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Theoretical Investigation of Spectroscopic and Thermodynamic Properties of 1-Acetyl-3-methyl-4-[3-(3-methoxybenzoxy)benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one by 6-311G(d) and 3-21G HF/DFT(B3LYP) Methods

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Abstract: In this study, theoretically spectral and thermodynamic values of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one was calculated and compared with experimental values. For this purpose, firstly, this compound has been optimized using 6-311G(d) and 3-21G HF/DFT(B3LYP) basis sets. ^{1}H-NMR and ^{13}C-NMR spectral values were calculated according to the method of GIAO using Gaussian G09W Software program. Theoretical and experimental values were plotted according to δexp=a+b. δ calc. The standard error values were found via the Sigma plot with regression coefficient of a and b constants. Futhermore, the vibrational frequency of title compound have been calculated by using 6-311G(d) and 3-21G HF/DFT(B3LYP) basis sets and these values are multiplied with appropriate adjustment factors. In the identification of calculated IR data was used the veda4f program. Also, the molecular structure, the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO), electronic transition, Natural Bonding Orbital (NBO) analysis, total static dipole moment (μ), the mean polizability (<α>), the anisotropy of the polarizability (Δα), the mean first-order hyperpolarizability (<β>), electronegativity(χ), hardness(η), molecular electrostatic potential maps (MEP) and Mulliken atomic charges of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy) benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule have been investigated by using DFT(B3LYP) and HF levels with 6-311G(d) and 3-21G basis sets.

Keywords: 4,5-Dihydro-1*H*-1,2,4-triazol-5-on, Gaussian 09W, GIAO, B3LYP, HF, 6-311G(d), 3-21G basis sets

Introduction

4,5-dihydro-1*H*-1,2,4-triazol-5-one and its derivatives constitute one of the most biologically active classes of compounds having a wide spectrum of activities such as antifungal, antimicrobial (Zhang et al., 2014), anti-HIV, antihypertensive (Ali, Ragab, Farghaly, & Abdalla, 2011), analgesic (Uzgören-Baran et al., 2012), antiviral, hypocholesteremic, anti-inflammatory (El-Serwy, Mohamed, Abbas, & Abdel-Rahman, 2013), antitumor (Chen et al., 2016), antioxidant properties. Some researchers have reported theoretical the electronic, structural properties and spectroscopic (IR, NMR, UV) parameters of 4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives (Jin et al., 2014; Al-tamimi, 2016; Gatfaoui et al., 2017; Pokharia et al., 2017; Süleymanoğlu et al., 2017)

The quantum-chemical calculation methods have been extensively used to predict the theoretical spectroscopic, thermodynamic and electronic properties of molecule systems. The quantum-chemical calculation methods have been widely used to predict the theoretical, structural, spectroscopic (IR, NMR, and UV) and electronic properties of molecular systems. The quantum chemical methods provide support experimental methods. In addition, many theoretical properties such as vibrational spectroscopy, molecular geometry, electronic and

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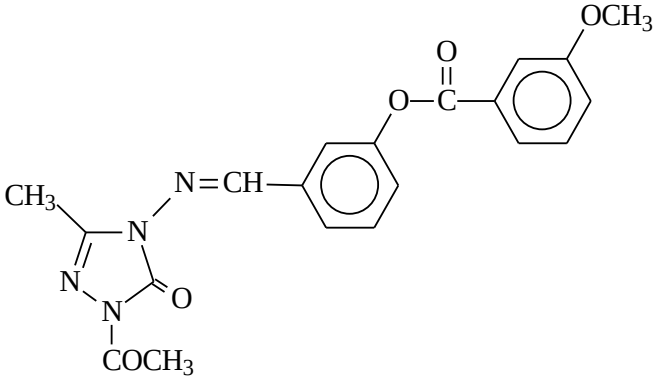
thermodynamic properties, ^{13}C and ^{1}H NMR chemical shifts, Mulliken atomic charges and HOMO-LUMO energies can be examined by using some theoretical methods. The electronic spectroscopy provides important information on electron transitions and electronic properties in molecular systems. The ^{1}H and ^{13}C NMR chemical shifts of molecule in solvent and in the gas phase can be calculated by using the DFT/B3LYP and Hartree Fock (HF) methods. Also, the geometric parameters (dihedral angles, bond angles and bond lenghts), vibrational frequencies, Mulliken atomic charges, electronic properties, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the calculated optimized molecule can be determined by using the DFT/B3LYP and Hartree Fock (HF) methods. All structural electronic and thermodynamic calculations were performed by using Gaussian G09W program (Frisch et al., 2009) and GaussView 5.0 program package (Frisch, Nielson, & Holder, 2003)

In this paper, theoretically spectral and thermodynamic values of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one was calculated and compared with experimental values [hilal tez]. For this purpose, firstly, this compound has been optimized using 6-311G(d) and 3-21G HF/DFT(B3LYP) basis sets. ^{1}H-NMR and ^{13}C-NMR spectral values were calculated according to the GIAO method (Wolinski, Hilton, & Pulay, 1990). Theoretical and experimental values (Medetalibeyoğlu, & Yüksek 2018) were plotted according to $\delta exp=a+b.\ \delta$ calc. The standard error values were found via the Sigma plot with regression coefficient of a and b constants. Futhermore, the vibrational frequency of title compound have been calculated by using 6-311G(d) and 3-21G HF/DFT(B3LYP) basis sets and these values are multiplied with appropriate adjustment factors. In the identification of calculated IR data was used the veda4f program (Jamróz, 2004). Also, the molecular structure, the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO), electronic transition, Natural Bonding Orbital (NBO) analysis, total static dipole moment (μ), the mean polizability ($<\alpha>$), the anisotropy of the polarizability ($\Delta\alpha$), the mean first-order hyperpolarizability ($<\beta>$), electronegativity(χ), hardness(η), molecular electrostatic potential maps (MEP) and Mulliken atomic charges of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy) benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule have been investigated by using DFT(B3LYP) and HF levels with 6-311G(d) and 3-21G basis sets.

