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Theoretical (6-311G(d,p)/ 3-21G) and Spectroscopic (^{13}C/ ^{1}H-NMR, FT-IR) Analyses pf 3-Propyl-4-[3-(2-Methylbenzoxy)-Benzylidenamino]-4,5-Dihydro-1*h*-1,2,4-Triazol-5-One Molecule

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Abstract: The molecule was studied with the method Density Functional Theory (DFT) using two different the basis sets (6-311G(d,p)/ 3-21G) in the Gaussian 09W program. First, the most stable three-dimensional shape of the molecule was determined with the GaussView5.0 program (Dennington et al., 2009). Based on the structure of this optimized molecule, spectroscopic properties (FT-IR, ^{13}C/ ^{1}H-NMR), the electronic properties (electron affinity (A), ionization potential (I), electronegativity (χ), chemical hardness and softness, electrophilic and nucleophilic index), HOMO-LUMO energies and $\Delta E g$ energy, the geometric properties (bond length and angle) ve the thermodynamic properties (thermal energy (E), thermal capacity (CV), entropy (S)) were calculated with DFT/ 6-311G(d,p) and 3-21G. In addition, the total energy of the molecule, mulliken atomic charge values, dipole moment, molecular electron potential (MEP), total density and contour surface maps were determined. The electrophilic and nucleophilic regions of the structure were confirmed. Theoretical calculations of ^{13}C/ ^{1}H-NMR isotropic shift values were performed in gas phase and solvent (DMSO) acording to GIAO method and regression analyzes were by compare with experimental values of computational data. R^{2} values were calculated and regression graphs were created. FT-IR (Infrared) vibration frequency values were calculated from the Veda4f program. The theoretical vibration frequency values were compared with the experimental IR values. Experimental data obtained from the literature.

Keywords: 1,2,4-Triazole-5-one, Giao, Mep, Homo-Lumo.

Introduction

Compounds containing the 4,5-dihydro-1*H*-1,2,4-triazol-5-one ring are antimicrobial (Turan-Zitouni et.al., 2005; Bayrak et.al., 2010), antitumor, anti-HIV (Ikizler et.al, 1998), antifungal (Sancak et.al.,2010), anticancinogenic (Guzeldemirci et. al., 2010), inflammation preventive (Aytac et.al.,2009), antiviral (Hashem et.al., 2007), antioxidant (Gürsoy-Kol et.al., 2016), with biological properties (Chohan et.al., 2010), with pharmacological properties (Kucukguzel et.al., 2000), antimycobacterial (Klimeová et.al., 2004) have been reported in many different studies. Quantum chemical calculations have been used commonly to theoretically estimate the structure, electronic properties, thermodynamics, spectroscopy of molecular systems. (Yüksek et.al., 2005) Theoretical calculations investigated for the molecule were calculated with the Gaussian 09 quantum chemistry program (Frisch et.al., 2009) on an equipped computer. Assential calculations were carried out using the Density Functional Theory DFT method with the restricted B3LYP (Kohn et.al., 1996; Becke
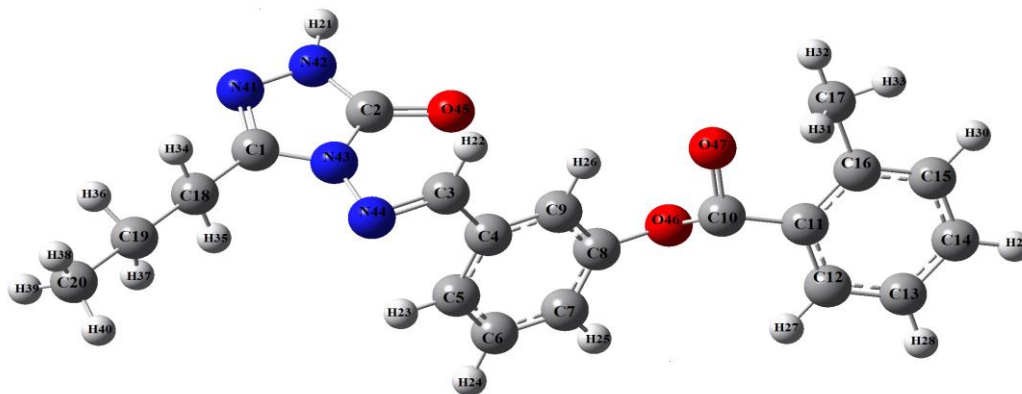
Figure 1. The Gaussview structure of the molecule.

