Caucasian Journal of Science

Volume: 6, Issue: 1, Year : 2019 www.cjoscience.com e-ISSN: 2148-6840

Experimental (FT-IR, NMR) and Theoretical (B3PW91, B3LYP, HF) Analyses of 2-(3-Ethyl-4,5-Dihydro-1*H*-1,2,4-Triazol-5-on-4-yl)-azomethine)-Benzoic Acide

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Araştırma Makalesi Research Article	Kimya Chemistry	Geliş Tarihi/Received 24.04.2019	Kabul Tarihi/Accepted 30.06.2019

Abstract: 2-(3-Ethyl-4,5-dihydro-1*H*-1,2,4-triazol-5-on-4-yl)-azomethine)-benzoic acid has been optimized using DFT(B3PW91, B3LYP) and HF methods with 6-311G++(d,p) basis sets. Then, ^{13}C-NMR and ^{1}H-NMR spectral values according to GIAO method were calculated using Gaussian G09W program package in gas phase and in DMSO solvent. Theoretical and experimental values were plotted according to δ exp=a+b. d calc. Theoretical spectral values of molecule were calculated and compared with experimental values. The veda4f program was used in defining FT-IR data. 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(B3PW91,B3LYP) and HF methods. Then, these values are multiplied with scala factors. IR spectrums were drawn with obtained values according to HF and DFT method. In addition, the molecular surfaces such as the electron spin potential (ESP), the molecular electrostatic potential (MEP), the total density, the electron density, the electrostatic potential of the molecule were designated. Also, electronegativity (χ), global hardness (η), softness (σ), electron affinity (A) and ionization potential (I), highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) energy, E_{LUMO}-E_{HOMO} energy gap (ΔE*g*), the thermodynamics properties (entropy S^0, heat capacity CV^0 and enthalpy H^0), bond angles, bond lengths, mulliken atomic charges, total energy, dipole moments, were calculated with Gaussian 09W program on the computer.

Keywords: B3LYP, HF, Veda4f, HOMO-LUMO.

1. INTRODUCTION

Schiff bases (-HC=N-) are the most important organic compounds that they are obtained by condensation between a primary amine and an aldehyde or ketone to form an azomethine or imine group (Puchtler, 1981). 1,2,4-Triazole derivatives are known for several biological applications (Asiri et al., 2013; Ma et al., 2016; Nair et al., 2006; Yadav et al., 2001; Wang et al., 2001; Dash et al., 1984; Xia et al., 2014). Otherwise, Schiff bases have been used as bacteriocides, insecticides, pesticides, fungicides (Aydoğan et al., 2001; Azam et

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al 2007). In the last year, thereotical properties of Schiff bases were investigated on a computer. In this study, we investigated thereotical features of molecule. All theoretical calculations for the target compound were with the Gaussian 09W program (Frisch et al., 2009) on a personal computer. For this, firstly, molecule was optimized by using the DFT and HF methods with the restricted B3LYP/ B3PW91 (Frisch et al., 2009; Wolinski et al 1990) level of theory, 6-311G++(d,p) basis set, for all atoms. Optimized structure is the most stable structure of the molecule. The theoretical calculations $^{1}H/^{13}C$-NMR were performed by using DFT(B3PW91, B3LYP)/HF 6-311G++(d,p) and $^{1}H/^{13}C$-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 (Wolinski et al., 1990). The visualization of all results has been performed using GaussView 5 (GaussView, 2009). Theoretical and experimental values were inserted into the grafic according to equatation of δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Experimental data obtained from the literature (Yüksek et al 2006). Then, from this form, dipole moments, LUMO-HOMO, total energy, bond lengths, mulliken charges and bond angles, 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, finally, the Veda4f program was used in defining IR data (Jamroz, 2004). The theoretical vibrational spectra were calculated at the B3LYP, B3PW91 /HF 6-311G++(d,p) basis sets in the gas phase and these data are scaled with factors (Merrich et al., 2007) for 6-311G++(d,p) basis set. Theoretical IR spectra were obtained from these scaled values.