Result and Discussion

Geometry of title molecule was optimized at the HF and B3LYP levels of theory along with standard 6-311G(d) and 3-21G basis sets. The vibrational frequencies were calculated by HF and B3LYP methods. The ^{1}H-NMR and ^{13}C-NMR shielding values were calculated according to GIAO (Gauge Including Atomic Orbital) method. (Wolinski, Hilton, & Pulay, 1990; Dodds, McWeeny, & Sadlej, 1980). Time–dependent density functional theory (TD-DFT) was used to compute oscillator strengths, excitation energies for electronic transitions from ground to excited states (Bauernschmitt, & Ahlrichs, 1996; Casida et al., 1998; Stratmann et al., 1998). Some quantum chemical descriptors (bond lengths, bond angles, UV-Vis values, dipole moments, Mulliken atomic charges, HOMO-LUMO energies and total energy) are calculated at the DFT/6-311G(d) and DFT/3-21G, HF/6-311G(d) and HF/3-21G levels. All the calculations were carried out with the Gaussian 09W software (Frisch et al., 2009).

1-Acetyl-3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one



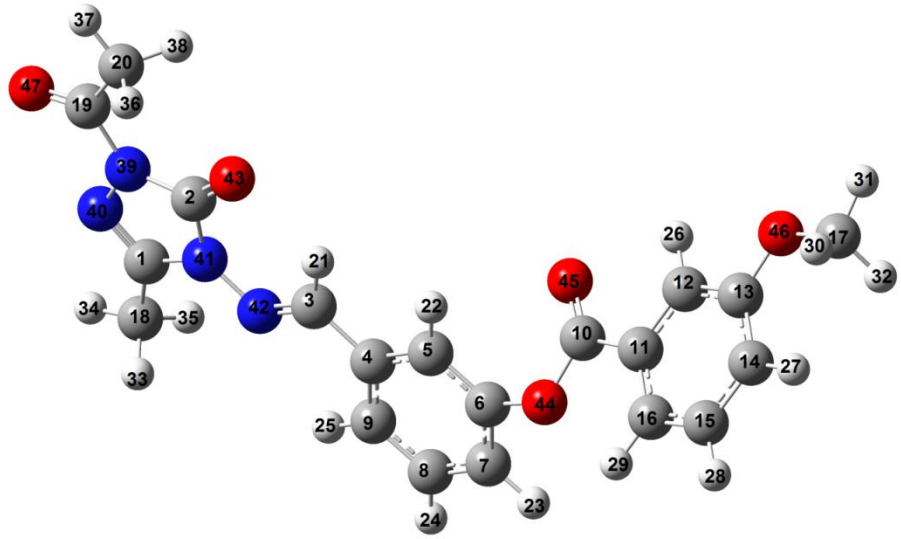


Figure 1. The optimized molecular structure of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy)benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one

Table 1. The calculated ^{1}H and ^{13}C NMR isotropic chemical shifts of title compound (with respect to TMS, all values in ppm) (6-311G(d))

	$\delta_{Exp.}$	$\delta_{cal.}$ **HF (Vacuum)**	$\delta_{cal.}$ **HF (DMSO)**	**Different**	**Different (DMSO)**	$\delta_{cal.}$ **B3LYP (Vacuum)**	$\delta_{cal.}$ **B3LYP (DMSO)**	**Different**	**Different (DMSO)**
C1	146.71	150.20	153.41	-3.49	-6.70	139.83	143.55	6.88	3.16
C2	151.07	154.29	154.84	-3.22	-3.77	142.67	143.22	8.40	7.85
C3	147.81	153.55	154.39	-5.74	-6.58	143.16	144.04	4.65	3.77
C4	134.71	139.26	138.85	-4.55	-4.14	125.87	125.57	8.84	9.14
C5	126.25	130.22	129.66	-3.97	-3.41	120.14	120.05	6.11	6.20
C6	154.45	157.84	157.43	-3.39	-2.98	142.43	141.51	12.02	12.94
C7	125.47	126.42	127.68	-0.95	-2.21	117.50	118.35	7.97	7.12
C8	130.03	131.76	133.15	-1.73	-3.12	120.71	121.61	9.32	8.42
C9	120.24	123.58	124.19	-3.34	-3.95	114.46	115.21	5.78	5.03
C10	164.33	166.45	167.95	-2.12	-3.62	151.38	153.22	12.95	11.11
C11	130.36	134.36	133.50	-4.00	-3.14	122.62	121.69	7.74	8.67
C12	122.15	124.75	122.84	-2.60	-0.69	115.25	113.24	6.90	8.91
C13	159.43	165.22	165.40	-5.79	-5.97	149.57	149.42	9.86	10.01
C14	114.39	115.28	117.95	-0.89	-3.56	104.12	106.59	10.27	7.80
C1	130.1	131.71	133.27	-1.53	-3.09	120.83	122.37	9.35	7.81

