functions are used. According to this calculations result, the highest bond length is between C(19)-C(20) atoms that this values are 1.54/1.54 Å for B3LYP/ B3PW91 6-311G(d,p). Besides, respectively, the bond lengths in the triazole ring N44-N45, N46-N47, N44-C1, C2-O48, C2-N46, N46-C1, N47=C3 are calculated 1.38/1.37; 1.37/1.36; 1.29/1.29; 1.21/1.21; 1.42/ 1.42; 1.28/ 1.28 Å for B3LYP 6-311G(d,p) basis sets (table 4).

Table 4. The calculated bond lengths with B3LYP/B3PW91 6-311G(d,p)

Bağ Açıları	B3LYP	B3PW91	Bağ Açıları	B3LYP	B3PW91
N(44)-C(1)-N(46)	111.27	111.18	H(26)-C(7)-C(8)	120.41	120.35
N(44)-N(45)-H(22)	120.48	120.46	C(7)-C(8)-O(49)	125.37	125.35
H(22)-N(45)-C(2)	125.07	124.95	O(49)-C(17)-H(31)	111.48	111.50
N(45)-C(2)-O(48)	129.98	129.99	O(49)-C(17)-H(32)	111.21	111.26
O(48)-C(2)-N(46)	128.45	128.90	O(49)-C(17)-H(33)	105.69	105.81
N(45)-C(2)-N(46)	101.16	101.10	C(7)-C(8)-C(9)	118.99	118.97
N(44)-C(1)-C(19)	124.77	124,93	C(8)-C(9)-O(50)	118.84	118.80
C(1)-C(19)-C(20)	113.60	113.51	C(9)-O(50)-C(10)	118.07	117.68
C(1)-C(19)-H(37)	106.65	106.65	O(50)-C(10)-O(51)	122.62	122.70
C(1)-C(19)-H(38)	109.02	108.94	O(50)-C(10)-C(11)	125.96	125.88
C(19)-C(20)-C(21)	113.60	112.17	C(10)-C(11)-C(16)	123.09	123.10
C(19)-C(20)-H(39)	108.74	108.75	C(10)-C(11)-C(12)	117.87	117.80
C(19)-C(20)-H(40)	109.08	109.04	C(11)-C(12)-H(27)	118.60	118.54
C(20)-C(21)-H(41)	111.32	111.34	H(27)-C(12)-C(13)	120.33	120.42
H(42)-C(20)-C(21)	111.68	111.30	C(12)-C(13)-H(28)	119.45	119.46
H(43)-C(21)-C(22)	111.05	111.10	H(28)-C(13)-C(14)	121.08	121.07
H(41)-C(21)-H(42)	107.67	107.63	C(13)-C(14)-O(52)	124.52	124.44
H(42)-C(21)-H(43)	107.64	107.66	C(13)-C(14)-C(15)	119.80	119.80
H(41)-C(21)-H(43)	107.69	107.60	C(14)-O(52)-C(18)	118.80	118.47
C(1)-N(46)-C(2)	108.29	108.28	O(52)-C(18)-H(34)	111.42	111.46
N(46)-N(47)-C(3)	119.92	118.92	O(52)-C(18)-H(35)	111.41	111.46
N(47)-C(3)-H(23)	122.29	122.30	O(52)-C(18)-H(36)	105.71	105.83
H(22)-C(3)-C(4)	118.22	118.40	H(34)-C(18)-H(36)	109.33	109.23
C(3)-C(4)-C(5)	122.21	122.15	H(35)-C(18)-H(36)	109.34	109.23
C(3)-C(4)-C(9)	119.08	119.07	H(34)-C(18)-H(35)	109.52	109.50
C(4)-C(5)-H(24)	118.62	118.54	C(14)-C(15)-H(29)	118.34	118.36
C(4)-C(5)-C(6)	120.16	120.13	H(29)-C(15)-C(16)	121.40	121.41
C(5)-C(6)-H(25)	119.98	119.99	C(15)-C(16)-H(30)	120.04	120.05
C(5)-C(6)-C(7)	120.93	120.91	H(30)-C(16)-C(11)	119.56	119.56
H(25)-C(6)-C(7)	119.08	119.08			
C(6)-C(7)-H(26)	119.69	119.71			

In the literature, the N-N, C=O N=C bond lengths are measured as 1.40, 1.21, 1.28, Å (Sudha et al. 2018). The calculated bond length values are consistent with literature values. The highest bond angle is between N(45)-

