Research Article

Compared of Theoretical Properties of Novel 1-(Morpholine-4-yl-methyl)-3-(*p*-methoxybenzyl)-4-(4-isopropylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one According to Two Methods

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Abstract In this study, 1-(morpholine-4-yl-methyl)-3-(*p*-methoxybenzyl)-4-(4-isopropylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule was optimized by using the B3LYP/HF 6-31G(d) and B3LYP/HF 6-311G(d) different two method. This optimized structure used to calculation of the various theoretical properties of the compounds. IR absorption frequencies of analyzed molecule were calculated by two methods. Then, they were compared with each other and experimental data, which are shown to be accurate. Infrared spectra were composed by using the data obtained from both methods. The veda4f program, was used in defining IR data, which were calculated theoretically. ^{1}H NMR and ^{13}C NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W. Experimental and theoretical values were inserted into the graphic according to equation δ exp=a+b. δ calc. The standard error values were found via Sigma Plot program with regression coefficient of a and b constants. Additionally, bond angles, bond lengths, mulliken charges, the HOMO-LUMO energy, E_{LUMO}-E_{HOMO} energy gap (ΔEg), dipole moment, electronegativity (χ), electron affinity (A), global hardness (η), softness (S), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP), total energy of the molecule and thermodynamic parameters of this compound was investigation by using the B3LYP/HF 6-31G(d) and B3LYP/HF 6-311G(d) basis sets.

Keyword: 1,2,4-Triazol-5-one, Veda4f, GIAO, HOMO-LUMO

1. Introduction

Schiff bases (-HC=N-) are well-known organic compounds that they are obtained by condensation between a primary amine and an aldehyde or ketone to form an azomethine or imine group [1]. These compounds are generally formed by reaction of an aldehyde with a primary amine, where R, may be an alkyl or an aryl group. Schiff bases that include aryl substituents are fundamentally more stable and more easily synthesized, while those which contain alkyl substituents are comparatively unstable. Many studies have lately been made using Schiff bases [2-8]. Schiff bases are inhibit as antifungal, antitumor and antibacterial agents and they have been used as pesticides, herbicides and insecticides, too [9, 10]. In the last year, theoretical properties of Schiff bases were investigated on a computer. In this study, we examined theoretical features of [2-Methoxy-4-(3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl)-azomethinphenyl acetate molecule. All theoretical calculations for the target compound were with the Gaussian 09 quantum chemistry program [11] on a personal computer. For this, firstly, molecule were optimized by using the Density Functional Theory (DFT) and Hartree Fock (HF) methods with the restricted B3LYP [11, 12] level of theory, 6-31G(d) and 6-311G (d) basis sets, for all atoms. Optimized structure is the most stable structure of the

molecule. Then from this form, dipole moments, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), total energy of the molecule, bond lengths, bond angles and mulliken charges, 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. In addition, The theoretical calculations ^{1}H-NMR and ^{13}C-NMR were performed by using DFT/HF 6-31G(d) and DFT/HF 6-311G(d) level. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 [12]. The visualization of all results has been performed using GaussView 5 [13]. Theoretical and experimental values were inserted into the graphic according to equation of δ exp_a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Finally, the theoretical vibrational spectra were calculated at the B3LYP/DFT/HF 6-31G(d) and 6-311G (d) basis sets in the gas phase and these data are scaled with 0.9613 and 0,8929 factors for 6-31G(d) basis set and 0.9905 and 0.9516 factors for 6-311G(d) basis set [14]. The data obtained according to DFT and HF method are formed using theoretical infrared spectrum. The veda4f program was used in defining IR data [15]. The experimental and theoretical IR spectra are given in Fig. 5, 6.

2. Materials and Methods
2.1 Experimental
Melting points were check on WRS-2A Microprocessor Melting-Point Apparatus. The IR spectra were measured on Alpha-P Bruker FT-IR Spectrometer. ^{1}H- and ^{13}C-NMR spectra were recorded in deuterated dimethyl sulfoxide with TMS as internal standard on a Bruker 400 MHz spectrometer, respectively. Yield: 78%, m.p. 96 [0]C. IR (υ, cm-1): 3035 (=CH), 1706 (C=O), 1608 (C=N), 1570 (C=C). ^{1}H-NMR (DMSO-d6): δ 1.22 (d, 6H, CH(CH$_3$)$_2$; J=6,80 Hz), 2.59-2.60 (m, 4H, CH$_2$NCH$_2$), 2.95 (hept, 1H, CH(CH$_3$)$_2$; J=6,80 Hz), 3.58 (m, 4H, CH$_2$OCH$_2$), 3.70 (s, 3H, OCH$_3$), 4.01(s, 2H, CH$_2$Ph, 4,56 (s, 2H, NCH$_2$N, 6.88; 7.25; 7.38; 7,73 (d, 2H, ArH; J=8.40 Hz), 9.65 (s, 1H, N=CH). ^{13}C-NMR (DMSO-d$_6$): δ 23.52 (2CH3), 30.07 (CH$_2$Ph), 33.15 (CH), 50.01 (CH$_2$NCH$_2$), 55.01 (OCH$_3$), 66.04 (CH$_2$OCH$_2$+NCH$_2$N), 113.95; 126.99; 127.40; 127.89; 129.74; 131.04; 145.22; 158.15 (Arom-C), 150.32 (Triazole C3), 152.39 (Triazole C5) 154.24 (N=CH).

2.2 Theoretical
The quantum chemical calculations were carried out with density functional theory (DFT) and Hartree-Fock (HF) methods using 6-31G(d) and 6-311G(d) different two basis set at the Gaussian 09W program package on a computing system [11]. Firstly, the compound was optimized by using the B3LYP/6-31G (d) and HF/6-31G (d) basis sets [11,12]. Thus, the most stable geometrical conformer of compound was obtained. Then, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with method of GIAO [12]. The veda4f program was used in defining IR data [15]. Theoretically calculated IR data are multiplied with appropriate scale factors [14]. Scale dft and hf values obtained according to HF and DFT method are formed using theoretical infrared spectrum. Otherwise, bond angles, bond lengths, the HOMO-LUMO energy and mulliken charges of compound were calculated theoretically on the computer. The temperature addicted thermodynamic parameters (thermal energies **E**, thermal capacity **CV**, entropy **S**) were calculated from the vibrational frequency calculations of the title compound in the gas phase using the DFT/HF 6-31G(d) and 6-311G(d) level. In addition, E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (S), ionization potential (I), chemical potential (Pi), electrophilic index (ω), Nucleophilic index (IP), total energy of the molecule, dipole moments were calculated.
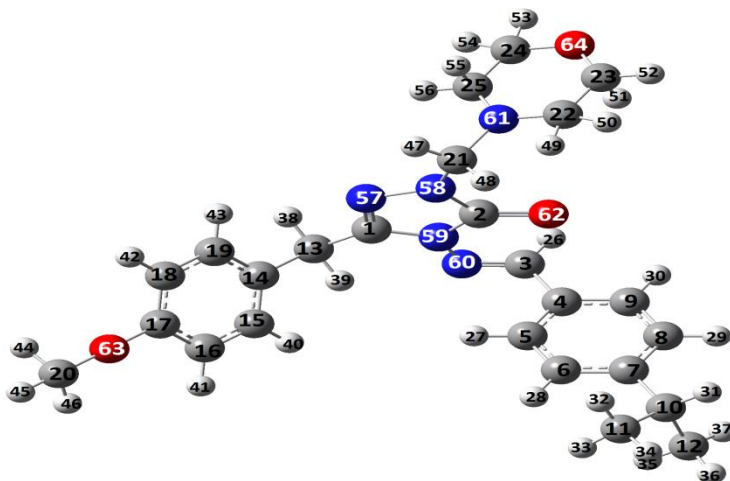
3. Result and Discussion
3.1 Computational Details

Figure 1: The Gaussview structure of the molecule

Table 1: ^{13}C and ^{1}H-NMR (DMSO) isotropic chemical shifts (δ/ppm) (6-31G(d))