5	8								
C16	120.57	124.11	124.29	-3.54	-3.72	113.33	113.72	7.24	6.85
C17	55.47	53.54	54.08	1.93	1.39	35.30	35.77	20.17	19.70
C18	11.21	12.35	12.44	-1.14	-1.23	0.49	0.70	10.72	10.51
C19	166.00	164.44	168.07	1.56	-2.07	151.44	155.51	14.56	10.49
C20	23.43	24.57	24.86	-1.14	-1.43	11.43	11.76	12.00	11.67
H21	9.67	9.56	9.54	0.11	0.13	8.94	8.95	0.73	0.72
H22	7.64	7.21	7.26	0.43	0.38	6.62	6.82	1.02	0.82
H23	7.52	6.86	7.10	0.66	0.42	6.65	6.90	0.87	0.62
H24	7.62	7.12	7.38	0.50	0.24	6.85	7.12	0.77	0.50
H25	7.84	7.74	7.86	0.10	-0.02	7.57	7.72	0.27	0.12
H26	7.82	7.57	7.39	0.25	0.43	7.43	7.23	0.39	0.59
H27	7.35	6.33	6.70	1.02	0.65	6.06	6.47	1.29	0.88
H28	7.56	7.03	7.29	0.53	0.27	6.79	7.09	0.77	0.47
H29	7.76	7.45	7.56	0.31	0.20	7.18	7.31	0.58	0.45
H30	3.88	3.19	3.37	0.69	0.51	2.51	2.71	1.37	1.17
H31	3.88	3.69	3.76	0.19	0.12	3.08	3.14	0.80	0.74
H32	3.88	3.18	3.36	0.70	0.52	2.51	2.71	1.37	1.17
H33	2.37	2.00	2.17	0.37	0.20	1.52	1.72	0.85	0.65
H34	2.37	1.83	1.87	0.54	0.50	1.46	1.43	0.91	0.94
H35	2.37	2.00	2.16	0.37	0.21	1.51	1.70	0.86	0.67
H36	2.50	2.14	2.26	0.36	0.24	1.56	1.70	0.94	0.80
H37	2.50	1.60	1.64	0.90	0.86	1.14	1.16	1.36	1.34
H38	2.50	2.17	2.28	0.33	0.22	1.57	1.70	0.93	0.80

Table 2. The calculated ^{1}H and ^{13}C NMR isotropic chemical shifts of title compound (with respect to TMS, all values in ppm) (3-21G)

	$\delta_{Exp.}$	**$\delta_{cal.}$ HF (Vacuum)**	**$\delta_{cal.}$ HF (DMSO)**	**Different**	**Different (DMSO)**	**$\delta_{cal.}$ B3LYP (Vacuum)**	**$\delta_{cal.}$ B3LYP (DMSO)**	**Different**	**Different (DMSO)**
C1	146.71	115.89	118.01	30.82	28.70	112.50	115.35	34.21	31.36
C2	151.0	117.47	117.63	33.60	33.44	115.33	115.50	35.74	35.57

	7								
C3	147.81	118.63	119.15	29.18	28.66	116.07	116.63	31.74	31.18
C4	134.71	100.14	99.57	34.57	35.14	92.70	92.11	42.01	42.60
C5	126.25	90.74	90.19	35.51	36.06	84.32	83.77	41.93	42.48
C6	154.45	120.91	120.89	33.54	33.56	111.04	110.87	43.41	43.58
C7	125.47	88.41	89.38	37.06	36.09	84.08	84.94	41.39	40.53
C8	130.03	93.76	94.93	36.27	35.10	88.87	89.99	41.16	40.04
C9	120.24	87.52	87.90	32.72	32.34	83.16	83.63	37.08	36.61
C10	164.33	133.24	133.85	31.09	30.48	128.53	129.30	35.80	35.03
C11	130.36	96.43	95.69	33.93	34.67	90.09	89.27	40.27	41.09
C12	122.15	88.40	86.89	33.75	35.26	85.49	83.70	36.66	38.45
C13	159.43	124.42	124.48	35.01	34.95	115.72	115.40	43.71	44.03
C14	114.39	83.18	85.14	31.21	29.25	78.28	80.36	36.11	34.03
C15	130.18	94.30	95.55	35.88	34.63	88.97	90.44	41.21	39.74
C16	120.57	88.15	88.20	32.42	32.37	83.96	84.43	36.61	36.14
C17	55.47	31.56	31.19	23.91	24.28	15.60	16.19	39.87	39.28
C18	11.21	-6.41	-6.56	17.62	17.77	-17.72	-17.73	28.93	28.94
C19	166.00	127.55	129.97	38.45	36.03	125.39	128.54	40.61	37.46
C20	23.43	4.34	4.44	19.09	18.99	-7.78	-7.60	31.21	31.03
H21	9.67	9.24	9.21	0.43	0.46	8.68	8.65	0.99	1.02
H22	7.64	7.78	7.70	-0.14	-0.06	7.37	7.28	0.27	0.36
H23	7.52	5.81	6.10	1.71	1.42	5.74	6.06	1.78	1.46
H24	7.62	6.10	6.42	1.52	1.20	5.90	6.26	1.72	1.36
H25	7.84	6.86	6.99	0.98	0.85	6.78	6.96	1.06	0.88
H26	7.82	6.66	6.48	1.16	1.34	6.81	6.56	1.01	1.26
H27	7.35	5.25	5.68	2.10	1.67	4.95	5.44	2.40	1.91
H28	7.56	6.03	6.34	1.53	1.22	5.75	6.13	1.81	1.43
H29	7.76	6.63	6.78	1.13	0.98	6.49	6.70	1.27	1.06
H30	3.88	2.74	2.98	1.14	0.90	1.74	2.03	2.14	1.85
H3	3.88	3.39	3.51	0.49	0.37	2.73	2.82	1.15	1.06

H31	3.88	2.74	2.98	1.14	0.90	1.74	2.03	2.14	1.85
H32	2.37	1.53	1.71	0.84	0.66	0.82	1.04	1.55	1.33
H33	2.37	1.14	1.18	1.23	1.19	0.59	0.62	1.78	1.75
H34	2.37	1.53	1.71	0.84	0.66	0.82	1.04	1.55	1.33
H35	2.50	1.96	2.05	0.54	0.45	1.17	1.29	1.33	1.21
H36	2.50	0.99	1.05	1.51	1.45	0.42	0.45	2.08	2.05
H37	2.50	1.96	2.05	0.54	0.45	1.17	1.29	1.33	1.21
H38									