2. MATERIALS AND METHODS

2.1. Experimental

IR: υ (cm^{-1}) 3363 (NH), 1719, 1671 (C=O), 1614(C=N), 763 (1,2-disubstituted benzene ring). ^{1}H NMR (DMSO-d6, 400 MHz): δ ppm 1.79 (t, 3H, CH_3, J=7.40 Hz), 2.66 (q, 2H, CH_2, J=7.40 Hz), 7.54-7.69 (m, 2H, ArH), 7.91 (d, 1H, ArH), 8.01 (d, 2H, Ar-H), 10.40 (s, 1H, N=CH), 11.85 (s, 1H, NH), 11.85 (s, 1H, COOH). ^{13}C-NMR (DMSO-d6, 100 MHz): δ ppm 9.98 (CH_3), 18.46 (CH_2), 133.7, 130.22 (2C), 132.07 (2C), 130.72, 131.53 (2C), 126.73(2C) (arom-C), 148.01 (triazole C3), 152.50 (N=CH), 151.21 (triazole C5), 167.78 (COOH).

2.2. Theoretical

The quantum chemical calculations were carried out with Density Functional Theory (DFT) and Hartree-Fock (HF) methods using 6-311G++(d,p) basis sets at the Gaussian 09W program package on a computing system (Frisch et al., 2009). Firstly, the compound was optimized by using the DFT(B3PW91, B3LYP)/HF methods and 6-311G++(d,p) basis set (Frisch et al., 2009; Wolinski et al., 1990). Then, ^{13}C/ ^{1}H-NMR isotropic shift values were calculated with method of GIAO (Wolinski et al., 1990). The veda4f program was used in defining IR data (Jamroz, 2004). Theoretically calculated IR data are scaled with appropriate scala factors (Merrich et al., 2007). Scaled DFT and HF values are formed using theoretical infrared spectrum. Besides, the HOMO-LUMO energy, bond angles, bond lengths 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 6-311G++(d,p) levels. 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, dipole moment were calculated.

3. RESULT AND DISCUSSION

3.1. Computational Details

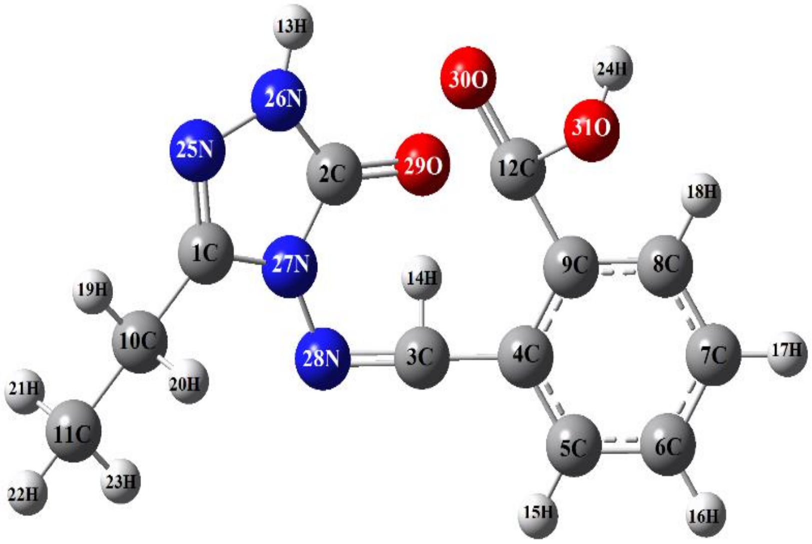


Figure 1. The Gaussview structure of the molecule.

Table 1. ^{1}H/ ^{13}C-NMR(DMSO) isotropic chemical shifts (δ/ppm) B3PW91, B3LYP, HF(6-311G++(d,p))

No	Experimental	B3PW91/6311d,p	Differ B3PW91	B3LYP/6311d,p	Differ B3LYP	HF/6311d,p	Differ hf
C1	148,1	151,53	-3,43	157,71	-9,61	147,34	0,76
C2	151,21	149,63	1,58	155,07	-3,86	144,14	7,07
C3	152,5	154,65	-2,15	159,01	-6,51	151,67	0,83
C4	133,7	138,88	-5,18	144,02	-10,32	132,75	0,95
C5	130,22	129,6	0,62	133,48	-3,26	121,83	8,39
C6	132,07	135,58	-3,51	139,67	-7,6	130,15	1,92
C7	130,72	131,86	-1,14	135,8	-5,08	122,65	8,07
C8	131,53	133	-1,47	137,27	-5,74	127,32	4,21
C9	126,73	128,46	-1,73	133,27	-6,54	118,85	7,88
C10	18,46	19,56	-1,1	23,88	-5,42	8,64	9,82
C11	9,98	9,31	0,67	12,97	-2,99	12,46	-2,48
C12	167,78	167,70	0,08	172,74	-4,96	156,22	11,56
H13	11,85	8,46	3,39	8,42	3,43	7,48	4,37
H14	10,4	11,72	-1,32	11,55	-1,15	10,42	-0,02
H15	7,91	9,40	-1,49	3,24	4,67	8,50	-0,59
H16	7,68	8,93	-1,25	8,77	-1,09	8,51	-0,83
H17	7,58	8,63	-1,05	8,45	-0,87	8,26	-0,68
H18	8,01	9,43	-1,42	9,28	-1,27	9,01	-1
H19	2,66	3,29	-0,63	3,18	-0,52	2,59	0,07
H20	2,66	3,08	-0,42	3,79	-1,13	3,02	-0,36
H21	1,79	1,75	0,04	1,67	0,12	1,20	0,59
H22	1,79	2,01	-0,22	1,94	-0,15	1,42	0,37
H23	1,79	2,13	-0,34	2,05	-0,26	1,48	0,31
H24	11,85	7,30	4,55	7,18	4,67	6,47	5,38