No	Exp.	B3LYP	Differ.	B3LYP	Differ.	HF	Differ.	HF	Differ.
C1	144.91	149.46	150.46	-4.55	-5.55	144.48	146.67	0.43	-1.76
C2	154.21	152.26	152.86	1.95	1.35	147.15	147.68	7.06	6.53
C3	152.39	154.54	155.44	-2.15	-3.05	148.87	149.88	3.52	2.51
C4	131.01	137.23	136.10	-6.22	-5.09	126.57	125.53	4.44	5.48
C5	127.89	128.23	127.64	-0.34	0.25	123.30	122.85	4.59	5.04
C6	126.99	128.62	129.24	-1.63	-2.25	123.38	123.44	3.61	3.55
C7	150.30	154.39	156.54	-4.09	-6.24	148.11	149.77	2.19	0.53
C8	126.99	131.66	132.17	-4.67	-5.18	120.69	121.07	6.30	5.92
C9	127.89	136.06	136.44	-8.17	-8.55	130.22	130.63	-2.33	-2.74
C10	33.45	47.66	47.50	-14.21	-14.05	29.47	29.23	3.98	4.22
C11	23.53	33.10	32.44	-9.57	-8.91	20.27	19.81	3.26	3.72
C12	23.53	32.90	32.66	-9.37	-9.13	20.27	19.81	3.26	3.72
C13	30.92	42.49	42.18	-11.57	-11.26	27.94	27.49	2.98	3.43
C14	135.65	140.47	140.64	-4.82	-4.99	130.02	130.35	5.63	5.30
C15	128.67	132.30	132.42	-3.63	-3.75	126.49	126.42	2.18	2.25
C16	128.49	131.27	131.74	-2.78	-3.25	124.57	124.81	3.92	3.68
C17	126.77	129.55	129.82	-2.78	-3.05	123.26	123.53	3.51	3.24
C18	128.49	131.38	131.47	-2.89	-2.98	124.62	124.86	3.87	3.63
C19	128.67	130.71	130.57	-2.04	-1.90	126.45	126.39	2.22	2.28
C20	66.03	74.30	74.05	-8.27	-8.02	56.28	56.12	9.75	9.91
C21	49.99	58.50	58.28	-8.51	-8.29	41.27	40.95	8.72	9.04
C22	66.03	73.89	73.73	-7.86	-7.70	55.76	55.61	10.27	10.42
C23	66.03	74.50	74.40	-8.47	-8.37	55.65	55.48	10.38	10.55
C24	49.99	59.16	58.86	-9.17	-8.87	40.74	40.48	9.25	9.51
H25	9.62	10.99	10.93	-1.37	-1.31	10.31	10.27	-0.69	-0.65
H26	7.72	9.14	9.16	-1.42	-1.44	8.89	8.95	-1.17	-1.23
H27	7.37	8.35	8.56	-0.98	-1.19	7.75	7.95	-0.38	-0.58
H28	7.37	8.01	8.20	-0.64	-0.83	7.90	8.11	-0.53	-0.74
H29	7.72	8.07	8.21	-0.35	-0.49	8.06	8.25	-0.34	-0.53

H30	2.95	3.58	3.72	-0.63	-0.77	2.76	2.92	0.19	0.03
H31	1.22	2.89	2.05	-1.67	-0.83	1.48	1.41	-0.26	-0.19
H32	1.22	2.11	2.19	-0.89	-0.97	1.49	1.56	-0.27	-0.34
H33	1.22	2.14	2.20	-0.92	-0.98	1.55	1.61	-0.33	-0.39
H34	1.22	2.06	2.01	-0.84	-0.79	1.49	1.42	-0.27	-0.20
H35	1.22	2.12	2.17	-0.90	-0.95	1.50	1.61	-0.28	-0.39
H36	1.22	2.09	2.16	-0.87	-0.94	1.48	1.56	-0.26	-0.34
H37	4.09	4.64	4.76	-0.55	-0.67	4.04	4.22	0.05	-0.13
H38	4.09	4.64	4.80	-0.55	-0.71	4.00	4.19	0.09	-0.10
H39	7.34	8.37	8.56	-1.03	-1.22	7.86	8.06	-0.52	-0.72
H40	7.32	8.25	8.43	-0.93	-1.11	7.92	8.11	-0.60	-0.79
H41	7.23	8.11	8.28	-0.88	-1.05	7.87	8.06	-0.64	-0.83
H42	7.32	8.20	8.34	-0.88	-1.02	7.94	8.12	-0.62	-0.80
H43	7.34	8.40	8.42	-1.06	-1.08	7.92	8.11	-0.58	-0.77
H44	4.57	4.63	4.79	-0.06	-0.22	3.93	4.04	0.64	0.53
H45	4.57	5.23	5.27	-0.66	-0.70	4.62	4.67	-0.05	-0.10
H46	2.59	3.81	3.80	-1.22	-1.21	2.52	2.46	0.07	0.13
H47	2.59	3.13	3.23	-0.54	-0.64	2.06	2.19	0.53	0.40
H48	3.56	4.34	4.57	-0.78	-1.01	3.55	3.65	0.01	-0.09
H49	3.56	4.48	4.35	-0.92	-0.79	3.29	3.30	0.27	0.26
H50	3.56	4.51	4.61	-0.95	-1.05	3.38	3.46	0.18	0.10
H51	3.56	4.51	4.49	-0.95	-0.93	3.64	3.72	-0.08	-0.16
H52	2.59	3.33	3.46	-0.74	-0.87	2.46	2.49	0.13	0.10
H53	2.59	3.27	3.37	-0.68	-0.78	2.45	2.46	0.14	0.13

Table 2: ^{13}C and ^{1}H-NMR (DMSO) isotropic chemical shifts (δ/ppm) (6-311G(d))

No	Exp.	B3LYP	Differ.	B3LYP	Differ.	HF	Differ.	HF	Differ.
C1	144.91	149.46	150.46	-4.55	-5.55	144.48	146.67	0.43	-1.76
C2	154.21	152.26	152.86	1.95	1.35	147.15	147.68	7.06	6.53
C3	152.39	154.54	155.44	-2.15	-3.05	148.87	149.88	3.52	2.51
C4	131.01	137.23	136.10	-6.22	-5.09	126.57	125.53	4.44	5.48
C5	127.89	128.23	127.64	-0.34	0.25	123.30	122.85	4.59	5.04
C6	126.99	128.62	129.24	-1.63	-2.25	123.38	123.44	3.61	3.55
C7	150.30	154.39	156.54	-4.09	-6.24	148.11	149.77	2.19	0.53
C8	126.99	131.66	132.17	-4.67	-5.18	120.69	121.07	6.30	5.92
C9	127.89	136.06	136.44	-8.17	-8.55	130.22	130.63	-2.33	-2.74
C10	33.45	47.66	47.50	-14.21	-14.05	29.47	29.23	3.98	4.22
C11	23.53	33.10	32.44	-9.57	-8.91	20.27	19.81	3.26	3.72
C12	23.53	32.90	32.66	-9.37	-9.13	20.27	19.81	3.26	3.72
C13	30.92	42.49	42.18	-11.57	-11.26	27.94	27.49	2.98	3.43
C14	135.65	140.47	140.64	-4.82	-4.99	130.02	130.35	5.63	5.30
C15	128.67	132.30	132.42	-3.63	-3.75	126.49	126.42	2.18	2.25
C16	128.49	131.27	131.74	-2.78	-3.25	124.57	124.81	3.92	3.68
C17	126.77	129.55	129.82	-2.78	-3.05	123.26	123.53	3.51	3.24
C18	128.49	131.38	131.47	-2.89	-2.98	124.62	124.86	3.87	3.63
C19	128.67	130.71	130.57	-2.04	-1.90	126.45	126.39	2.22	2.28
C20	66.03	74.30	74.05	-8.27	-8.02	56.28	56.12	9.75	9.91
C21	49.99	58.50	58.28	-8.51	-8.29	41.27	40.95	8.72	9.04
C22	66.03	73.89	73.73	-7.86	-7.70	55.76	55.61	10.27	10.42