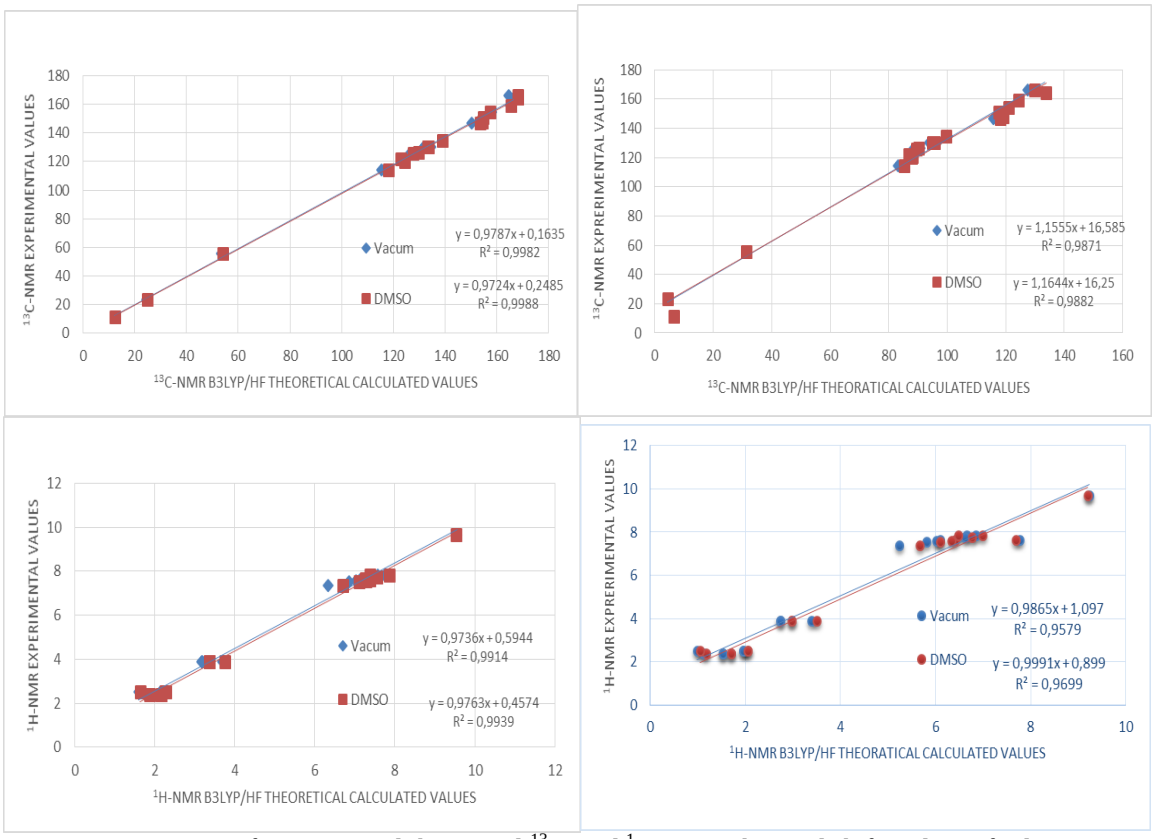


Figure 2. Comparison of experimental/theoretical ^{13}C- and ^{1}H-NMR chemical shifts values of title compound with 6-311G(d)(a)/B3LYP, HF, B3LYP(DMSO) ve HF(DMSO) ve 3-21G(b)/B3LYP, HF, B3LYP(DMSO) ve HF(DMSO) methods

Table 3. The calculated IR frequencies of title compound (6-311G)

	Vibration Frequencies	**HF**	**B3LYP**
1	τ COCC(51),τ NCCC(37), τ CNNC(10)	5	14
2	τ CCCC(14), τ COCC(27), τ CCCN(14), τ CNNC(12), τ NCCN(10)	12	17
3	τ CCOC(65),τ NCCC(13), τ COCC(29), τ CCCC(20)	16	18
4	τ NCNN(30), τ CCNN(18), τ NCCN(38)	35	36
5	τ CCCC(28), τ COCC(19)	37	40
6	δ COC(22), δ CCO(12), τ COCC(19), τ CCNC(15)	52	51
7	τ CCNC(60)	65	67
8	δ CCN(18), δ CNN(10), δ NCC(10), τ COCC(25), τ CCCC(10)	67	74
9	τ COCC(65), τ HCOC(11)	70	84