3.2. The relation between R values of the compound

There is such a relationship between R^{2}-values of the compound. B3PW91/6-311G++(d,p) (DMSO): ^{1}H:0.7632, ^{13}C: 0.9985; B3LYP/6-311G++(d,p) (DMSO): ^{1}H: 0.6358, ^{13}C: 0.9982; HF/6-311G++(d,p) (DMSO): ^{1}H: 0.7083,^{13}C: 0.9923. 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				^{1}H			
	R^{2}	**S. hata**	**a**	**b**	**R^{2}**	**S. hata**	**a**	**b**
B3PW91	0.9985	2.0120	0.9904	-0.2375	0.7632	2.0352	0.9674	0.1931
B3LYP	0.9982	2.2364	0.9831	-3.8994	0.6358	2.406	0.9372	0.9011
HF	0.9923	4.6442	1.0081	3.9851	0.7083	2.154	0.9850	0.7193

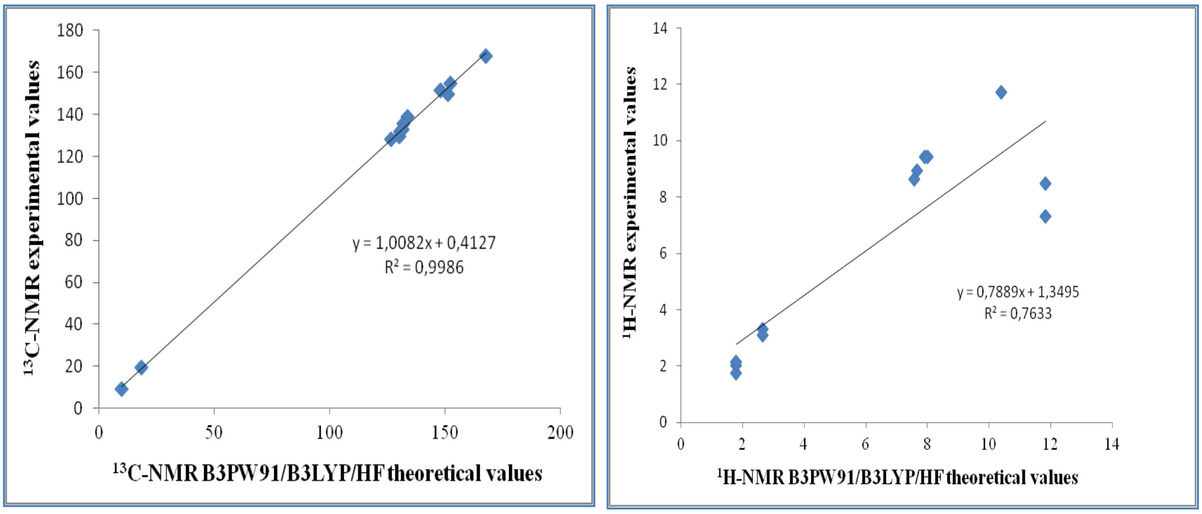


Figure 2. The correlation graphs for B3PW91/B3LYP/HF 6-311G++(d,p) /DMSO chemical shifts

3.3. The vibration frequency of the compound

Theoretically IR values were calculation veda 4f programme and scala values were obtain. The calculated harmonic vibrational frequency values were scaled with 0.9576 for B3PW91/6-311++G(d,p) level, 0.9671 for B3LYP/6-311++G(d,p) level, 0.9489 for HF/6-311++G(d,p) level (Merrich et al., 2007). The possitive frequency in the data was found. IR spectrums were drawn with obtained values according to DFT(B3PW91/B3LYP), HF methods. Theoretical IR values were compare with experimental IR values. The result of this compare were found corresponding with each other of values.