C23	66.03	74.50	74.40	-8.47	-8.37	55.65	55.48	10.38	10.55
C24	49.99	59.16	58.86	-9.17	-8.87	40.74	40.48	9.25	9.51
H25	9.62	10.99	10.93	-1.37	-1.31	10.31	10.27	-0.69	-0.65
H26	7.72	9.14	9.16	-1.42	-1.44	8.89	8.95	-1.17	-1.23
H27	7.37	8.35	8.56	-0.98	-1.19	7.75	7.95	-0.38	-0.58
H28	7.37	8.01	8.20	-0.64	-0.83	7.90	8.11	-0.53	-0.74
H29	7.72	8.07	8.21	-0.35	-0.49	8.06	8.25	-0.34	-0.53
H30	2.95	3.58	3.72	-0.63	-0.77	2.76	2.92	0.19	0.03
H31	1.22	2.89	2.05	-1.67	-0.83	1.48	1.41	-0.26	-0.19
H32	1.22	2.11	2.19	-0.89	-0.97	1.49	1.56	-0.27	-0.34
H33	1.22	2.14	2.20	-0.92	-0.98	1.55	1.61	-0.33	-0.39
H34	1.22	2.06	2.01	-0.84	-0.79	1.49	1.42	-0.27	-0.20
H35	1.22	2.12	2.17	-0.90	-0.95	1.50	1.61	-0.28	-0.39
H36	1.22	2.09	2.16	-0.87	-0.94	1.48	1.56	-0.26	-0.34
H37	4.09	4.64	4.76	-0.55	-0.67	4.04	4.22	0.05	-0.13
H38	4.09	4.64	4.80	-0.55	-0.71	4.00	4.19	0.09	-0.10
H39	7.34	8.37	8.56	-1.03	-1.22	7.86	8.06	-0.52	-0.72
H40	7.32	8.25	8.43	-0.93	-1.11	7.92	8.11	-0.60	-0.79
H41	7.23	8.11	8.28	-0.88	-1.05	7.87	8.06	-0.64	-0.83
H42	7.32	8.20	8.34	-0.88	-1.02	7.94	8.12	-0.62	-0.80
H43	7.34	8.40	8.42	-1.06	-1.08	7.92	8.11	-0.58	-0.77
H44	4.57	4.63	4.79	-0.06	-0.22	3.93	4.04	0.64	0.53
H45	4.57	5.23	5.27	-0.66	-0.70	4.62	4.67	-0.05	-0.10
H46	2.59	3.81	3.80	-1.22	-1.21	2.52	2.46	0.07	0.13
H47	2.59	3.13	3.23	-0.54	-0.64	2.06	2.19	0.53	0.40
H48	3.56	4.34	4.57	-0.78	-1.01	3.55	3.65	0.01	-0.09
H49	3.56	4.48	4.35	-0.92	-0.79	3.29	3.30	0.27	0.26
H50	3.56	4.51	4.61	-0.95	-1.05	3.38	3.46	0.18	0.10
H51	3.56	4.51	4.49	-0.95	-0.93	3.64	3.72	-0.08	-0.16
H52	2.59	3.33	3.46	-0.74	-0.87	2.46	2.49	0.13	0.10
H53	2.59	3.27	3.37	-0.68	-0.78	2.45	2.46	0.14	0.13

3.2. The relation between R^2 values of the compound

The optimized R^2 values of the compound: B3LYP/631G(d) (DMSO): [13]C: 0.9815, [1]H: 0.9807; HF/631G(d,p) (DMSO): [13]C: 0.9915, [1]H: 0.9807

The optimized R^2 values of the compound: B3LYP/6311G(d) (DMSO): [13]C: 0.9891, [1]H: 0.9902; HF/6311G(d,p) (DMSO): [13]C: 0.9906, [1]H: 0.9798. There is such a relationship between R^2-values of the compound. Found standard error rate and a, b constants regression values were calculated according to formula exp =a +b. δ calc Eq. These values for compound were given in the table **3**. Theoretical and experimental carbon and proton chemical shifts ratios between according to R^2 and a, b values, linear a correlation were observed.

Table 3: The correlation data for chemical shifts of the molecules

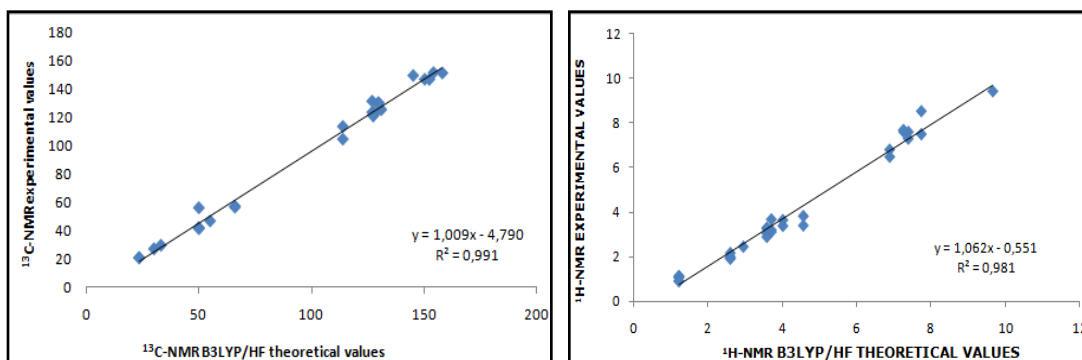|		[13]C				[1]H			
		R	S. hata	a	b	R	S. hata	a	b
6-31G	DFT	0.9815	6.4084	1.0546	-12.191	0.9807	0.3357	0.9234	0.5884
	HF	0.9915	4.3428	0.9823	5.5069	0.9807	0.3357	0.9234	0.5884
6-311G	DFT	0.9891	4.9084	0.9849	-12.574	0.9902	0.2386	0.9909	-0.3745
	HF	0.9906	4.5536	0.9241	0.9301	0.9798	0.3432	0.9457	0.3929

Figure 3: The correlation graphs for B3LYP/HF 631G(d) chemical shifts of the molecule
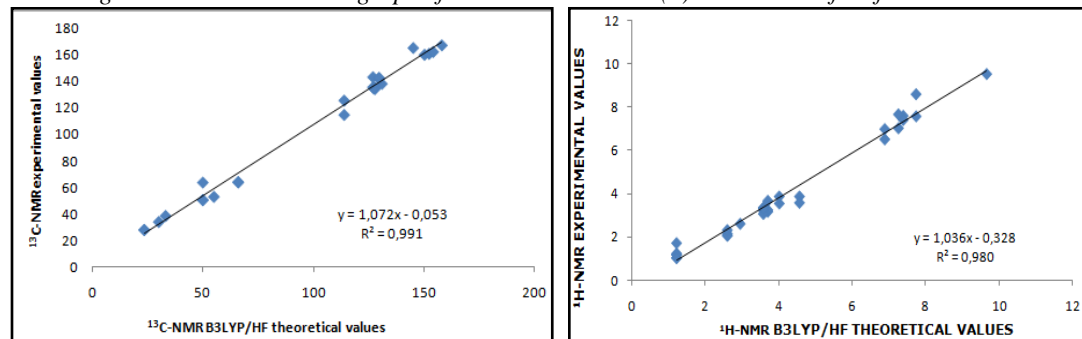

Figure 4: The correlation graphs for B3LYP/HF 6311G(d) chemical shifts of the molecule

3.3. The vibration frequency of the compound

Theoretically IR values were calculation veda 4f programme and scale values were obtain. Theoretically calculated IR data are multiplied with appropriate scale factors respectively 0.9613, 0.8929 for DFT/HF 631G (d) and 0.9905, 0.9516 factors for DFT/HF6311G (d) basis sets. The positive frequency in the data was found. IR spectrums were drawn with obtained values according to HF and DFT method. Theoretically IR values were compare with experimentally IR values. The result of this compare were found corresponding with each other of values.