10	τ CCCN(18), τ CNNC(15), τ CCNN(23),τ NNCN(10), τ NCNN(11)	91	94
11	δ COC(15), δ CCC(13), τ CCNN(27), τ CNNC(19)	130	128
12	δ CCO(13), τ CNNC(12), τ CCNN(18)	140	137
13	δ NCC(10), δ NCN(13), δ NNC(10), δ CCC(12)	161	157
14	τ HCCN(55), τ CNNC(12), τ NCNN(21)	172	161
15	τ CCCC(12), τ NCNN(13)	176	166
16	τ HCCN(69)	185	171
17	τ CNNC(28), τ NNCN(11), τ HCCN(56)	192	177
18	δ CCC(12), δ COC(19)	196	199
19	δ NCN(10), δ CCC(14), τ HCOC(12), τ COCC(13), τ OCCC(24), τ CCCC(18)	225	215
20	δ CCC(12), δ COC(19), δ CCN(14), τ HCOC(12), τ CCCC(18), τ OCCC(12)	226	219
21	τ CCCC(15), τ NCNN(14), τ CCCN(33), τ NCCN(22)	228	237
22	ν CC(13), δ NCN(15), δ CCO(10)	250	244
23	δ COC(28), τ CCCN(14)	270	264
24	τ COCC(10), τ HCOC(45), τ CCCC(25)	292	280
25	δ COC(21), δ OCO(15)	307	296
26	δ CCN(37)	339	327
27	τ NCNN(11), τ CNNC(16), τ NNCN(14), τ CCCN(10), τ CCNN(34), τ NCCN(10)	365	350
28	τ CNNC(35), τ CCNN(11)	375	364
29	δ CCO(19), δ CNN(15), δ OCN(23), δ CCN(29)	391	371
30	δ CCN(25), δ OCN(18)	396	377
31	δ CCC(38), δ COC(10), δ OCO(10), τ CCCC(12)	439	426
32	δ CCN(10), τ CCCC(30)	457	437
33	ν NC(10), δ CCN(11), τ CCCC(18)	468	444
34	τ CCCC(12), τ HCCC(15), τ CCOC(11), τ CCCN(10)	480	457
35	δ CCC(12), δ NNC(13), δ CCO(13)	496	467
36	δ CCC(21), δ COC(10)	507	496
37	δ COC(12), δ CCC(13), τ OCCC(37), τ OCOC(12), τ HCCC(11)	581	551
38	δ COC(20), δ CCC(14), τ CCCC(12), τ OCCC(29)	583	567
39	τ HCCN(11), τ ONNC(24)	600	583
40	δ CCC(10), τ ONNC(15)	612	583
41	δ CCC(11), τ HCCN(16), τ ONNC(32)	613	592
42	δ OCO(10), τ CCOC(26), τ CCCN(19), τ COCC(13), τ CCCC(15)	624	598
43	ν CC(26), δ OCC(32), τ NNCN(21)	629	606
44	ν CC(17), δ CCC(11), δ NNC(16),τ NNCN(11)	675	654
45	τ NNCN(21), τ CNNC(31), τ NCNN(16), τ CNNC(13)	690	655
46	δ NCC(11), δ CNN(11), δ CCN(11), δ OCN(18), δ CCC(10)	699	675
47	δ CCC(14), τ CCCC(18), τ HCCC(18)	711	683
48	δ CCC(18), τ CCCC(18), τ OCCC(10), τ HCCC(27)	716	686
49	τ CCCC(15), τ HCCC(37), τ CCOC(20)	725	691
50	ν CC(10), δ CCC(13), τ ONNC(41)	796	739
51	τ OCOC(45), τ HCCC(24)	808	753
52	ν NN(13), τ NCNN(11), τ ONNC(41)	816	769
53	δ OCO(12), τ HCCC(30)	830	789
54	τ OCOC(23), τ HCCC(50)	848	802
55	τ OCOC(29), τ HCCC(49)	861	809
56	τ HCCC(15)	874	826
57	ν OC(20), τ HCCC(19)	926	875
58	ν CC(22), ν NN(11), τ HCCC(42)	955	891
59	ν OC(11), τ HCCC(49)	966	896
60	ν CC(15), ν NC(11), ν NN(10), δ NNC(10), τ HCCC(25)	967	913
61	τ HCCC(39)	982	917
62	τ HCCC(39)	985	918
63	ν OC(10), ν CC(13), δ CCC(11), τ HCCC(42)	998	957
64	ν CC(19), δ HCH(11), τ HCCN(29), τ HCCC(55)	1020	961
65	ν CC(30), δ CCC(32), δ HCH(10), τ HCCN(25)	1027	968
66	ν CC(21), δ CCC(21), τ HCCC(56)	1034	968

67	ν CC(25), δ CCC(23), τ HCCC(46)	1044	1002
68	τ HCCC(59), τ HCNN(85)	1051	1006
69	ν CC(17), δ CCC(23), δ HCH(19), τ HCCN(47)	1077	1008
70	δ HCH(17), τ HCCC(39), τ HCNN(89)	1082	1022
71	δ HCH(19), τ HCCN(53)	1114	1059
72	ν OC(60), δ HCH(21), τ CNNC(10), τ HCCN(57)	1117	1061
73	ν CC(19), δ HCC(22), δ HCH(21), τ HCCN(58)	1124	1067
74	ν CC(10), ν OC(48), δ HCH(26), δ NNC(11), τ HCCN(10), τ HCOC(26)	1126	1079
75	ν OC(11), ν CC(14), δ HCC(20)	1137	1084
76	ν CC(18), δ HCC(23)	1142	1099
77	ν CC(11), ν NC(21), δ HCC(21), δ NNC(13)	1144	1111
78	ν CC(21), ν NN(26), τ HCCN(17)	1156	1136
79	ν CC(25), δ HCC(40)	1168	1167
80	ν NN(18), δ HCC(14), δ HCH(26), τ HCOC(26), τ HCCN(16)	1204	1172
81	δ HCC(33)	1219	1181
82	δ HCC(26), δ HCH(25), τ HCOC(26)	1232	1185
83	ν NC(15), ν NN(11), δ OCC(12), δ HCC(20), τ HCOC(11)	1251	1197
84	ν CC(15), δ HCC(19), δ HCH(11), τ HCOC(18)	1262	1199
85	ν OC(11), ν CC(11), δ HCC(12), τ HCOC(11)	1266	1222
86	ν NN(22), ν NC(13), δ NCN(12)	1296	1246
87	ν OC(17), ν CC(20), δ NCN(11)	1310	1276
88	ν CC(16), ν OC(42)	1325	1286
89	ν NN(13), ν NC(32), δ OCN(10)	1361	1303
90	ν OC(17), δ HCC(20)	1368	1311
91	δ HCC(30)	1373	1313
92	ν CC(22), δ HCC(78)	1376	1343
93	ν CC(24), ν NC(17), δ HCC(17), δ CNN(12), δ HCH(13)	1413	1349
94	ν NC(11), δ HCN(37), δ NNC(10), δ HCH(11)	1440	1370
95	δ HCH(92), δ HCN(10)	1477	1407
96	δ HCH(64), δ HCN(15)	1481	1417
97	ν CC(16), δ HCH(14)	1500	1435
98	δ HCH(72), τ HCCN(23)	1516	1458
99	ν CC(14), δ HCC(10), δ HCH(50), τ HCCN(15)	1524	1459
100	ν CC(13), δ HCH(24), δ HCC(12)	1528	1465
101	δ HCH(76), τ HCCN(22)	1530	1475
102	δ HCH(76), τ HCCN(24)	1534	1475
103	δ HCH(61)	1546	1480
104	δ HCH(55), δ HCN(10), τ HCCN(19)	1549	1486
105	δ HCH(72), δ HCN(37), τ HCOC(12)	1562	1498
106	δ HCH(71), τ HCOC(10)	1570	1509
107	δ HCC(40), δ HCH(16), δ CCC(12)	1574	1511
108	δ HCC(27), δ CCC(14)	1577	1515
109	ν CC(32), δ HCC(10), δ CCC(17)	1691	1610
110	ν CC(32), δ HCC(11), δ CCC(15)	1698	1611
111	ν CC(21), δ HCC(14)	1717	1628
112	ν CC(31)	1718	1638
113	ν NC(64), ν CC(12)	1796	1647
114	ν NC(64)	1802	1663
115	ν OC(40)	1859	1772
116	ν OC(88)	1904	1786
117	ν OC(50)	1921	1811
118	ν CH(91)	3030	2982
119	ν CH(92)	3059	3025
120	ν CH(97)	3070	3036
121	ν CH(50)	3086	3041
122	ν CH(100)	3117	3078
123	ν CH(100)	3135	3095
124	ν CH(46)	3149	3117