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

No	Deneysel	B3LYP 3-21G/DMSO	Fark/DMSO	B3LYP/6-311G/DMSO	Fark/DMSO
C1	146.93	134.70	12.23	153.21	-6.28
C2	152.66	133.71	18.95	153.76	-1.10
C3	151.26	135.39	15.87	153.80	-2.54
C4	135.22	117.53	17.69	139.83	-4.61
C5	120.69	104.81	15.88	124.31	-3.62
C6	130.27	112.28	17.99	133.90	-3.63
C7	125.08	106.36	18.72	127.88	-2.80
C8	151.03	138.43	12.60	157.70	-6.67
C9	128.13	107.23	20.90	130.42	-2.29
C10	165.19	151.77	13.42	168.33	-3.14
C11	126.25	111.24	15.01	129.95	-3.70
C12	131.89	115.09	16.80	136.54	-4.65
C13	125.47	109.90	15.57	129.77	-4.30
C14	133.08	116.84	16.24	138.65	-5.57
C15	130.84	115.30	15.54	136.02	-5.18
C16	140.20	127.13	13.07	151.59	-11.39
C17	21.23	22.78	-1.55	25.07	-3.84
C18	26.62	25.14	1.48	30.52	-3.90
C19	18.85	19.28	-0.43	23.17	-4.32
C20	13.46	10.90	2.56	12.14	1.32
H21	11.88	6.71	5.17	8.06	3.82
H22	9.77	10.05	-0.28	10.88	-1.11
H23	7.77	7.70	0.07	9.00	-1.23
H24	7.60	7.10	0.50	8.45	-0.85
H25	8.12	6.78	1.34	8.18	-0.06
H26	7.79	8.38	-0.59	8.31	-0.52
H27	7.43	8.14	-0.71	9.38	-1.95
H28	7.62	6.96	0.66	8.26	-0.64
H29	7.47	7.12	0.35	8.44	-0.97
H30	7.45	7.01	0.44	8.29	-0.84
H31	2.61	2.86	-0.25	3.53	-0.92
H32	2.61	2.85	-0.24	3.67	-1.06
H33	2.61	2.07	0.54	2.94	-0.33
H34	2.66	1.93	0.73	2.98	-0.32
H35	2.66	2.88	-0.22	3.93	-1.27
H36	1.69	1.60	0.09	2.59	-0.90
H37	1.69	1.39	0.30	2.41	-0.72
H38	0.95	0.74	0.21	1.52	-0.57
H39	0.95	0.67	0.28	1.49	-0.54
H40	0.95	0.70	0.25	1.71	-0.76

et.al., 1993; Becke et.al., 1988) level of theory, using 6-31G(d,p) basis sets, for all atoms (Kotan et.al., Beytur et al., 2019). In this study, IR absorption frequencies of analyzed molecules were calculated Then, they were compared with experimental data (Ulufer, 2002), which are shown to be accurate.

Method

In this study, the Gaussian 09W package program, which is a very comprehensive program, was used. First of all, with the B3LYP/6-311G(d,p) and 3-21G(d,p) basis sets of Density Functional Theory, the most stable low-energy optimized structure of atoms and molecules has been established. Each atom was then given a number. From this optimized structure, all geometric, electronic, thermodynamic and spectroscopic theoretical values of the molecule were calculated (Frisch et al., 2009). IR vibration frequency values were calculated with the Veda 4f program (Jamróz, 2004). The ^{1}H-NMR and ^{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 (Ulufer, 2002) and the difference values were found, and these values were δ exp=a+b. δ calc. plotted according to the equation. The regression coefficient and standard error values of constants a and b were found using the Sigmaplot program. The dipole moment, HOMO-LUMO energy, total energy, bond angle, bond length, mulliken atomic charges of the target molecule were calculated. In addition, MEP surface maps were determined.
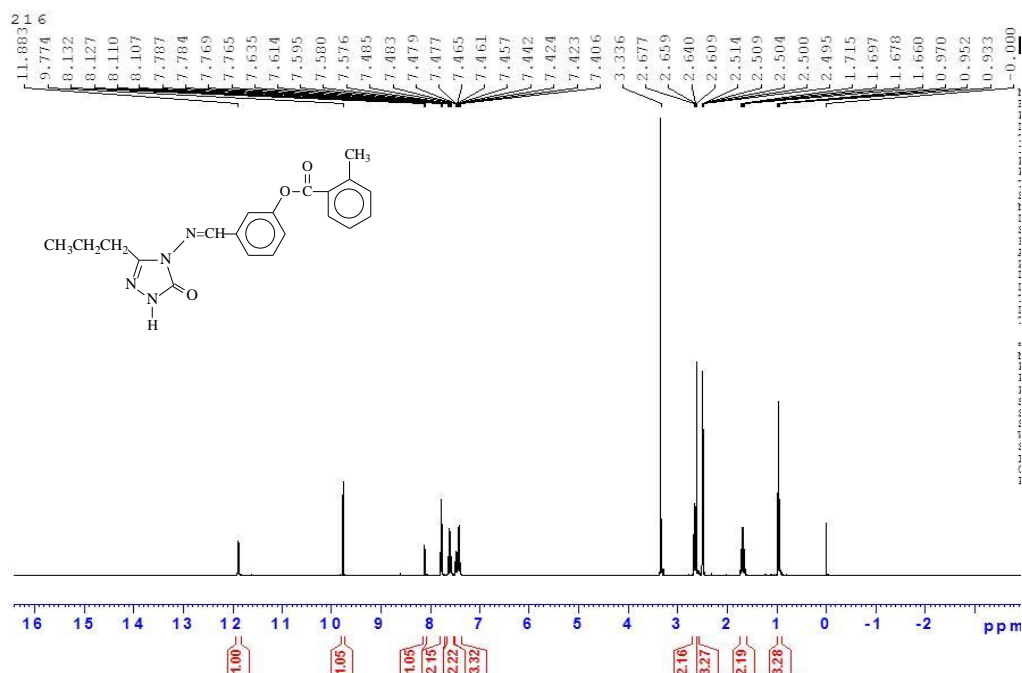
Results and Discussion