Table 4: Significant vibrational frequencies (cm^{-1})

Significant vibrational frequencies	Experimental	B3LYP/HF 6-31G(d)		B3LYP/HF 6-311G(d)	
	IR (cm^{-1})	Skalalı DFT	Skalalı HF	Skalalı DFT	Skalalı HF
ν C=C	1570	1593	1620	1596	1605
ν C=N	1608	1614	1704	1628	1697
ν C=O	1706	1768	1712	1768	1726
ν =CH	3035	3091	3039	3162	3218
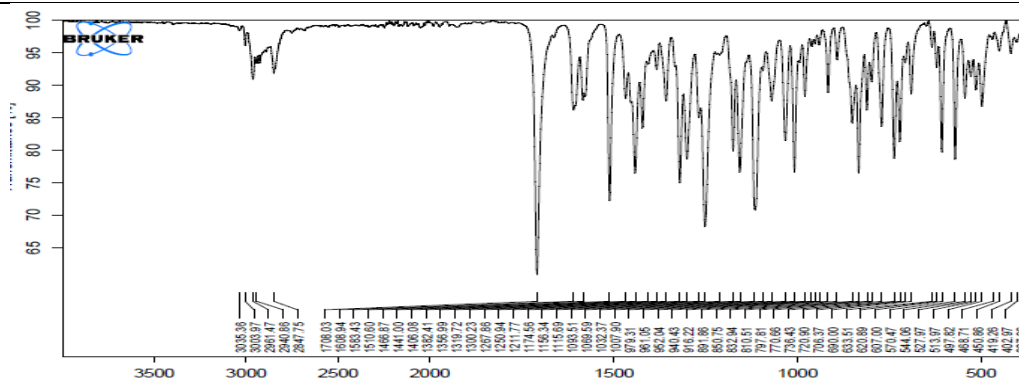
Figure 5: Experimental IR spectrum

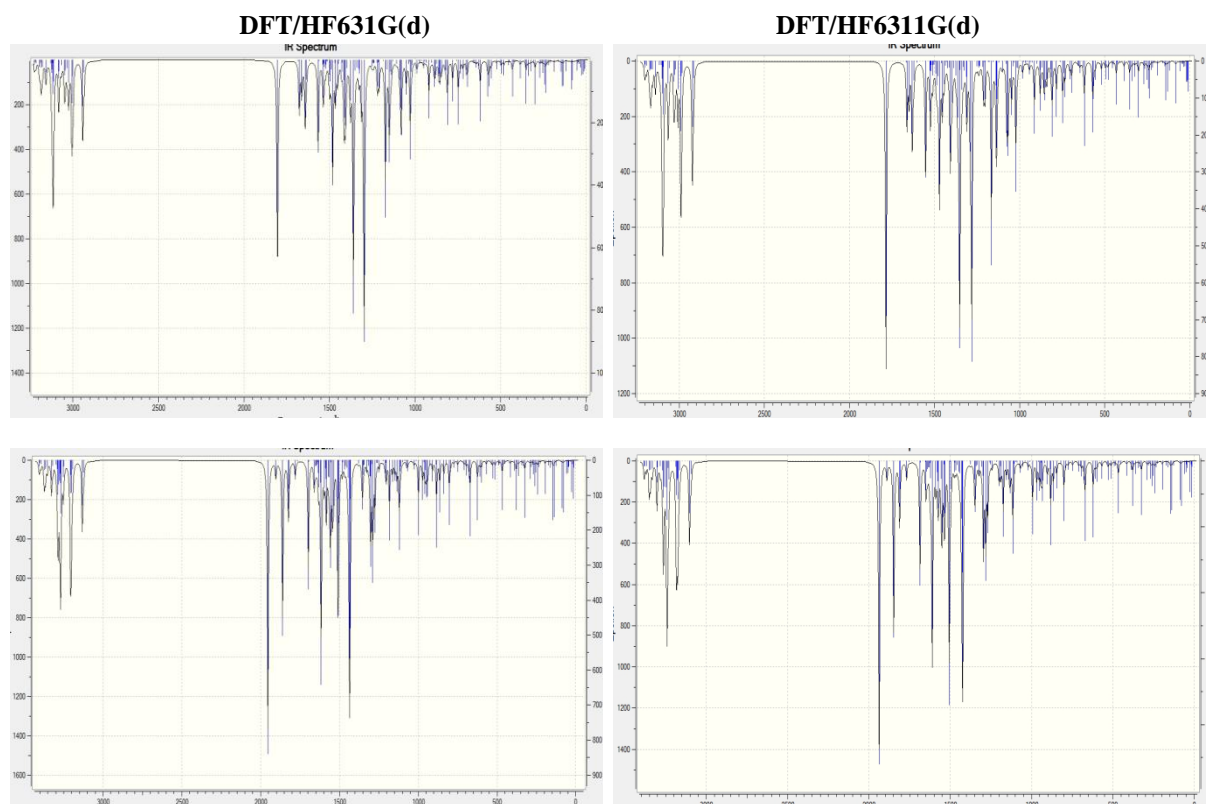**DFT/HF631G(d)**   **DFT/HF6311G(d)**

Figure 6: Theoretical IR spectrums and simulated with B3LYP/DFT/HF 631G(d) and
B3LYP/DFT/HF 6311G(d) levels of the molecule

3.4 Molecular Geometry

The molecular geometric parameters such as bond lengths, bond angles, Mulliken atomic charges calculated by using the HF and DFT/B3LYP methods with 6-31G(d) basis set obtained data are precondition in Table 5-7. According to this result, the longest bond length is between C10-C11 and C10-C12 atoms that this values are 1.54/1.53 Å for DFT/HF 6-31G(d) and 1.53/1.53 Å for DFT/HF 6-311G(d). Besides, respectively, the bond lengths in the triazole ring N57-N58, N57-C1, C2-O62, C2-N59, N59-C1, N58-C2 are calculated 1.38/1.37, 1.30/1.26, 1.22/1.20, 1.41/1.38, 1.38/1.37, 1.37/1.35 Å for DFT/HF 6-31G(d) and 1.38/1.37, 1.29/1.26, 1.21/1.19, 1.41/1.38, 1.38/1.37, 1.37/1.34 Å for DFT/HF 6-311G(d) basis sets (table 5). In the literature, the N=C, N-N, C=O bond lengths are measured as 1.280, 1.404, 1.212 Å [16, 17]. The highest bond angle is between C(2)-N(59)-O(60) atoms, which is $130.49/129.34^{o'}$ (table 6). The calculated Mulliken atomic charges [18] calculated by using the Hartree Fock (HF) and DFT/B3LYP methods with 6-31G(d) and 6-311G(d) basis sets. The electronegative oxygen (O) and nitrogen (N) atoms have negative atomic charge values. The carbon atoms surrounded by electronegative atoms have positive atomic charge values. The C1 atom surrounded by two electronegative atoms (N57, N58) and C2 atom which is surrounded by three electronegative atoms (N58, N59, O62) have the highest positive charges values. All hydrogen atoms of the compound (**3**) have positive atomic charge values (table 7).