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

vibrational frequencies	Experimental (cm^{-1})	B3PW91/B3LYP/HF 6-311G++(d,p)		
	IR	Scaled B3PW91	Scaled B3LYP	Scaled HF
ν NH	3363	3523	3557	3728
ν C=O	1719, 1671	1716	1733	1873
ν C=N	1614	1586	1601	1785

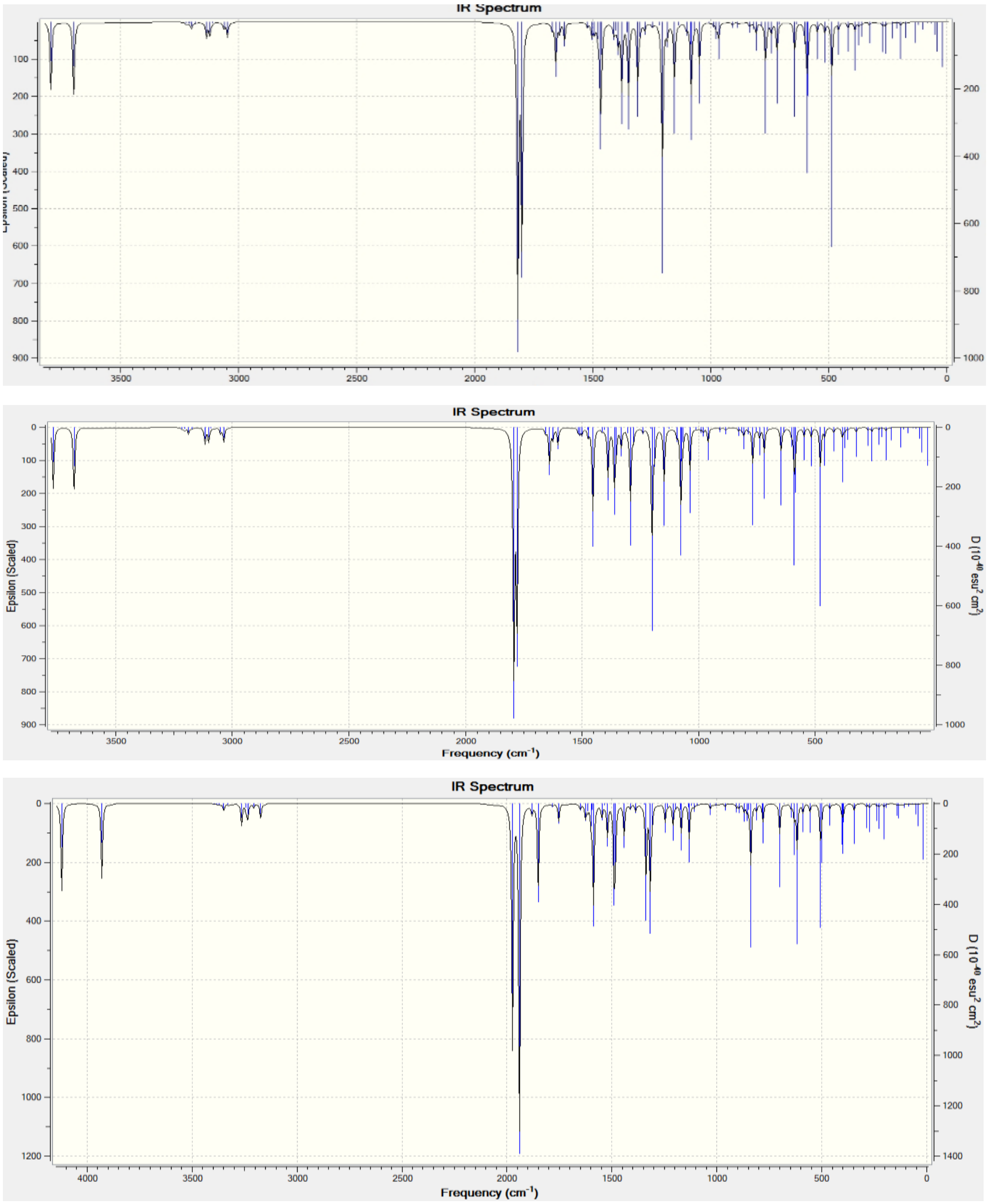


Figure 3. Theoretical IR spectrums and simulated with B3PW91/B3LYP/HF 6-311G ++(d,p)