Computational Details

The Relation between R Values of the Compound

There is such a relationship between R^2-values of the compound. B3LYP/3-21G(d,p) (DMSO): ^{1}H: 0,8768, ^{13}C: 0,9946; B3LYP/6-311G(d,p) (DMSO): ^{1}H: 0,8956, ^{13}C: 0,9978. These values for compound were seen in the table 2. Theoretical and experimental carbon/proton chemical shifts ratios between acording to a, b values, R^2 lineer a correlation were observed.

Table 2. The correlation data for chemical shifts

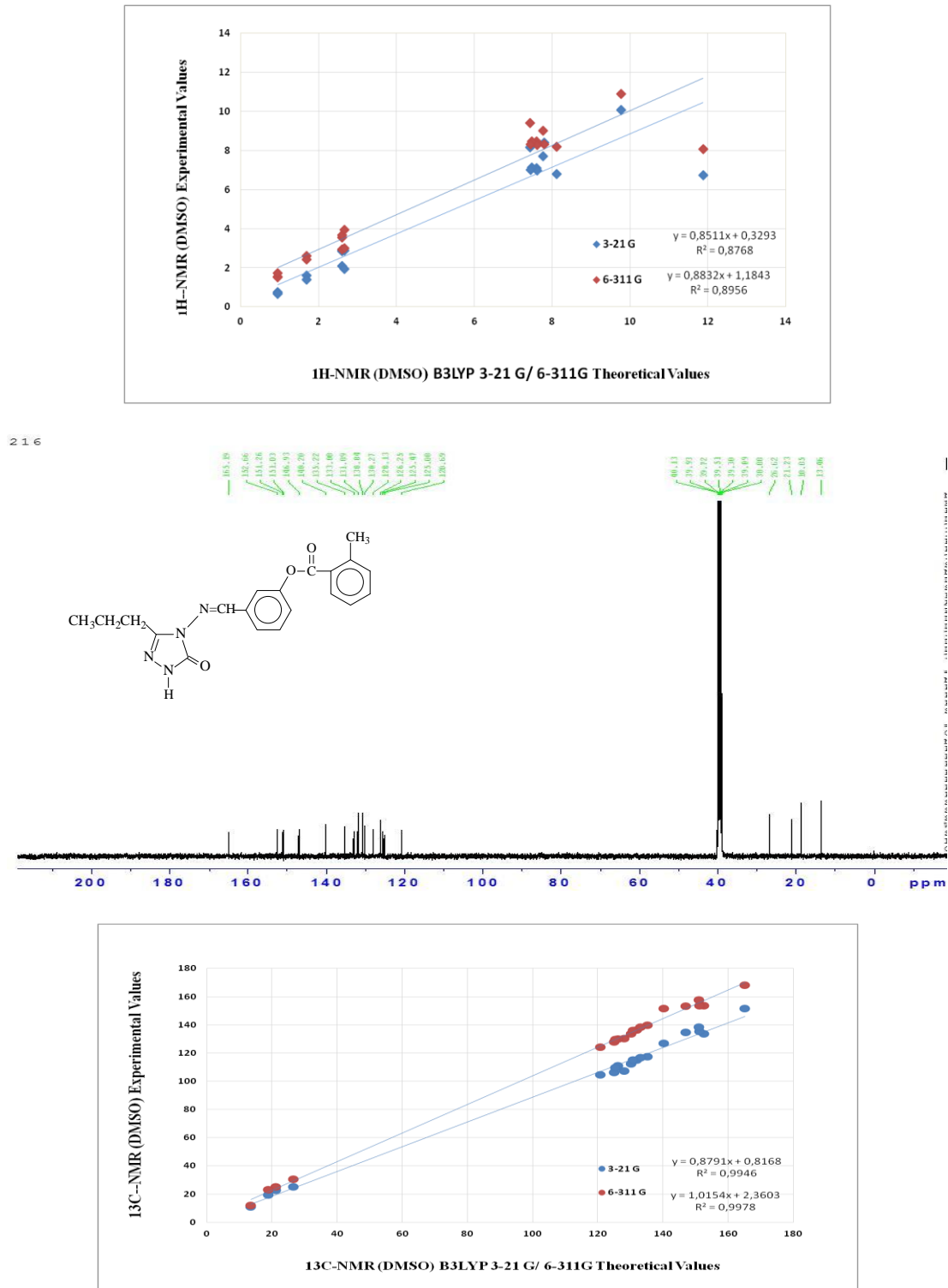|	^{13}C-NMR/ R^2	^{1}H-NMR /R^2
3-21G(d,p)	0.9946	0.8768
6-311G(d,p)	0.9978	0.8956