Table 5: The calculated bond lengths with B3LYP/HF 631G(d) /6-311G(d) of the molecule

bond lengths	DFT 6-31	HF 6-31	DFT6-311	HF6-311	bond lengths	DFT6-31	HF6-31	DFT6-311	HF6-311
C(1)-C(13)	1.49	1.49	1.494	1.496	C(7)-C(8)	1.39	1.38	1.396	1.384
C(1)-N(57)	1.30	1.26	1.297	1.267	C(8)-H(29)	1.08	1.07	1.086	1.075
C(1)-N(59)	1.38	1.37	1.386	1.375	C(8)-C(9)	1.39	1.38	1.391	1.387
N(57)-N(58)	1.38	1.37	1.383	1.372	C(9)-H(30)	1.08	1.07	1.086	1.076
N(58)-C(2)	1.37	1.35	1.372	1.349	C(4)-C(9)	1.40	1.38	1.399	1.384

C(2)-N(59)	1.41	1.38	1.417	1.387	C(7)-C(10)	1.52	1.52	1.520	1.520
C(2)-O(62)	1.22	1.20	1.217	1.197	C(10)-H(31)	1.09	1.08	1.096	1.086
N(59)-N(60)	1.37	1.36	1.371	1.366	C(10)-C(11)	1.54	1.53	1.539	1.533
C(13)-H(38)	1.09	1.08	1.093	1.082	C(11)-H(32)	1.09	1.08	1.092	1.084
C(13)-H(39)	1.09	1.08	1.091	1.081	C(11)-H(33)	1.09	1.08	1.093	1.085
C(13)-C(14)	1.52	1.51	1.521	1.519	C(11)-H(34)	1.09	1.08	1.094	1.085
C(14)-C(15)	1.39	1.37	1.391	1.378	C(10)-C(12)	1.54	1.53	1.538	1.534
C(15)-H(40)	1.08	1.07	1.085	1.075	C(12)-H(35)	1.09	1.08	1.092	1.085
C(15)-C(16)	1.39	1.39	1.396	1.392	C(12)-H(36)	1.09	1.08	1.094	1.085
C(16)-C(17)	1.39	1.38	1.395	1.382	C(12)-H(37)	1.09	1.08	1.093	1.084
C(16)-H(41)	1.08	1.07	1.082	1.072	N(58)-C(21)	1.44	1.43	1.448	1.438
C(17)-O(63)	1.36	1.34	1.363	1.346	C(21)-H(47)	1.10	1.08	1.099	1.079
O(63)-C(20)	1.41	1.39	1.418	1.397	C(21)-H(48)	1.09	1.07	1.090	1.087
H(44)-C(20)	1.09	1.07	1.095	1.084	C(21)-N(61)	1.45	1.44	1.450	1.440
H(45)-C(20)	1.09	1.08	1.095	1.084	N(61)-C(22)	1.46	1.45	1.463	1.452
H(46)-C(20)	1.09	1.08	1.088	1.078	C(22)-H(49)	1.09	1.04	1.106	1.084
C(17)-C(18)	1.40	1.39	1.401	1.394	C(22)-H(50)	1.10	1.08	1.094	1.094
C(18)-H(42)	1.08	1.07	1.084	1.074	C(22)-C(23)	1.52	1.52	1.525	1.518
C(18)-C(19)	1.38	1.37	1.384	1.373	C(23)-H(51)	1.10	1.08	1.100	1.088
C(19)-H(43)	1.08	1.07	1.085	1.075	C(23)-H(52)	1.09	1.08	1.091	1.081
N(60)-C(3)	1.28	1.26	1.285	1.257	C(23)-O(64)	1.42	1.39	1.420	1.397
C(3)-H(26)	1.08	1.07	1.086	1.074	O(64)-C(24)	1.42	1.40	1.422	1.398
C(3)-C(4)	1.46	1.47	1.463	1.474	C(24)-H(53)	1.09	1.08	1.091	1.088
C(4)-C(5)	1.40	1.39	1.404	1.394	C(24)-H(54)	1.10	1.08	1.100	1.081
C(5)-H(27)	1.08	1.07	1.083	1.073	C(24)-C(25)	1.52	1.51	1.523	1.517
C(5)-C(6)	1.38	1.37	1.385	1.376	C(25)-H(55)	1.10	1.09	1.106	1.094
C(6)-H(28)	1.08	1.07	1.085	1.075	C(25)-H(56)	1.09	1.08	1.092	1.081
C(6)-C(7)	1.40	1.39	1.404	1.397	C(25)-N(61)	1.46	1.45	1.465	1.454

Table 6: The calculated bond angles with B3LYP/HF 631G(d)/ 6-311G(d) of the molecule

Bond Angles	B3LYP 6-31	HF 6-31	B3LYP 6-311	HF 6-311	Bond Angles	B3LYP 6-31	HF6-31	B3LYP 6-311	HF 6-311
N(57)-C(1)-N(59)	111.35	111.23	111.29	111.22	H(28)-C(6)-C(7)	120.58	119.83	119.72	119.88
N(57)-N(58)-C(2)	113.22	112.55	113.14	112.54	C(6)-C(7)-C(8)	117.82	117.86	117.75	117.79
N(57)-N(58)-C(21)	122.06	122.13	122.08	122.24	C(7)-C(8)-H(29)	119.38	119.71	119.43	119.75
C(21)-N(58)-C(2)	124.48	125.14	124.48	125.06	C(7)-C(8)-C(9)	121.18	121.07	121.21	121.10
N(58)-C(2)-O(62)	129.03	128.90	129.19	128.98	C(8)-C(9)-H(30)	119.85	119.46	119.70	119.39
O(62)-C(2)-N(59)	128.88	128.38	128.71	128.31	C(8)-C(9)-C(4)	120.71	120.75	120.77	120.77
C(2)-N(59)-N(60)	130.49	130.34	130.34	130.38	C(7)-C(10)-C(11)	111.86	111.87	111.89	111.90
C(1)-N(59)-N(60)	121.35	121.38	121.54	121.45	C(7)-C(10)-C(12)	111.80	111.87	111.85	111.89
N(57)-C(1)-C(13)	124.47	124.62	124.60	124.64	C(7)-C(10)-H(31)	107.01	106.97	106.94	106.93
N(59)-C(1)-C(13)	124.13	124.09	124.06	124.09	H(31)-C(10)-C(11)	107.40	107.32	107.34	107.29
C(1)-C(13)-H(38)	106.25	106.39	106.57	106.46	C(10)-C(11)-H(32)	111.24	111.49	111.33	111.24
C(1)-C(13)-H(39)	109.05	109.07	109.04	109.06	C(10)-C(11)-H(33)	111.34	111.49	111.51	111.66
C(1)-C(13)-C(14)	113.69	112.91	113.46	113.00	C(10)-C(11)-H(34)	110.53	110.44	110.64	110.53
H(38)-C(13)-H(39)	107.72	107.91	107.62	107.76	C(10)-C(12)-H(35)	111.34	111.49	111.51	111.67
H(38)-C(13)-C(14)	110.23	110.22	110.12	110.16	C(10)-C(12)-H(36)	110.52	110.44	110.67	110.52
H(39)-C(13)-C(14)	109.67	110.13	109.81	110.18	C(10)-C(12)-H(37)	111.23	111.12	111.33	111.24
C(13)-C(14)-C(15)	121.27	121.73	121.47	121.80	H(35)-C(12)-H(36)	107.65	107.67	107.52	107.54
C(13)-C(14)-C(19)	120.58	120.33	120.47	120.35	H(35)-C(12)-H(37)	107.75	107.84	107.63	107.71
C(14)-C(15)-H(40)	119.51	119.71	119.60	119.75	H(36)-C(12)-H(37)	108.18	108.11	107.98	107.97
C(14)-C(15)-C(16)	121.59	121.67	121.60	121.71	H(32)-C(11)-H(33)	107.75	107.86	107.66	107.73
H(40)-C(15)-C(16)	118.88	118.61	118.78	118.52	H(32)-C(11)-H(34)	108.17	108.10	108.00	107.96
C(15)-C(16)-C(17)	119.51	119.59	119.62	119.66	H(33)-C(11)-H(34)	107.63	107.66	107.50	107.52