3.4. Molecular Geometry

The molecular geometric parameters such as bond angles, bond lengths calculated by using the HF method and B3PW91/B3LYP functionals in DFT method with 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(10)-C(11) atoms that this values are 1.538/1.532/1.532 Å for B3LYP/B3PW91/HF 6-311G++(d,p). Besides, respectively, the bond lengths in the triazole ring N25-N26, N25-C1, C2-O29, C2-N27, N27-C1 are calculated 1,380/1.370/1.369; 1,297/1.295/1,268; 1.216/1,214/1.196; 1.420/1.415/1.387 Å for B3LYP/B3PW91/HF 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 (Ocak et al., 2003; Ustabaş et al., 2007). The calculated bond length values are consistent with literature values.

The highest bond angle is between N(26)-C(2)-O(29) atoms, which is $130.11/130.13/129.63^0$ for B3LYP/B3PW91/HF 6-311G++(d,p) basis sets (table 5). The calculated Mulliken atomic charges (Mulliken, 1955) calculated by using the HF and B3LYP/B3PW91 methods 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 (N25, N27) and C2 atom which is surrounded by three electronegative atoms (N26, N27, O29) have negative charges values. All hydrojen atoms of the compound (H13-H24) have positive atomic charge values (table 6).

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

Bond Lengths	B3LYP	B3PW91	HF	Bond Lengths	B3LYP	B3PW91	HF
C(1)-N(25)	1.297	1.295	1.268	C(3)-H(14)	1.082	1.084	1.071
C(1)-N(27)	1.390	1.386	1.380	C(3)-C(4)	1.475	1.470	1.487
C(1)-C(10)	1.490	1.485	1.493	C(4)-C(5)	1.402	1.399	1.388
N(25)-N(26)	1.380	1.370	1.369	C(5)-H(15)	1.082	1.083	1.072
N(26)-H(13)	1.006	1.005	0.990	C(5)-C(6)	1.388	1.386	1.383
N(26)-C(2)	1.368	1.364	1.346	C(6)-H(16)	1.084	1.085	1.075
C(2)-N(27)	1.420	1.415	1.387	C(6)-C(7)	1.394	1.392	1.383
C(2)-O(29)	1.216	1.214	1.196	C(7)-H(17)	1.083	1.084	1.074
N(27)-N(28)	1.371	1.362	1.368	C(7)-C(8)	1.389	1.387	1.382
C(10)-H(19)	1.091	1.092	1.082	C(8)-H(18)	1.081	1.082	1.072
C(10)-H(20)	1.093	1.094	1.084	C(8)-C(9)	1.401	1.398	1.389
C(10)-C(11)	1.538	1.532	1.532	C(9)-C(12)	1.489	1.485	1.491
C(11)-H(21)	1.092	1.092	1.085	C(12)-O(30)	1.209	1.207	1.185
C(11)-H(22)	1.092	1.093	1.085	C(12)-O(31)	1.357	1.351	1.326
C(11)-H(23)	1.091	1.092	1.083	O(31)-H(24)	0.968	0.967	0.945
N(28)-C(3)	1.285	1.283	1.256				

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

Bond Angles	B3LYP	B3PW91	HF	Bond Angles	B3LYP	B3PW91	HF
N(25)-C(1)-N(27)	111.090	111.028	111.051	N(27)-N(28)-C(3)	118.503	118.477	118.454
N(25)-N(26)-H(13)	120.418	120.403	120.930	N(28)-C(3)-H(14)	122.473	122.521	122.901
H(13)-N(26)-C(2)	125.182	125.042	125.310	H(14)-C(3)-C(4)	119.345	119.525	118.949
N(26)-C(2)-O(29)	130.115	130.134	129.638	C(3)-C(4)-C(5)	119.139	119.064	118.578
O(29)-C(2)-N(27)	128.717	128.776	128.461	C(3)-C(4)-C(9)	122.452	122.486	122.681
N(26)-C(2)-N(27)	101.160	101.081	101.897	C(4)-C(5)-H(15)	118.231	118.133	118.820
N(25)-C(1)-C(10)	124.920	125.090	125.085	C(4)-C(5)-C(6)	121.323	121.288	120.988
C(1)-C(10)-H(19)	106.495	106.461	106.416	C(5)-C(6)-H(16)	119.732	119.737	119.629
C(1)-C(10)-H(20)	108.819	108.723	108.719	C(5)-C(6)-C(7)	120.090	120.087	120.189
H(19)-C(10)-C(11)	110.358	110.520	108.132	H(15)-C(5)-C(6)	120.171	120.571	120.188
H(20)-C(10)-C(11)	109.657	109.758	110.012	C(6)-C(7)-H(17)	120.454	119.737	120.502
C(1)-C(10)-C(11)	113.483	113.391	113.017	H(16)-C(6)-C(7)	119.955	120.170	120.179
H(19)-C(10)-H(20)	107.837	107.790	108.132	C(7)-C(8)-H(18)	120.214	120.458	119.994
C(10)-C(11)-H(21)	110.836	110.871	110.760	H(18)-C(8)-C(9)	118.915	119.960	119.291
C(10)-C(11)-H(22)	110.032	110.122	109.820	C(7)-C(8)-C(9)	120.863	120.831	120.712