Figure 2. The experimental and theoretical ^{13}C/ ^{1}H-NMR correlation graphs for B3LYP 6-311G(d,p) and B3LYP 3-21G(d,p) DMSO chemical shifts

The Vibration Frequency of the Compound

Theoretically IR values were calculation veda 4f program and scale values were obtain. The calculated harmonic vibrational frequency values were scaled with 0.9671 for B3LYP 3-21 G level, 0.9688 for 6-311G(d,p) level (Merrick et al., 2007). The positive frequency in the data was found. IR spectrums were drawn

with obtained values according to DFT method. Theoretically IR values were compare with experimentally IR values and found corresponding with each other of values.

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

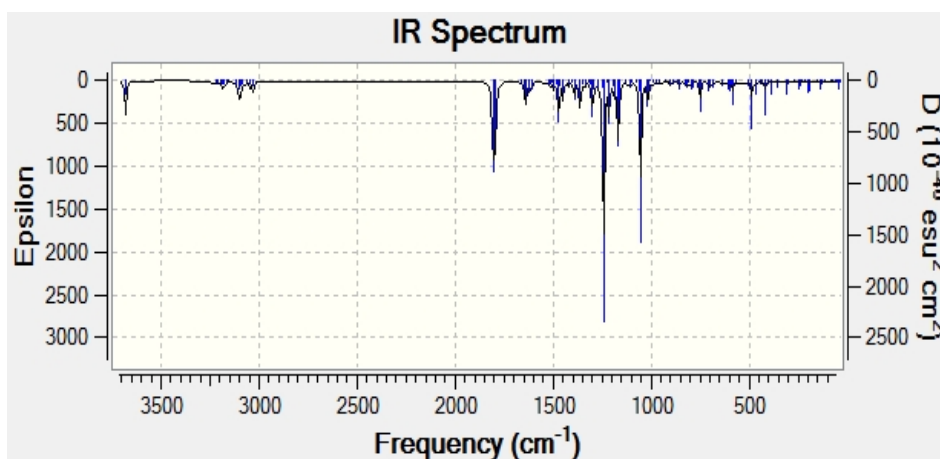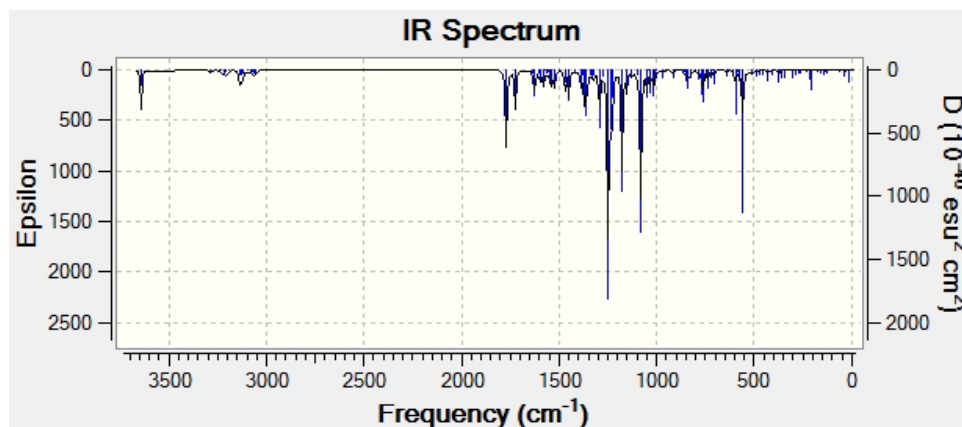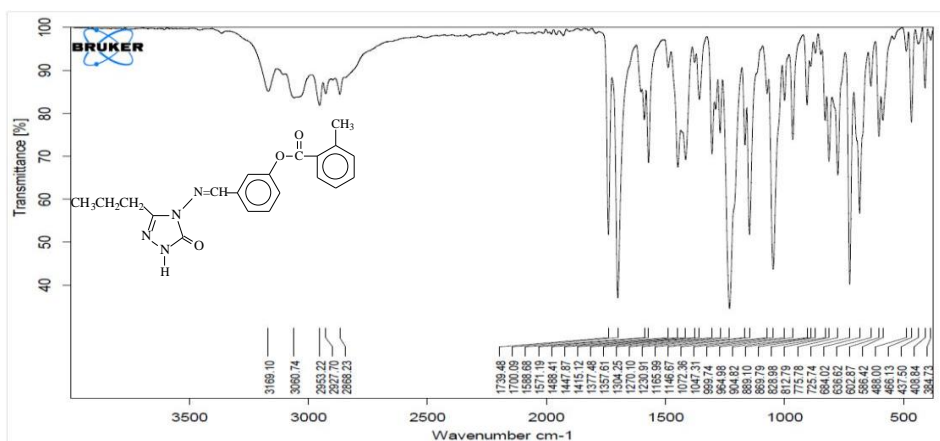| Experimental IR	Scaled B3LYP 3-21G	Scaled B3LYP 6-311G	Experimental IR
ν (NH)	3169	3514	3565
ν (C=O)	1739. 1700	1708. 1664	1737. 1750
ν (C=N)	1589	1577	1613
ν (COO)	1231	1248	1259