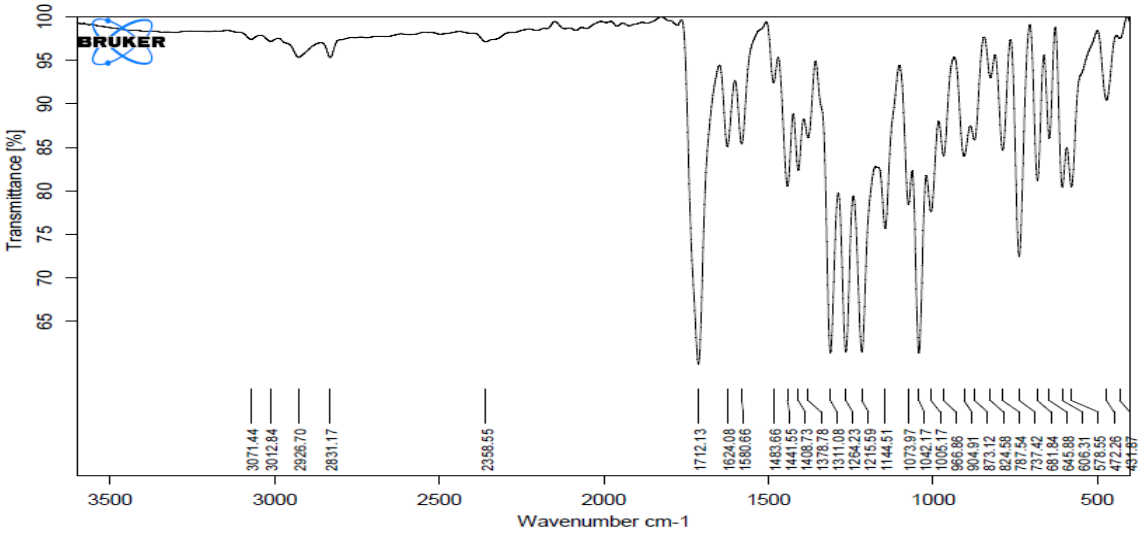
125	ν CH(92)	3152	3122
126	ν CH(97)	3159	3131
127	ν CH(52)	3188	3142
128	ν CH(54)	3191	3145
129	ν CH(34)	3202	3147
130	ν CH(42)	3211	3169
131	ν CH(67)	3220	3176
132	ν CH(46)	3222	3180
133	ν CH(57)	3227	3185
134	ν CH(56)	3236	3187
135	ν CH(48)	3238	3193

Table 4. The calculated IR frequencies of title compound (3-21G)