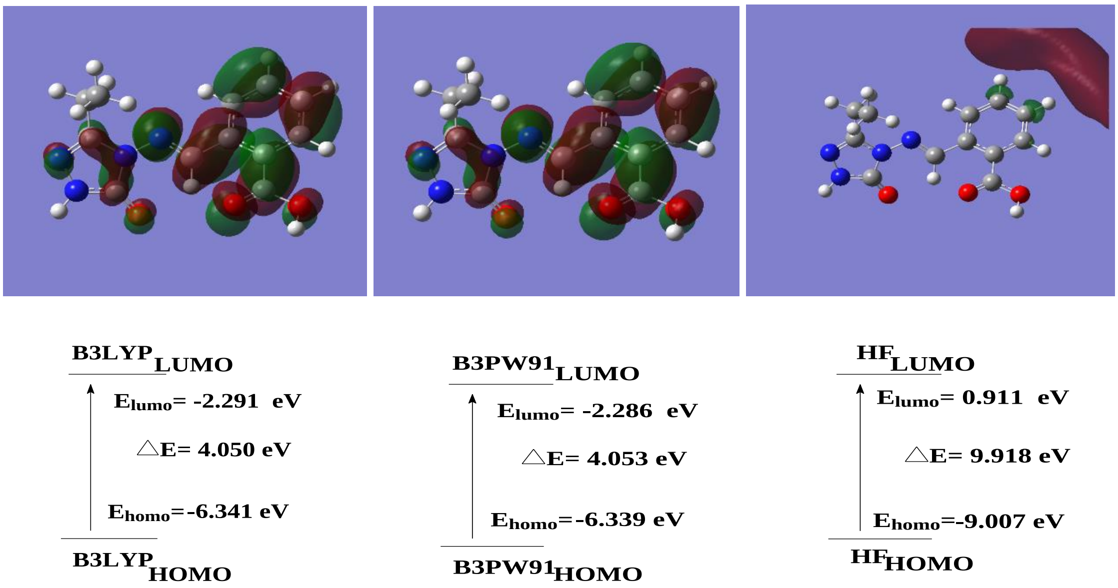
C(10)-C(11)-H(23)	111.222	111.208	111.406	C(9)-C(12)-O(30)	125.733	125.589	124.940
H(21)-C(11)-H(22)	108.118	108.089	108.155	C(9)-C(12)-O(31)	112.699	112.707	113.276
H(22)-C(11)-H(23)	108.045	107.997	108.092	C(12)-O(31)H(24)	106.524	106.246	108.291
H(21)-C(11)-H(23)	108.486	108.448	108.509	O(30)-C(12)O(31)	121.558	121.693	121.778
C(1)-N(27)-C(2)	108.376	108.379	108.167				

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

	B3LYP	**B3PW91**	**HF**		**DFT**	**B3PW91**	**HF**
C1	-0.157	-0.180	0.024	**H17**	0.165	0.203	0.199
C2	0.430	0.447	0.717	**H18**	0.206	0.239	0.254
C3	-0.193	-0.211	-0.894	**H19**	0.190	0.223	0.02
C4	0.136	0.063	0.229	**H20**	0.150	0.176	0.164
C5	0.110	0.207	-0.298	**H21**	0.147	0.170	0.146
C6	-0.301	-0.380	-0.282	**H22**	0.155	0.184	0.149
C7	-0.328	-0.400	0.467	**H23**	0.158	0.184	0.175
C8	-0.082	-0.108	0.008	**H24**	0.295	0.299	0.279
C9	-0.414	-0.472	0.282	**N25**	-0.040	-0.018	-0.027
C10	0.026	-0.198	0.207	**N26**	-0.219	-0.246	-0.314
C11	-0.139	-0.568	-0.281	**N27**	-0.018	0.029	-0.139
C12	-0.457	-0.062	-0.450	**N28**	-0.025	0.021	0.033
H13	0.388	0.422	0.433	**O29**	-0.355	-0.337	-0.484
H14	0.225	0.245	0.279	**O30**	-0.249	-0.230	-0.340
H15	0.176	0.209	0.225	**O31**	-0.161	-0.1340	-0.244
H16	0.183	0.224	0.218				

3.5. 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 4.050/4.053/9.918 e.v. for B3PW91/B3LYP/HF 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.