Figure 3. Experimental and theoretical IR spectrums simulated with B3LYP 3-21G(d,p) and B3LYP 6-311G(d,p)

Molecular Geometry

The molecular geometric parameters such as bond angles, mulliken atomic charges, bond lengths calculated by using the and B3LYP functional in DFT method with 3-21G(d,p)/ 6-311G(d,p) basis set and data are summarized in Table 4-6. According to this result, the highest bond length is between C(18)-C(19) atoms that this values are 1.555/1.544 Å for B3LYP 3-21G(d,p)/ 6-311G(d,p). Besides, respectively, the bond lengths in the triazole ring N41-N42, N41-C1, C2-O45, C2-N43, N43-C1 are calculated 1.43/1.38; 1.31/1.29; 1.23/1.21;1.43/1.42, 1.39/ 1.39 Å for B3LYP 3-21G(d,p)/ 6-311G(d,p) basis sets (table 4). In the literature, the N-N, N=C, C=O bond lengths are measured as 1.404, 1.280, 1.212 Å (Sudha et al. 2018).

The calculated bond length values are consistent with literature values. The highest bond angle is between H(21)-N(42)-C(2) atoms, which is $126.510/125.116^0$ for B3LYP 3-21G(d,p)/ 6-311G(d,p) basis sets (table 5). The calculated Mulliken atomic charges (Mulliken, 1955) calculated by using the B3LYP method with 3-21G(d,p) and 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 (N41, N43) and C2 atom which is surrounded by three electronegative atoms (N42, N43, O45) have negative charges values. All hydrogen atoms of the compound (H22-H40) have positive atomic charge values (table 6).

Table 4. The calculated bond lengths with B3LYP 3-21G/ B3LYP 6-311G(d,p)

	Bond Length	B3LYP 3-21G	B3LYP 6-311G		Bond Length	B3LYP 3-21G	B3LYP 6-311G
1	C(1)-N(41)	1.316	1.296	27	C(6)-C(7)	1.394	1.395
2	C(1)-N(43)	1.397	1.391	28	C(7)-H(25)	1.081	1.082
3	C(1)-C(18)	1.482	1.490	29	C(7)-C(8)	1.397	1.389
4	N(41)-N(42)	1.438	1.380	30	C(8)-O(46)	1.409	1.392
5	N(42)-H(21)	1.008	1.005	31	C(8)-C(9)	1.395	1.390
6	N(42)-C(2)	1.376	1.368	32	C(9)-H(26)	1.077	1.081
7	C(2)-O(45)	1.237	1.215	33	O(46)-C(10)	1.399	1.378
8	C(2)-N(43)	1.433	1.420	34	C(10)-O(47)	1.229	1.203
9	N(43)-N(44)	1.410	1.369	35	C(10)-C(11)	1.480	1.488
10	C(18)-H(34)	1.093	1.092	36	C(11)-C(12)	1.404	1.403
11	C(18)-H(35)	1.094	1.093	37	C(11)-C(16)	1.415	1.416
12	C(18)-C(19)	1.555	1.544	38	C(12)-H(27)	1.079	1.080
13	C(19)-H(36)	1.094	1.093	39	C(12)-C(13)	1.389	1.387
14	C(19)-H(37)	1.096	1.095	40	C(13)-H(28)	1.083	1.083
15	C(19)-C(20)	1.541	1.530	41	C(13)-C(14)	1.396	1.392
16	C(20)-H(38)	1.095	1.093	42	C(14)-H(29)	1.084	1.083
17	C(20)-H(39)	1.096	1.094	43	C(14)-C(15)	1.393	1.392
18	C(20)-H(40)	1.094	1.093	44	C(15)-H(30)	1.084	1.084
19	N(44)-C(3)	1.297	1.284	45	C(15)-C(16)	1.401	1.399
20	C(3)-H(22)	1.084	1.086	46	C(16)-C(17)	1.518	1.508
21	C(3)-C(4)	1.465	1.466	47	C(17)-H(31)	1.093	1.091
22	C(4)-C(5)	1.403	1.403	48	C(17)-H(32)	1.093	1.091
23	C(4)-C(9)	1.403	1.400	49	C(17)-H(33)	1.093	1.091
24	C(5)-H(23)	1.081	1.082				
25	C(5)-C(6)	1.391	1.386				
26	C(6)-H(24)	1.083	1.083				

MEP Surface Analysis

Electrophilic and nucleophilic regions of the molecule were determined by drawing the MEP map of the molecule with the 3-21G(d,p) and 6-311G(d,p) basic sets of B3LYP method. Different values of electrostatic energy are indicated by different colors. Red means there is very negative electrostatic energy, blue means there is very positive electrostatic energy. When the MEP map is examined, the region of N41, N46, O45 and O47 atoms and are in red, the region of H21 acidic proton atom is in blue, while the around of C-H atoms are in yellow-green.