	Vibration Frequencies	**HF**	**B3LYP**
1	τ NCNC(16), τ CCCC(12), τ CNNC(25), τ COCC(17)	13	14
2	τ CCCC(13), τ COCC(34), τ CCOC(24)	17	17
3	δ NCC(18), δ CCO(12), δ CCC(22), δ COC(22), δ NNC(17)	25	24
4	τ CNNC(11), τ COCC(41), τ CCOC(34)	30	32
5	τ NCNN(32), τ CCNC(14), τ NNCC(23)	40	38
6	τ CCNC(65)	62	59
7	δ CCC(13), δ COC(28), δ NNC(16), τ HCOC(10), τ COCC(57)	66	68
8	δ COC(15), δ CCO(17), δ NNC(15), τ CCCC(10), τ COCC(48)	67	80
9	τ COCC(31), τ CCCC(22)	87	94
10	τ NCNC(10), τ NNCC(11), τ CCNN(18), τ CCCC(15)	102	98
11	δ CCC(11), δ COC(13), δ CCO(12), τ HCCN(29), τ NCNC(12), τ CNNC(14), τ CCNN(13)	124	123
12	δ CCO(12), δ CCC(17), δ COC(12), τ NCNC(18), τ CNNC(13), τ CCNN(22)	141	124
13	δ NCC(11), δ CNN(15), τ HCCN(48)	157	141
14	δ CNN(15), δ NCC(11), τ HCCN(50), τ CCNN(10)	167	157
15	τ HCCN(16), τ NCNC(11), τ CCNN(11), τ CCCC(27)	173	160
16	τ CCCC(15), τ HCCN(62)	179	169
17	τ NCNC(16), τ CNNC(19), τ CCNN(10)	185	183
18	δ COC(32)	194	196
19	τ HCOC(45), τ COCC(14), τ OCCC(18), τ CCCC(13)	210	209
20	δ CNN(22), δ CCN(22)	219	216
21	ν CC(14), δ COC(12), δ CCN(10)	248	247
22	τ CCCC(22)	263	257
23	δ COC(34), τ HCOC(21), τ CCCC(23)	270	269
24	δ CCO(10), δ CCC(11), δ COC(30), τ HCOC(11), τ CCCC(30)	273	272
25	τ CNNC(26), τ CCCC(17)	281	285
26	δ OCO(11), δ COC(16), δ CCN(23)	325	323
27	δ OCO(11), δ CCO(12), δ CNN(18), δ COC(13)	353	348
28	δ OCN(28), δ CCN(27), τ NCNN(17), τ NNCC(17), τ CNNC(20)	371	352
29	δ OCN(23), δ CCN(27), τ NCNN(17), τ NNCC(21), τ CCNN(37), τ CNNC(20)	372	363
30	δ OCN(23), δ CCN(27), τ NCNN(11), τ NNCC(10), τ CCNN(40)	375	364
31	δ OCC(13), δ CCN(12)	419	409
32	δ CCC(32), δ COC(10)	434	428
33	δ CCC(17), δ NNC(12)	454	446
34	τ CCCC(49)	464	447
35	τ HCCC(20), τ CCCC(42), τ CCOC(14), τ OCCC(10)	485	467
36	δ CCC(18)	495	488
37	δ CCC(16), δ COC(18), τ HCCC(13), τ CCCC(11), τ OCOC(15), τ OCCC(39)	557	550
38	δ CCC(16), δ COC(20), τ CCOC(34), τ CCCC(17), τ HCCC(12), τ OCOC(13), τ OCCC(21)	573	553
39	ν NN(10), ν CC(15), δ OCC(15), δ CNN(23), δ CCC(14)	581	570

40	ν NC(16), ν CC(29), δ OCC(34)	585	575
41	δ COC(19), δ CCC(28), δ CCO(14)	594	584
42	τ HCCN(14), τ ONNC(41)	614	595
43	ν CC(23), δ CCN(12), τ CCCC(17), τ CCOC(34)	634	608
44	ν CC(21), δ CCN(13), τ OCCC(23), τ CCCC(27)	637	626
45	δ OCN(12), δ NCC(13), δ CCC(14)	672	655
46	τ NCNC(19), τ ONNC(10), τ CNNC(12)	693	656
47	ν CC(14), δ CCC(28), τ ONNC(43), τ CCNN(13)	694	682
48	τ HCCC(31), τ CCCC(19)	727	702
49	τ HCCC(42), τ CCCC(30)	737	710
50	δ NCN(21)	749	730
51	τ ONNC(43), τ CCNN(13), τ HCCC(13), τ OCOC(55)	784	737
52	δ OCO(17), τ HCCC(12), τ OCOC(52)	790	743
53	ν OC(11), δ OCO(27)	801	770
54	δ NCC(11), δ NCN(12), τ ONNC(42), τ CCNN(15)	804	782
55	τ HCCC(34), τ CCCC(13)	862	810
56	τ HCCC(63), τ OCOC(10)	865	812
57	ν CC(11), ν OC(15), δ OCO(11), τ HCCC(54)	871	850
58	ν CC(13)	882	862
59	ν CC(23), ν OC(11), δ CCC(14), δ NCN(17), τ HCCN(14)	933	912
60	ν CC(21), δ NCN(13), τ HCCN(14), τ HCCC(46)	943	919
61	ν CC(10), ν OC(15), τ HCCC(54)	996	926
62	ν CC(14), ν OC(11), τ HCCC(33)	998	926
63	ν CC(28), δ CCC(10), τ HCCC(28)	1002	945
64	ν CC(13), δ CCC(22), τ HCCC(26)	1011	978
65	ν CC(32), ν OC(24), δ CCC(10), τ HCCC(34)	1017	985
66	ν NC(14), δ HCH(12), τ HCCN(31), τ HCCC(60), τ CCCC(14)	1040	995
67	ν NC(10), τ HCCC(51), τ HCNN(15)	1041	996
68	ν OC(55), ν NC(10), δ CCC(22), τ HCCC(51)	1050	996
69	ν NC(12), δ CCC(17), τ HCCN(14), τ HCCC(62)	1074	999
70	ν OC(34), δ CCC(22), τ HCCC(47)	1078	1012
71	ν NC(14), τ HCNN(82), τ HCCN(11)	1087	1044
72	δ CNN(12), δ HCC(18), δ CCC(12), τ HCCN(15)	1090	1047
73	δ HCH(20), τ HCCN(54)	1094	1065
74	ν CC(18), ν OC(13), δ HCC(17), δ CCC(12)	1099	1068
75	ν CC(18), δ HCC(15), δ CNN(14), τ HCNN(21)	1100	1073
76	δ HCH(21), τ HCCN(55), τ HCNN(24)	1100	1075
77	ν CC(12), δ HCC(19), τ HCNN(48), τ HCCN(21)	1107	1086
78	ν CC(18), δ NCN(12), τ HCCN(19), δ HCC(21)	1121	1091
79	ν CC(31), ν NC(10), ν NN(10), δ HCH(24), τ HCOC(25), τ HCCN(13)	1148	1120
80	ν NC(10), ν NN(10), ν CC(31), δ HCH(24), δ OCC(11), τ HCOC(26)	1155	1121
81	ν OC(13), ν CC(31), δ HCC(13), δ HCH(24), τ HCOC(26)	1156	1137
82	ν CC(10), δ HCC(12), δ HCH(15), τ HCOC(27)	1166	1150
83	ν CC(10), ν OC(12), δ HCC(14)	1171	1172
84	ν NN(13), ν CC(18), ν OC(13), δ HCC(17), δ HCH(13), τ HCOC(25)	1184	1180
85	δ HCC(39)	1218	1188
86	ν CC(14), ν OC(10), δ HCC(41)	1219	1202
87	ν CC(19), ν OC(13), δ HCC(12)	1243	1240
88	ν NC(42), ν NN(15)	1258	1250
89	ν CC(18), ν OC(36), δ HCH(13), τ HCOC(25)	1279	1257
90	ν CC(27), ν OC(23), δ HCC(10)	1294	1280
91	ν CC(27), ν NC(33), δ HCC(26), δ CNN(15)	1323	1294
92	ν CC(15), δ HCC (41)	1334	1309
93	δ HCN(10), δ HCC(50)	1348	1321
94	ν NC(14), δ HCN(19), δ HCC(28)	1363	1333
95	δ HCN(38)	1417	1384
96	δ HCH(95)	1436	1407
97	ν CC16), δ HCC(11), δ HCH(98)	1445	1417