C(2)-O(48) atoms, which is 129.98/129.99^0 for B3LYP/ B3PW91 6-311G(d,p) basis sets (table 5). The calculated Mulliken atomic charges (Mulliken, 1955) calculated by using the B3LYP, B3PW91 method with 6-311G(d,p) basis sets. The electronegative oxygen (O) and nitrogen (N) atoms have negative atomic charge values. The carbon atoms surrounded by electronegative atoms have negative atomic charge values. The C1 atom surrounded by two electronegative atoms (N44, N46) and C2 atom which is surrounded by three electronegative atoms (N45, N46, O48) have negative charges values. All hydrogen atoms of the compound (H22-43) have positive atomic charge values (table 6).

Table 5. The calculated bond angles with B3LYP/B3PW91 6-311G(d,p)

bond length	B3LYP	B3PW91	bond length	B3LYP	mPW1PW91
C(1)-N(44)	1.29	1.29	C(7)-C(8)	1.39	1.39
C(1)-N(46)	1.39	1.39	C(8)-O(49)	1.35	1.35
C(1)-C(19)	1.48	1.48	O(49)-C(17)	1.42	1.41
N(44)-N(45)	1.38	1.37	C(17)-H(31)	1.09	1.09
N(45)-H(22)	1.00	1.00	C(17)-H(32)	1.09	1.09
N(45)-C(2)	1.36	1.36	C(17)-H(33)	1.08	1.09
C(2)-N(46)	1.42	1.42	C(8)-C(9)	1.40	1.40
C(2)-O(48)	1.21	1.21	C(9)-O(50)	1.38	1.38
N(46)-N(47)	1.37	1.36	C(4)-C(9)	1.39	1.39
C(19)-H(37)	1.09	1.09	O(50)-C(10)	1.38	1.38
C(19)-H(38)	1.09	1.09	C(10)-O(51)	1.20	1.20
C(19)-C(20)	1.54	1.54	C(10)-C(11)	1.47	1.47
C(20)-H(39)	1.09	1.09	C(11)-C(12)	1.39	1.39
C(20)-H(40)	1.09	1.09	C(12)-H(27)	1.08	1.08
C(20)-C(21)	1.53	1.52	C(12)-C(13)	1.38	1.39
C(21)-H(41)	1.09	1.09	C(13)-H(28)	1.08	1.08
C(21)-H(42)	1.09	1.09	C(13)-C(14)	1.40	1.40
C(21)-H(43)	1.09	1.09	C(14)-C(15)	1.40	1.40
N(47)-C(3)	1.28	1.28	C(15)-H(29)	1.08	1.08
C(3)-H(23)	1.08	1.08	C(15)-C(16)	1.38	1.38
C(3)-C(4)	1.46	1.46	C(16)-H(30)	1.08	1.08
C(4)-C(5)	1.40	1.40	C(14)-O(52)	1.35	1.35
C(5)-H(24)	1.08	1.08	O(52)-C(18)	1.42	1.42
C(5)-C(6)	1.38	1.38	C(18)-H(34)	1.09	1.09
C(6)-H(25)	1.08	1.08	C(18)-H(35)	1.09	1.09
C(6)-C(7)	1.39	1.39	C(18)-H(36)	1.08	1.10
C(7)-H(26)	1.08	1.08			

Table 6. The calculated mulliken charges datas B3LYP/B3PW91 6-311G(d,p)

Atom	B3LYP	B3PW91	Atom	B3LYP	B3PW91	Atom	B3LYP	B3PW91
C1	0.337	0.379	C19	-0.179	-0.222	H37	0.130	0.149
C2	0.530	0.572	C20	-0.232	-0.278	H38	0.133	0.153
C3	0.143	0.172	C21	-0.297	-0.336	H39	0.116	0.134
C4	-0.143	-0.176	H22	0.249	0.257	H40	0.130	0.150
C5	-0.139	-0.033	H23	0.156	0.176	H41	0.105	0.119
C6	-0.032	-0.102	H24	0.103	0.116	H42	0.104	0.119
C7	-0.090	-0.119	H25	0.095	0.104	H43	0.112	0.127
C8	-0.107	0.225	H26	0.109	0.124	N44	-0.221	-0.244
C9	0.213	0.156	H27	0.111	0.121	N45	-0.313	0.333
C10	0.164	-0.171	H28	0.109	0.125	N46	-0.375	-0.409
C11	0.465	0.497	H29	0.107	0.119	N47	-0.209	-0.233
C12	-0.251	-0.290	H30	0.112	0.123	O48	0.385	-0.402
C13	-0.022	-0.024	H31	0.109	0.123	O49	-0.348	-0.390
C14	-0.138	-0.155	H32	0.118	0.132	O50	-0.387	-0.336
C15	0.189	0.197	H33	0.133	0.144	O51	-0.326	-0.343
C16	-0.095	-0.110	H34	0.116	0.130	O52	-0.341	-0.349
C17	-0.131	0.005	H35	0.133	0.144			
C18	0.005	-0.175	H36	0.115	0.128			