Table 5. The calculated bond angles with B3LYP 3-21G/ B3LYP 6-311G(d,p)

bond angle	B3LYP 3-21G	B3LYP 6-311G	bond angle	B3LYP 3-21G	B3LYP 6-311G
N(41)-C(1)-N(43)	112.039	111.165	C(5)-C(6)-H(24)	120.150	120.008
N(41)-N(42)-H(21)	119.515	120.460	C(5)-C(6)-C(7)	120.358	120.530
H(21)-N(42)-C(2)	126.510	125.116	H(24)-C(6)-C(7)	119.493	119.462
N(42)-C(2)-O(45)	101.250	130.065	C(6)-C(7)-H(25)	121.563	121.519
O(45)-C(2)-N(43)	127.934	128.755	H(25)-C(7)-C(8)	118.556	119.202
N(43)-C(1)-C(18)	125.203	108.324	C(7)-C(8)-O(46)	113.865	116.550
C(1)-C(18)-H(34)	107.770	106.623	O(46)-C(8)-C(9)	125.611	122.292
C(1)-C(18)-H(35)	108.687	108.559	C(8)-C(9)-H(26)	119.801	120.225
C(1)-C(18)-C(19)	111.816	114.179	C(8)-O(46)-C(10)	125.652	120.495
H(34)-C(18)-H(35)	109.318	107.958	O(46)-C(10)-O(47)	122.921	122.433
H(34)-C(18)-C(19)	109.937	110.061	O(47)-C(10)-C(11)	110.229	126.390
H(35)-C(18)-C(19)	109.268	109.261	C(11)-C(12)-H(27)	118.461	118.795
C(18)-C(19)-H(36)	108.054	108.942	H(27)-C(12)-C(13)	120.779	120.062
C(18)-C(19)-H(37)	108.236	107.580	C(12)-C(13)-H(28)	120.122	120.094
C(19)-C(20)-H(38)	110.738	111.651	H(28)-C(13)-C(14)	120.403	120.619
C(19)-C(20)-H(39)	110.470	111.194	C(13)-C(14)-H(29)	120.173	120.292
C(19)-C(20)-H(40)	110.817	111.651	H(29)-C(14)-C(15)	119.809	119.778
H(38)-C(20)-H(39)	107.841	107.392	C(14)-C(15)-H(30)	119.705	119.350
H(39)-C(20)-H(40)	108.331	107.780	H(30)-C(15)-C(16)	118.630	118.527
H(38)-C(20)-H(40)	108.548	107.844	C(11)-C(12)-C(13)	120.760	121.143
C(1)-N(43)-C(2)	109.324	108.324	C(12)-C(13)-C(14)	119.475	119.287
N(43)-N(44)-C(3)	117.283	119.222	C(16)-C(17)-H(31)	111.133	111.684
N(44)-C(3)-H(22)	122.331	122.094	C(16)-C(17)-H(32)	111.136	111.550
H(22)-C(3)-C(4)	117.887	117.792	C(16)-C(17)-H(33)	109.644	109.908
C(3)-C(4)-C(5)	119.627	122.481	H(31)-C(17)-H(32)	106.312	105.889
C(3)-C(4)-C(9)	117.901	117.927	H(31)-C(17)-H(33)	109.268	108.853
C(4)-C(5)-H(23)	118.869	119.110	H(32)-C(17)-H(33)	109.274	108.825
C(4)-C(5)-C(6)	119.627	120.005			
C(4)-C(9)-C(8)	119.226	119.558			
H(23)-C(5)-C(6)	119.998	120.885			

Table 6. The calculated mulliken charges datas B3LYP 3-21G/ B3LYP 6-311G(d,p)