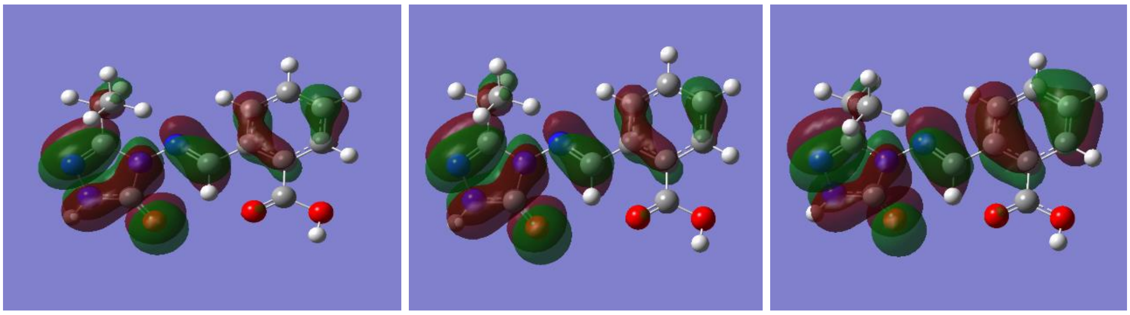


Figure 4. HOMO-LUMO energy of the molecule (6-311G++(d,p))

Table 7. The calculated electronic structure parameters of the molecule

		Hatree	**ev**	**kcal/mol**	**KJ/mol**
	LUMO	-0,08421	-2,29141	-52,842	-221,093
	HOMO	-0,23392	-6,36513	-146,786	-614,157
A	**elektron ilgisi**	0,08421	2,29141	52,842	221,093
I	İyonlaşma potansiyeli	0,23392	6,36513	146,786	614,157
ΔE	energy gap	0,14971	4,07371	93,9435	393,064
χ	electronegativity	0,159065	4,32827	99,8138	417,625
Pi	chemical potential	-0,159065	-4,32827	-99,8138	-417,625
ω	electrophilic index	0,000946978	0,02577	0,59423	2,48629
IP	Nucleophilic index	-0,01190681	-0,32399	-7,47156	-31,2613
S	molecular softness	13,3592	363,512	8382,91	35074,5
η	molecular hardness	0,074855	2,03686	46,9717	196,532

3.6. Thermodynamics properties, dipole moment and total energy of compound

Thermodynamics parameters were calculated with (B3PW91, B3LYP) functionals in DFT method and HF method at the 6-311G++(d,p) basis set at 298.150 K and under 1 atm pressure. All properties such as translational, electronic, vibrational and rotational partition functions, Entropy, Zero-point vibrational energy, Enthalpy were examined and were listened in table 8. The computed zero-point vibrational energy (ZPVE) values for all three levels were found as 149.26403, 148.60832, 160.02195 kcal/mol, respectively. The computed thermal energy (E), entropy(S) and heat capacity (Cv) values are 159.937/159.315/170124 kcal/mol; 136.077/136.277/132.667 cal; 63.558/ 63.774/59.400 cal for B3PW91/ B3LYP/ HF, respectively.

The dipole moment values were calculated as 1.4242, 1.4586, 5.0698 for DFT(B3PW91,B3LYP), HF methods and were shown in table 9.

The computed total energy values for molecule were obtained as -909.42648 Hartrees for B3LYP, -909.06629 Hartrees for B3PW91, -904.01237 Hartrees for HF (Table 10).