C(15)-C(16)-H(41)	119.36	119.07	119.18	118.95	N(58)-C(21)-H(47)	106.64	111.96	106.80	106.64
H(41)-C(16)-C(17)	121.11	121.32	121.18	121.38	N(58)-C(21)-H(48)	106.20	109.06	106.17	106.74
C(16)-C(17)-O(63)	124.81	124.78	124.87	124.87	N(58)-C(21)-N(61)	113.02	113.11	113.09	113.30
O(63)-C(17)-C(18)	115.68	115.80	115.80	115.86	C(21)-N(61)-C(22)	112.78	109.35	113.03	112.53
C(16)-C(17)-C(18)	119.49	119.41	118.44	119.26	C(21)-N(61)-C(25)	113.22	113.68	113.33	113.61
C(17)-C(18)-H(42)	118.51	118.57	118.41	118.51	N(61)-C(22)-H(49)	112.23	111.96	108.97	109.13
C(17)-C(18)-C(19)	120.16	120.17	120.26	120.26	N(61)-C(22)-H(50)	108.92	109.06	112.07	111.85
H(42)-C(18)-C(19)	121.31	121.24	121.32	121.22	H(49)-C(22)-H(50)	108.01	108.01	108.00	107.88
C(18)-C(19)-H(43	119.50	119.28	119.41	119.21	H(49)-C(22)-C(23)	108.82	109.05	108.87	109.07
O(63)-C(20)-H(44)	105.94	106.24	111.57	111.46	H(50)-C(22)-C(23)	109.57	109.35	109.53	109.28
O(63)-C(20)-H(45)	111.62	111.44	111.55	111.46	C(22)-C(23)-H(51)	110.67	110.63	109.29	109.38
O(63)-C(20)-H(46)	111.59	111.44	105.84	106.24	C(22)-C(23)-H(52)	109.22	109.39	110.82	110.65
H(44)-C(20)-H(45)	109.23	109.14	109.30	109.36	H(51)-C(23)-H(52)	108.86	108.68	108.82	108.55
H(44)-C(20)-H(46)	109.26	109.16	109.24	109.11	C(22)-C(23)-O(64)	111.35	111.03	111.42	111.22
H(45)-C(20)-H(46)	109.09	109.31	109.22	109.09	H(52)-C(23)-O(64)	106.50	106.92	109.98	112.19
N(58)-N(57)-C(1)	105.21	105.56	105.45	105.69	H(51)-C(23)-O(64)	110.16	110.11	106.42	106.95
N(59)-N(60)-C(3)	118.50	119.30	118.85	119.47	C(23)-O(64)-C(24)	110.74	112.17	110.89	110.01
N(60)-C(3)-H(26)	121.85	122.19	121.78	122.15	O(64)-C(24)-H(53)	106.42	106.86	106.34	106.89
H(26)-C(3)-C(4)	117.65	117.12	117.56	117.04	O(64)-C(24)-H(54)	110.08	110.02	109.92	109.94
C(3)-C(4)-C(5)	122.94	122.76	122.93	122.77	H(53)-C(24)-H(54)	108.77	108.63	108.73	108.50
C(3)-C(4)-C(9)	118.65	118.72	118.77	118.74	O(64)-C(24)-C(25)	111.35	111.02	111.37	111.16
C(4)-C(5)-C(6)	120.49	120.49	120.57	120.53	H(55)-C(25)-N(61)	111.25	111.24	111.03	111.10
C(4)-C(5)-H(27)	118.92	119.34	118.95	119.35	H(56)-C(25)-N(61)	109.10	109.39	109.21	109.52
H(27)-C(5)-C(6)	120.58	120.15	120.46	120.11	C(24)-C(25)-N(61)	109.47	109.44	109.59	109.64
C(5)-C(6)-H(28)	119.01	118.86	118.87	118.79	H(55)-C(25)-H(56)	107.57	107.72	107.60	107.54
C(5)-C(6)-C(7)	121.37	121.29	121.40	121.32					

Table 7: The calculated mulliken charges datas B3LYP/HF 631G(d)/ 6-311G(d) of the molecule

	DFT6-31	HF6-31	DFT6-311	HF6-311		DFT6-31	HF6-31	DFT6-311	HF6-311
C1	0.564	0.644	0.466	0.592	**H33**	0.144	0.158	0.201	0.203
C2	0.846	1.097	0,595	0.790	**H34**	0.144	0.163	0.207	0.210
C3	0.028	0.099	-0.064	0.040	**H35**	0.152	0.158	0.217	0.221
C4	0.135	-0.038	-0.009	-0.062	**H36**	0.144	0.163	0.207	0.218
C5	-0.163	-0.184	-0.162	-0.177	**H37**	0.144	0.173	0.202	0.204
C6	-0.190	-0.224	-0.209	-0.229	**H38**	0.180	0.220	0.251	0.265
C7	-0.195	0.062	0.107	0.072	**H39**	0.174	0.217	0.246	0.269
C8	-0.204	-0.244	-0.224	-0.249	**H40**	0.129	0.220	0193	0.228
C9	-0.183	-0.209	-0.205	-0.226	**H41**	0.130	0.218	0.207	0.235
C10	-0.162	-0.195	-0.298	-0.312	**H42**	0.139	0.208	0.202	0.231
C11	-0.440	-0.470	-0.593	-0.588	**H43**	0.143	0.209	0.201	0.229
C12	-0.440	-0.470	-0.593	-0.588	**H44**	0.170	0.192	0.218	0.208
C13	-0.417	-0.402	-0.580	-0.590	**H45**	0.151	0.161	0.208	0.206
C14	0.173	-0.002	0.048	0.001	**H46**	0.152	0.162	0.228	0.229
C15	-0.195	-0.199	-0.197	-0.214	**H47**	0.148	0.180	0.231	0.241
C16	-0.194	-0.288	-0.284	-0.318	**H48**	0.176	0.209	0.208	0.222
C17	0.375	0.435	0.266	0.348	**H49**	0.123	0.145	0.217	0.219
C18	-0.170	-0.247	-0.224	-0.257	**H50**	0.150	0.179	0.182	0.188
C19	-0.182	-0.193	-0.174	-0.185	**H51**	0.145	0.174	0.193	0.200
C20	-0.215	-0.186	-0.460	-0.412	**H52**	0.134	0.158	0.205	0.206
C21	0.008	0.111	-0.150	-0.067	**H53**	0.145	0.154	0.206	0.196
C22	-0.141	-0.145	.312	-0.282	**H54**	0.131	0.174	0.190	0.207
C23	-0.033	0.084	0.210	-0.155	**H55**	0.121	0.146	0.181	0.189
C24	0.036	0.004	-0.213	-0.159	**H56**	0.168	0.196	0.229	0.236
C25	-0.147	-0.149	-0.317	-0.287	**N57**	-0.351	-0.349	-0.227	-0.291
H26	0.208	0.282	0.258	0.300	**N58**	-0.370	-0.582	-0.309	-0.425

H27	0.151	0.228	0.211	0.239	N59	-0.437	-0.645	-0.380	-0.492
H28	0.127	0.203	0.192	0.219	N60	-0.312	-0.317	-0.206	-0.278
H29	0.129	0.204	0.192	0.218	N61	-0.393	-0.596	-0.300	-0.435
H30	0.140	0.218	0.203	0.228	O62	-0.551	-0.664	-0.405	-0.544
H31	0.132	0.174	0.206	0.217	063	-0.507	-0.652	-0.340	-0.454
H32	0.152	0.171	0.216	0.219	O64	-0.408	-0.625	-0.339	-0.462

3.5 Frontier molecular orbital analysis

Frontier molecular orbitals (FMO) (Figs. 6,7) determines the electric, electronic transitions, optical properties and kinetic stability [19]. HOMO-LUMO energy of compound was calculated using B3LYP/DFT 6-31G (d)/ 6-311G (d) levels of theory. The HOMO-LUMO energy gap is 4.33 e.v. for B3LYP/DFT basis set and 10.79 e.v. for B3LYP/HF 6-31G (d) basis set and 4.18 e.v. for B3LYP/DFTbasis set and 10.4 e.v. for B3LYP/HF 6-311G (d) (figure 4). Using HOMO-LUMO energy gap electronegativity (χ), electron affinity (A), global hardness (η), softness (S), chemical potential (μ), ionization potential (I), chemical potential (Pi), electrophilic index (ω), Nucleophilic index (IP) for the compound was calculated. These all properties are calculated as follows [20-22]:

$$\eta = (I - A)/2, \; \mu = -(I + A)/2, \; \chi = (I + A)/2, \; Pi = \chi, \; \omega = \mu^2 / 2\eta$$