MEP Surface Analysis

The molecular electron potential map allows us to identify the electronegative and electropositive atoms of the molecule. When we look at the MEP map, we see different colors because of the electron distribution. The nucleophilic regions with high electron density are in red, and the regions with low electron density, that is, electrophilic regions, are in blue. The region where the carbonyl group and other oxygens are located in the molecule is red in color because of its high electron density, while the surrounding of the N-H acidic proton is blue and were shown in Figure 4.

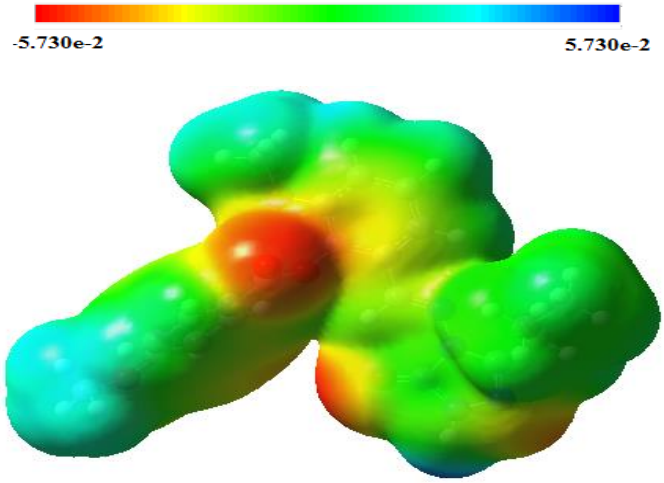


Figure 4**.** The calculated MEP and surface contour map of the molecule

Frontier molecular orbital analysis

Frontier molecular orbitals (FMO) identified optical and electric properties, kinetic stability, the electronic transitions (Fukui, 1982). The HOMO-LUMO energy values was calculated as 4.37/4.37 eV for B3LYP and B3PW91 functionals in the 6-311G(d,p) basis set (figure 5).