Table 8. The calculated thermodynamics parameters of the molecule

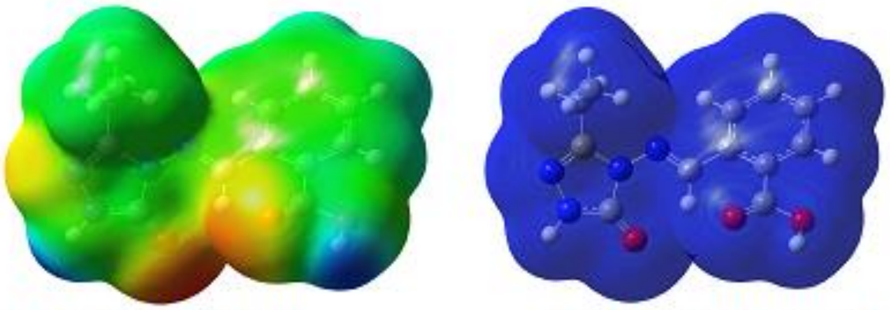
Parameters	B3PW91	B3LYP	HF
Rotational temperatures (Kelvin)			
A	0.03053	0.03035	0.03069
B	0.01057	0.01049	0.01040
C	0.00886	0.00879	0.00931
Rotational constants (GHZ)			
A	0.63618	0.63247	0.63949
B	0.22020	0.21866	0.21676
C	0.18463	0.18318	0.19399
Thermal Energies E(kcal/mol)			
Translational	0.889	0.889	0.889
Rotational	0.889	0.889	0.889
Vibrational	158.160	157.538	168.346
Total	159.937	159.315	170.124
Thermal Capacity CV(cal/mol-K)			
Translational	2.981	2.981	2.981
Rotational	2.981	2.981	2.981
Vibrational	57.597	57.813	53.438
Total	63.558	63.774	59.400
Entropy S(cal/mol-K)			
Translational	42.567	42.567	42.567
Rotational	33.785	33.806	33.746
Vibrational	59.725	59.904	56.353
Total	136.077	136.277	132.667
Zero-point correction (Hartree/Particle)	0.237867	0.236822	0.255011
Thermal correction to Energy	0.254876	0.253885	0.271109
Thermal correction to Enthalpy	0.255820	0.254829	0.272053
Thermal correction to Gibbs Free Energy	0.191166	0.190079	0.209019
Sum of electronic and zero-point Energies	-908.828431	-909.189658	-903.757362
Sum of electronic and thermal Energies	-908.811423	-909.172596	-903.741264
Sum of electronic and thermal Enthalpies	-908.810478	-909.171651	-903.740320
Sum of electronic and thermal Free Energies	-908.875133	-909.236401	-903.803354
Zero-point vibrational energy (Kcal/mol)	149.26403	148.60832	160.02195

Table 9. The calculated dipole moments datas of the molecule

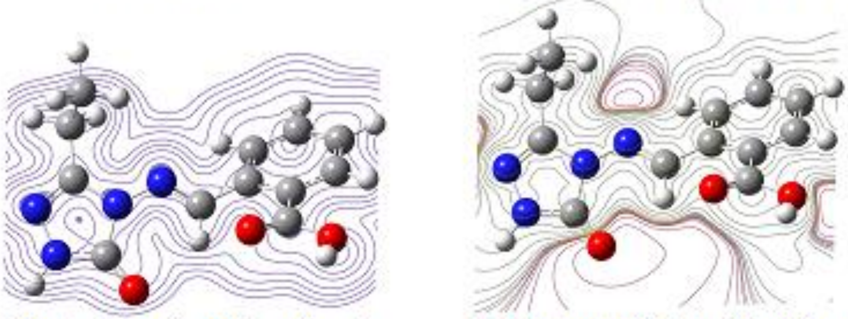
	μ_x	μ_y	μ_z	μ_{Toplam}
B3PW91	-0.5720	1.2889	0.1996	1.4242
B3LYP	-0.4443	1.3709	0.2255	1.4586
HF	1.3718	4.8685	0.3447	5.0698

Table 10. The calculated total energy datas of the molecule

Enerji (a.u.)	B3PW91	B3LYP	HF
	-909.06629	-909.42648	-904.01237



The MEP of the molecule Total density of the molecule



The Electron Density of the molecule The Electrostatic Potential of the molecule

Figure 5. The calculated molecular surfaces of the molecule

4. CONCLUSION

In this work, spectroscopic, electronic and geometric parameters of molecule are calculated by Hartree-Fock (HF) and B3LYP, B3PW91 functionals of Density Functional Theory (DFT) methods with the 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 possitive. 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 proton-carbon chemical shifts ratios between acording to a, b values and R^2 lineer a correlation were observed. 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 methods and 6-311G++(d,p) basis set. Result, obtained all data basis set were compared and these values were consistent with each other

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