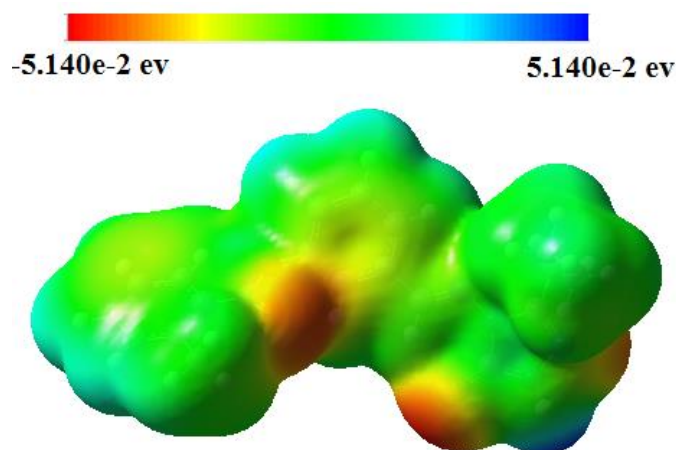| Atom	3-21G B3LYP	6-311G B3LYP	Atom	3-21G B3LYP	6-311G B3LYP
C1	0.660	0.342	H25	0.206	0.106
C2	0.948	0.534	H26	0.245	0.112
C3	0.109	0.133	H27	0.213	0.111
C4	-0.055	-0.173	H28	0.193	0.098
C5	-0.174	-0.015	H29	0.196	0.100
C6	-0.183	-0.103	H30	0.191	0.098
C7	-0.192	-0.056	H31	0.226	0.131
C8	0.301	0.152	H32	0.225	0.133
C9	-0.211	-0.010	H33	0.184	0.093
C10	0.710	0.436	H34	0.221	0.133
C11	-0.113	-0.215	H35	0.227	0.138
C12	-0.165	-0.003	H36	0.212	0.129
C13	-0.185	-0.094	H37	0.193	0.111
C14	-0.173	-0.067	H38	0.201	0.113
C15	-0.179	-0.076	H39	0.188	0.104
C16	0.029	-0.071	H40	0.189	0.109
C17	-0.587	-0.206	N41	-0.342	-0.216
C18	-0.429	-0.199	N42	-0.594	-0.313
C19	-0.384	-0.239	N43	-0.626	-0.374
C20	-0.554	-0.287	N44	-0.319	-0.207
H21	0.353	0.250	O45	-0.521	-0.387
H22	0.263	0.144	O46	-0.601	-0.374
H23	0.208	0.108	O47	-0.490	-0.325
H24	0.196	0.100			

Figure 4. The calculated MEP molecular surface of the molecule

Frontier Molecular Orbital Analysis

Frontier molecular orbitals (FMO) designated kinetic stability, the electronic transitions, electric and optical properties (Fukui, 1982). HOMO-LUMO energy values of compound was calculated with three computational levels and these values are 4.33/4.35 eV for B3LYP 3-21G(d,p) and 6-311G (d,p) basis sets (figure 4). Using HOMO-LUMO energy gap electron affinity (A), global hardness (η), electronegativity (χ), chemical potential (μ), softness (S), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP) for the compound was calculated and are showed in table 7.
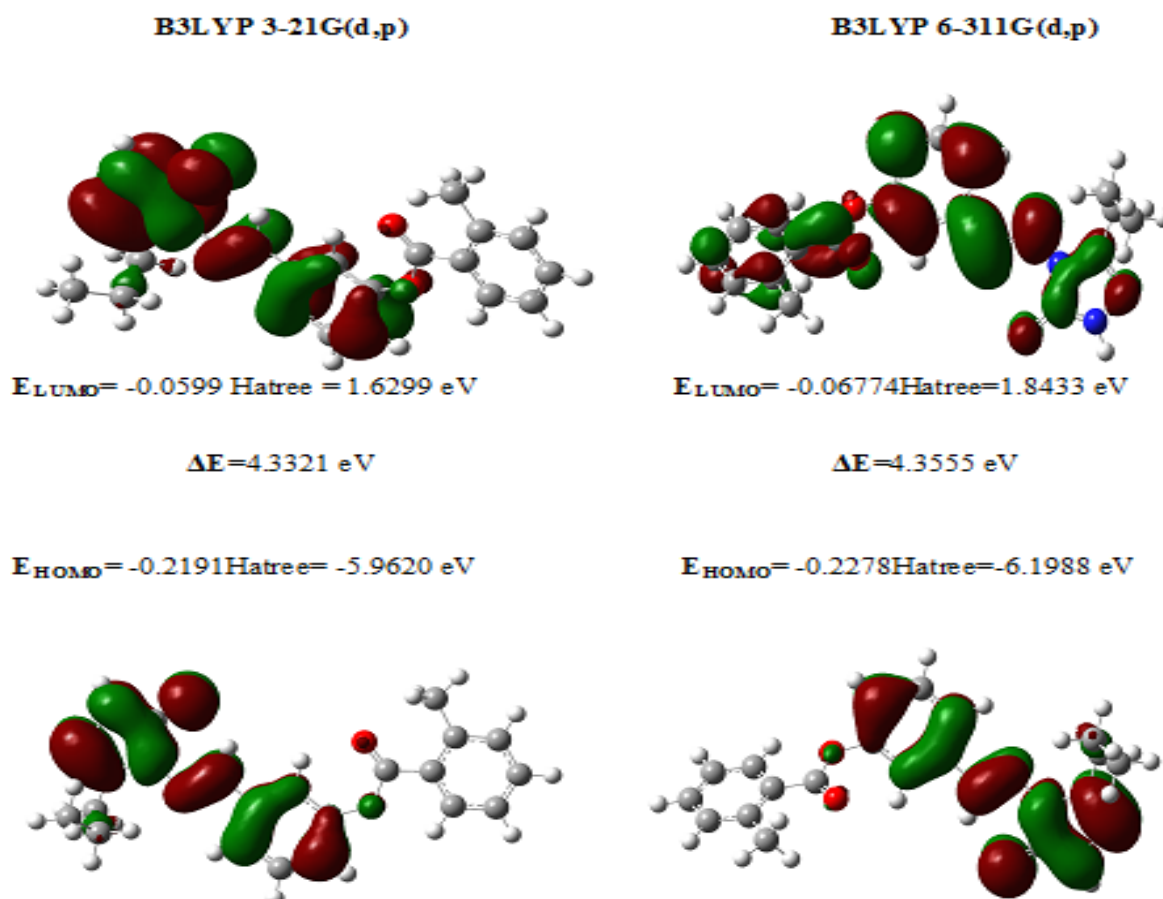
B3LYP 3-21G(d,p)