In this formula, I and A symbolised ionization potential and electron affinity of the compound, which are virtually obtained from HOMO and LUMO energies. Where I = $-E_{HOMO}$ and A= $-E_{LUMO}$ showed as per Janak theorem [23] and Perdew et al. [24]. The HOMO-LUMO energy gap in compound is 4.31; 10.79 e.v. All these parameters such as global hardness (η) chemical potential (μ), the global electrophilicity index (ω), electronegativity (χ), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP) have been calculated for the target compound using 6-31G (d) basis set and are showed in table 8.
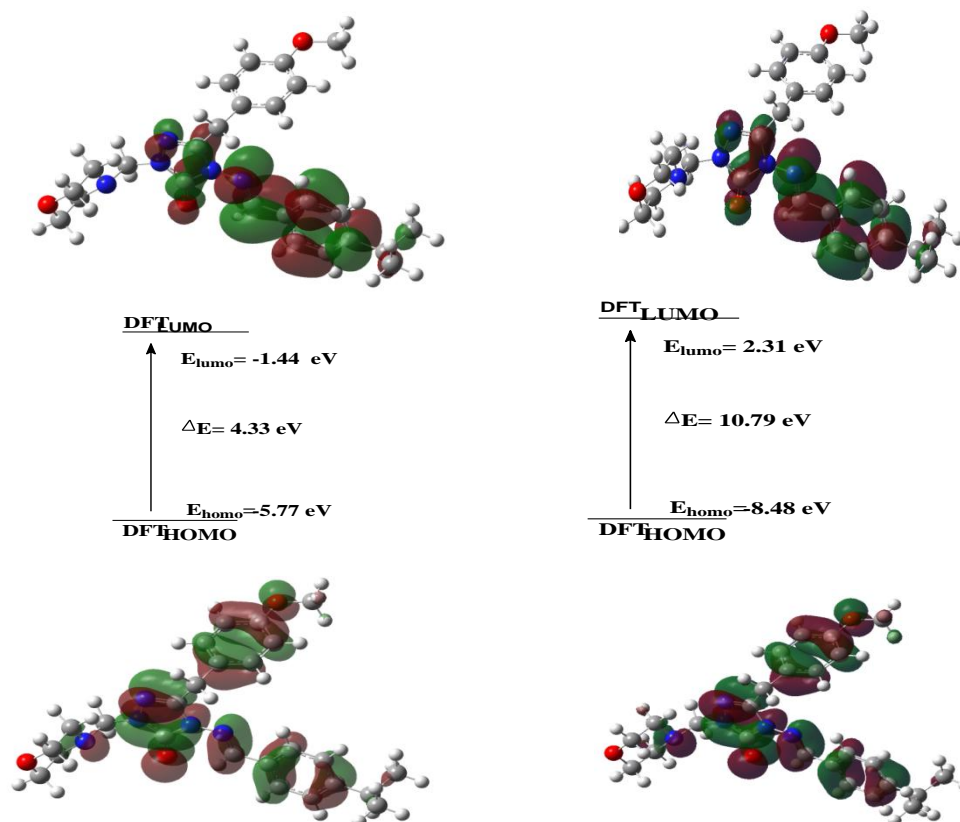

DFT$_{LUMO}$

E_{lumo}= -1.44 eV

$\triangle E$= 4.33 eV

E_{homo}=-5.77 eV

DFT$_{HOMO}$

DFT$_{LUMO}$

E_{lumo}= 2.31 eV

$\triangle E$= 10.79 eV

E_{homo}=-8.48 eV

DFT$_{HOMO}$

Figure 7: HOMO-LUMO energy of the molecule (6-31G)

DFT**LUMO**

E**lumo**= -1.58 eV

△E= 4.18 eV

E**homo**= -5.76 eV

DFT**HOMO**

DFT**LUMO**

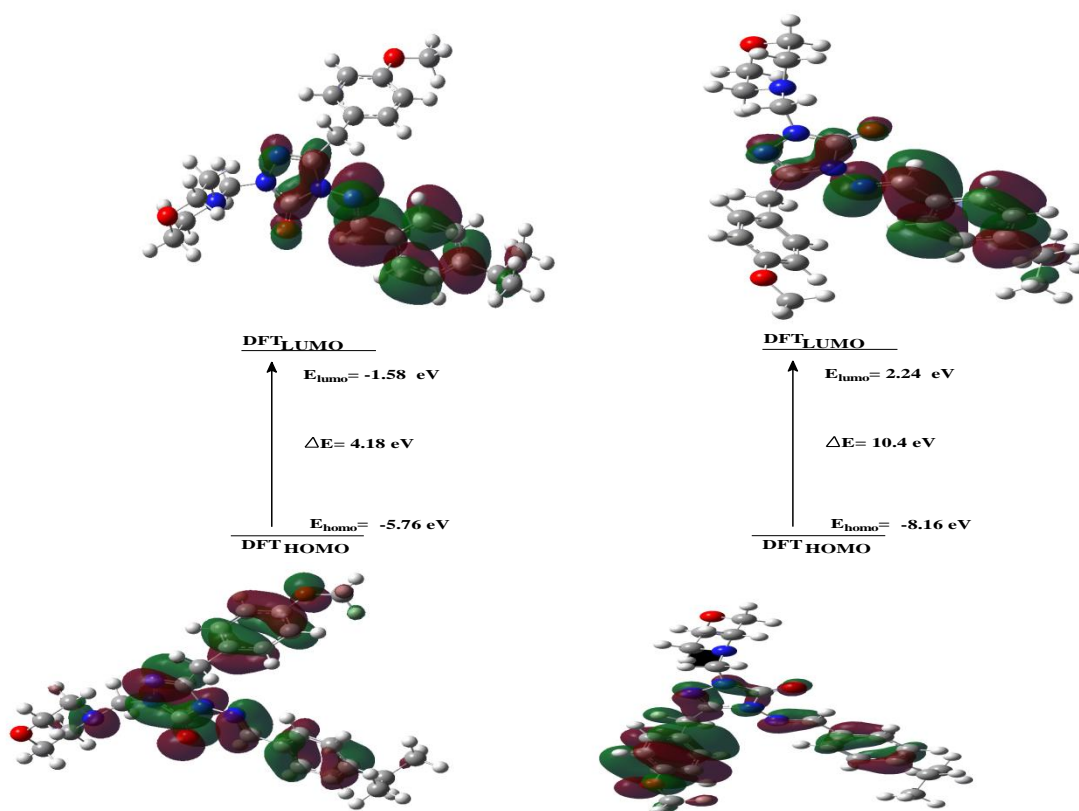E**lumo**= 2.24 eV

△E= 10.4 eV

E**homo**= -8.16 eV

DFT**HOMO**

Figure 8: HOMO-LUMO energy of the molecule (6-311G)

Table 8: The calculated electronic structure parameters of the molecule

		6-31G(d)				6-311G(d)			
		Hartree	**ev**	**kcal/mol**	**KJ/mol**	**Hartree**	**ev**	**kcal/mol**	**KJ/mol**
	LUMO	-0.05299	-1.44189	-33.2514	-139.125	-0.06155	-1.67482	-38.6228	-161.6
	HOMO	-0.21245	-5.78091	-133.313	-557.787	-0.22057	-6.00186	-138.408	-579.107
A	electron affinity	0.05299	1.44189	33.2514	139.125	0.06155	1.67482	38.6228	161.6
I	ionization potential	0.21245	5.78091	133.313	557.787	0.22057	6.00186	138.408	579.107
ΔE	energy gap	0.15946	4.33902	100.062	418.662	0.15902	4.32705	99.7855	417.507
χ	electronegativity	0.13272	3.6114	83.2822	348.456	0.14106	3.83834	88.5156	370.353
Pi	chemical potential	-0.13272	-3.6114	-83.2822	-348.456	-0.14106	-3.83834	-88.5156	-370.353
ω	electrophilic index	0.000702206	0.01911	0.44064	1.84364	0.000791042	0.02152	0.49638	2.07688
IP	Nucleophilic index	-0.01058177	-0.28794	-6.64009	-27.7824	-0.01121568	-0.30519	-7.03787	-29.4468
S	molecular softness	12.5423	341.286	7870.35	32929.9	12.5770	342.23	7892.13	33021
η	molecular hardness	0.07973	2.16951	50.0308	209.331	0.07951	2.16352	49.8928	208.754

3.6 Investigation of thermodynamics properties of compound

Thermodynamics parameters of molecule calculated with B3LYP/DFT/HF 631G (d) and B3LYP/DFT/HF 6311G (d) basis sets (table 9). Thermodynamic parameters of molecule (such as thermal energy, zero-point, vibrational energies (ZPVE), heat capacity, entropy, rotational temperatures and rotational constants) were calculated 298.150 K and 1 atm of pressure. In addition to, the standard thermodynamic functions of heat capacity CV^0, entropy S^0 and enthalpy H^0 were obtained at the B3LYP/DFT/HF 631G(d) and the B3LYP/DFT/HF 6311G(d) levels.