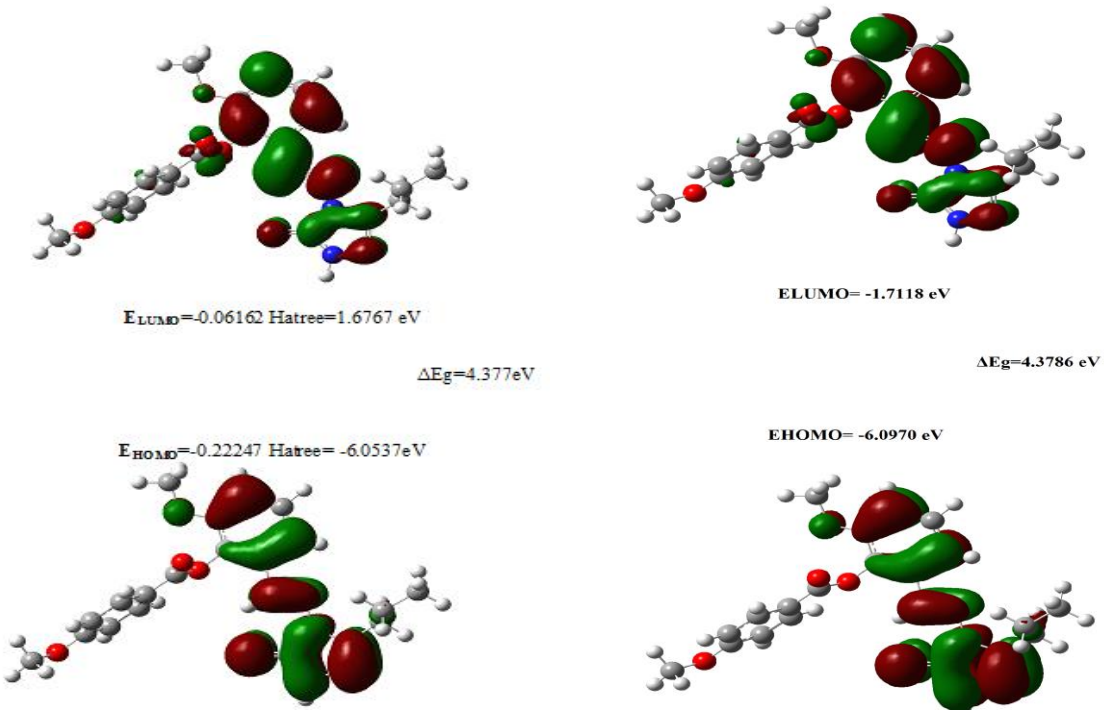


Figure 5. HOMO-LUMO energy of the molecule 6-311G(d,p)

Table 7. The calculated electronic structure parameters of the molecule

		B3LYP		B3PW91	
		Hatree	eV	Hatree	eV
	LUMO	-1,6767	-45,6242	-1,7184	-46,7589
	HOMO	-6,0537	-164,725	-6,097	-165,904
A	elektron ilgisi	1,6767	45,6242	1,7184	46,7589
I	İyonlaşma potansiyeli	6,0537	164,725	6,097	165,904
ΔE	energy gap	4,377	119,101	4,3786	119,145
χ	electronegativity	3,8652	105,175	3,9077	106,331
Pi	chemical potential	-3,8652	-105,175	-3,9077	-106,331
ω	electrophilic index	16,34784446	444,836	16,71543608	454,839
IP	Nucleophilic index	-8,4589902	-230,175	-8,55512761	-232,791
S	molecular softness	0,4569	12,4335	0,4568	12,4289
η	molecular hardness	2,1885	59,5506	2,1893	59,5724

Table 8. The calculated dipole moments datas of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
B3LYP	-1.9556	1.5362	0.3083	2.5059
B3PW91	2.0727	5.5753	-1.7611	6.2033

Table 9. The calculated total energy datas of the molecule

Energy(a.u.)	B3LYP	B3PW91
	-1408.9372	-1408.3805

Table 10. The calculated thermodynamics parameters of the molecule

Parameters	B3LYP	B3PW91
Rotational temperatures (Kelvin)		
A	0.00889	0.00897
B	0.00409	0.00410
C	0.00300	0.00301
Rotational constants (GHZ)		
A	0.18520	0.18695
B	0.08532	0.08553
C	0.06241	0.06273
Thermal Energies E(kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	273.264	274.209
Total	275.041	275.986
Thermal Capacity CV(cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	99.719	99.395
Total	105.680	105.356
Entropy S(cal/mol-K)		
Translational	43.925	43.925
Rotational	37.031	37.014
Vibrational	114.189	113.691
Total	195.145	194.631
Zero-point correction (Hartree/Particle)	0.409861	0.411456
Thermal correction to Energy	0.438306	0.439812
Thermal correction to Enthalpy	0.439251	0.440756
Thermal correction to Gibbs Free Energy	0.346531	0.348281
Sum of electronic and zero-point Energies	-1408.527436	-1407.969093
Sum of electronic and thermal Energies	-1408.498990	-1407.940737
Sum of electronic and thermal Enthalpies	-1408.498046	-1407.939793
Sum of electronic and thermal Free Energies	-1408.590766	-1408.032268
Zero-point vibrational energy (Kcal/mol)	257.19173	258.19228

Thermodynamics Properties

Thermodynamics parameters were calculated with the (B3LYP/ B3PW91) functionals of DFT method at 298.150 K and under 1 atm pressure and were summarized in the Table 10.

Conclusion

In this theoretical study, which supports all the experimentally obtained parameters, all the theoretical properties of the substance recorded in the literature have been studied. As a result, the experimental spectroscopic values of the molecule and the theoretical values obtained with the B3LYP and B3PW91 functions were compared. We observed that in all spectral calculation results, the values of both functions are very close to each other and to the experimental one. We were also able to find electrophilic and nucleophilic regions from the MEP map. Finally, we visualized the HOMO-LUMO orbitals of the molecule and calculated the energy gaps between them.

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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