B3LYP 6-311G(d,p)

E_{LUMO}= -0.0599 Hatree = 1.6299 eV

ΔE=4.3321 eV

E_{HOMO}= -0.2191 Hatree= -5.9620 eV

E_{LUMO}= -0.06774 Hatree=1.8433 eV

ΔE=4.3555 eV

E_{HOMO}= -0.2278 Hatree=-6.1988 eV

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

Table 7. The calculated electronic structure parameters of the molecule

		B3LYP 3-21G(d,p)		B3LYP 6-311G(d,p)	
		Hatree	ev	Hatree	ev
	LUMO	-0.0599	-1.62992	-0.06774	-1.84325
	HOMO	-0.2191	-5.96186	-0.2278	-6.1986
A	elektron ilgisi	0.0599	1.62992	0.06774	1.84325
I	İyonlaşma potansiyeli	0.2191	5.96186	0.2278	6.1986
ΔE	energy gap	0.1592	4.33194	0.16006	4.35534
χ	electronegativity	0.1395	3.79589	0.14777	4.02093
Pi	chemical potential	-0.1395	-3.79589	-0.14777	-4.02093
ω	electrophilic index	0.000774518	0.02108	0.000873766	0.02378
IP	Nucleophilic index	-0.0111042	-0.30215	-0.01182603	-0.32179
S	molecular softness	12.5628	341.843	12.4953	340.006
η	molecular hardness	0.0796	2.16597	0.08003	2.17767

Table 8. The calculated dipole moments datas of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
3-21G	0.1418	1.0885	-0.0173	1.0979
6-311G	0.5782	1.3859	0.1582	1.5100

Table 9. The calculated total energy datas of the molecule

Energy(a.u.)	B3lyp 3-21G	B3lyp 6-311G
	-1212.1405	-1219.1562

Table 10. The calculated thermodynamics parameters of the molecule

Rotational temperatures (Kelvin)	B3LYP/3-21G	B3LYP/6-311G
A	0.02219	0.02099
B	0.00307	0.00308
C	0.00275	0.00288
Rotational constants (GHZ)		
A	0.46236	0.43735
B	0.06401	0.06409
C	0.05740	0.05997
Thermal Energies E(kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	249.967	247.611
Total	251.744	249.389
Thermal Capacity CV(cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	85.689	87.156
Total	91.651	93.118
Entropy S(cal/mol-K)		
Translational	43.570	43.570
Rotational	36.491	36.501
Vibrational	92.706	98.410
Total	172.767	178.482
Zero-point correction (Hartree/Particle)	0.377112	0.372743
Thermal correction to Energy	0.401180	0.397426
Thermal correction to Enthalpy	0.402125	0.398370
Thermal correction to Gibbs Free Energy	0.320037	0.313568
Sum of electronic and zero-point Energies	-1211.763415	-1218.783521
Sum of electronic and thermal Energies	-1211.739346	-1218.758837
Sum of electronic and thermal Enthalpies	-1211.738402	-1218.757893
Sum of electronic and thermal Free Energies	-1211.820489	-1218.842695
Zero-point vibrational energy (Kcal/mol)	236.64133	233.89962

Thermodynamics Properties

Thermodynamics parameters were calculated with (B3LYP) functional in the both two basis set of DFT method at 298.150 K and under 1 atm pressure (Table 10).

Conclusion

In this work, spectroscopic, electronic and geometric parameters of molecule are calculated by B3LYP functional of DFT method with the 3-21G(d,p) and 6-311G (d,p) basis sets at the program package Gaussian G09W. FT-IR vibrational frequencies and spectrums were obtained. The FT-IR data was found positive. This result showed that the structure of the compound was stable. The chemical shifts in the calculations FT-IR and ^{1}H/^{13}C-NMR vibrational frequencies are found to be compatible with the experimental data. Theoretical and experimental carbon chemical shifts ratios between according to R^2 lineer a correlation was observed, but there is a slight deviation in the H-NMR correlation graph. The reason for this deviation is the N-H acidic proton (H21) in the molecule. Obtained spectroscopic parameters are compared with experimental data and with each other. In addition, the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO), bond angles, bond lengths, mulliken charges, E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronic parameters, thermodynamics properties, dipole moments, total energy were calculated with different basis sets such as 3-21 G(d,p)/ 6-311G(d,p) basis set. Result, obtained all data basis set were compared and these values were consistent with each other. The closest results to the experimental values are the results obtained with the 6-311 G(d,p) base set.

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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