Table 9: The calculated thermodynamics parameters of the molecule

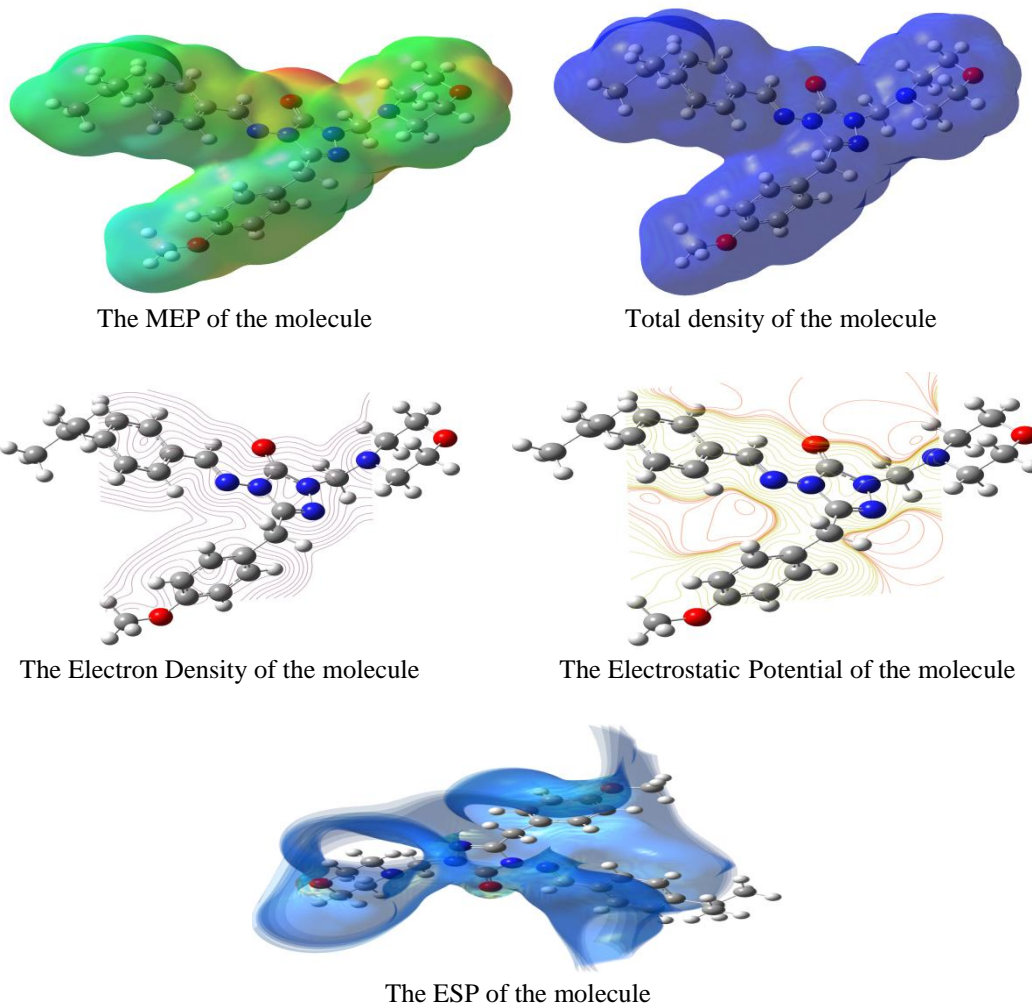| **Rotational temperatures (Kelvin)**	**DFT6-31G**	**HF6-31G**	**DFT6-311G**	**HF6-311G**
A	0.00614	0.00611	0.00599	0.00609
B	0.00301	0.00308	0.00303	0.00307
C	0.00215	0.00219	0.00215	0.00218
Rotational constants (GHZ)				
A	0.12804	0.12731	0.12485	0.12682
B	0.06264	0.06426	0.06318	0.06406
C	0.04489	0.04572	0.04480	0.04553
Thermal Energies E(kcal/mol)				
Translational	0.889	0.889	0.889	0.889
Rotational	0.889	0.889	0.889	0.889
Vibrational	355.683	379.853	354.008	377.792
Total	357.460	381.631	355.785	379.569
Thermal Capacity CV(cal/mol-K)				
Translational	2.981	2.981	2.981	2.981
Rotational	2.981	2.981	2.981	2.981
Vibrational	111.939	103.312	112.198	103.673
Total	117.900	109.274	118.160	109.635
Entropy S(cal/mol-K)				
Translational	44.196	44.196	44.196	44.196
Rotational	38.032	37.994	38.051	38.005
Vibrational	128.968	121.478	127.992	121.765
Total	211.196	203.669	210.239	203.967
Zero-point correction (Hartree/Particle)	0.538645	0.578972	0.536002	0.575637
Thermal correction to Energy	0.569649	0.608167	0.566980	0.604882
Thermal correction to Enthalpy	0.570593	0.609111	0.567924	0.605826
Thermal correction to Gibbs Free Energy	0.470247	0.512342	0.468033	0.508915
Sum of electronic and zero-point Energies	-1470.175959	-1460.960727	-1470.504987	1461.249451
Sum of electronic and thermal Energies	-1470.144955	-1460.931532	-1470.474009	1461.220206
Sum of electronic and thermal Enthalpies	-1470.144011	-1460.930587	-1470.473065	1461.219262
Sum of electronic and thermal Free Energies	-1470.244357	-1461.027357	-1470.572956	1461.316173
Zero-point vibrational energy (Kcal/mol)	338.00493	363.31015	336.34649	361.21756

Table 10: The calculated dipole moments datas of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
6-31G Dft	1.7624	2.2748	3.1793	4.2882
Hf	3.6656	5.2544	1.6045	6.6045
6-311G Dft	1.9693	2.6717	3.2927	4.6752
Hf	4.8302	0.5011	0.3110	4.8660

Table 11: The calculated total energy datas B3LYP/HF of the molecule

Enerji (a.u.)	DFT	HF
6-31 G	-1470.7146	-1461.5398
6-311 G	-1471.0409	-1461.8250

The MEP of the molecule

Total density of the molecule

The Electron Density of the molecule

The Electrostatic Potential of the molecule

The ESP of the molecule
Figure 8: The calculated molecular surfaces of the molecule (6-31G(d))

4. Conclusion

In this work, electronic, geometric and spectroscopic parameters of molecule are calculated by Density Functional Theory (DFT) and Hartree-Fock (HF) methods with the 631G(d) and 6311G(d) basis sets of the program package Gaussian G09W. Obtained spectroscopic parameters are compared with experimental data. In addition, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), bond angles, bond lengths, mulliken charges, E_{LUMO}-E_{HOMO} energy gap ($\Delta E g$), electronegativity (χ), electron affinity (A), global

hardness (η), softness (σ), ionization potential (I), total energy of the molecule, thermodynamics properties, dipole moments were calculated with B3LYP/HF/DFT 631G (d) and 6311G (d) basis sets. Furthermore, IR vibrational frequencies and IR spectrums were obtained. The IR data was found positive. This result showed that the structure of the compound was stable. The chemical shifts in the calculations ^{1}H-NMR and ^{13}C-NMR and IR vibrational frequencies are found to be compatible with the experimental data. Theoretical and experimental carbon and proton chemical shifts ratios between according to R^2 and a, b values, linear a correlation were observed. Result, obtained all data with the B3LYP/HF/DFT 6-31G(d) and 6-311G (d) basis sets were compared with each other.

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