98	δ HCH(95), δ HCN(17), δ HCC(10)	1453	1419
99	ν CC(12), δ HCC(15)	1458	1431
100	δ HCH (72), τ HCCN(24)	1470	1453
101	δ HCC(10), δ HCH(72)	1483	1453
102	δ HCH(66), τ HCCN(25)	1488	1472
103	δ HCC(27), δ HCH(76), τ HCCN(24)	1497	1482
104	δ HCC(20), δ CCC(10), δ HCH(74), τ HCCN(26)	1504	1483
105	δ HCH(76), δ HCC(47), τ HCCN(23), δ CCC(10)	1508	1488
106	ν CC(19), δ HCC(24), δ HCH(74), τ HCCN(26)	1513	1493
107	δ HCH(76), τ HCOC(11)	1525	1503
108	δ HCH(74)	1534	1514
109	ν CC(26), ν NC(39), δ HCC(10), δ CCC(10)	1598	1537
110	ν CC(41), ν NC(13), δ HCH(14), δ HCC(17)	1600	1557
111	ν CC(24), δ HCC(20), δ CCC(10)	1613	1557
112	ν CC(34), δ HCC(16), δ CCC(10)	1623	1567
113	ν NC(43), ν CC(30), δ CCC(17)	1649	1572
114	ν CC(21), ν NC(45), δ HCC(11)	1671	1585
115	ν OC(83)	1726	1676
116	ν OC(85)	1744	1684
117	ν OC(46)	1777	1713
118	ν CH(91)	2907	2924
119	ν CH(92)	2933	2967
120	ν CH(96)	2946	2977
121	ν CH(94)	2957	2978
122	ν CH(100)	2985	3016
123	ν CH(100)	3003	3032
124	ν CH(46)	3016	3051
125	ν CH(92)	3018	3060
126	ν CH(96)	3029	3071
127	ν CH(51)	3062	3080
128	ν CH(52)	3064	3093
129	ν CH(36)	3083	3096
130	ν CH(67)	3091	3121
131	ν CH(66)	3092	3123
132	ν CH(29)	3097	3126
133	ν CH(56)	3108	3134
134	ν CH(48)	3119	3152
135	ν CH(26)	3138	3168



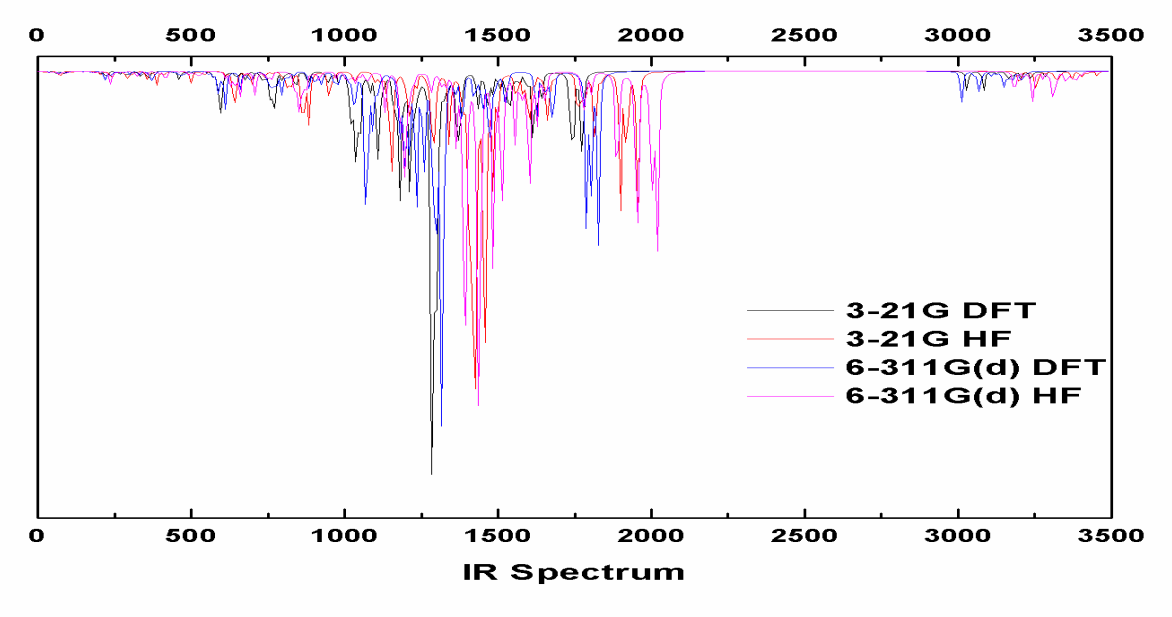
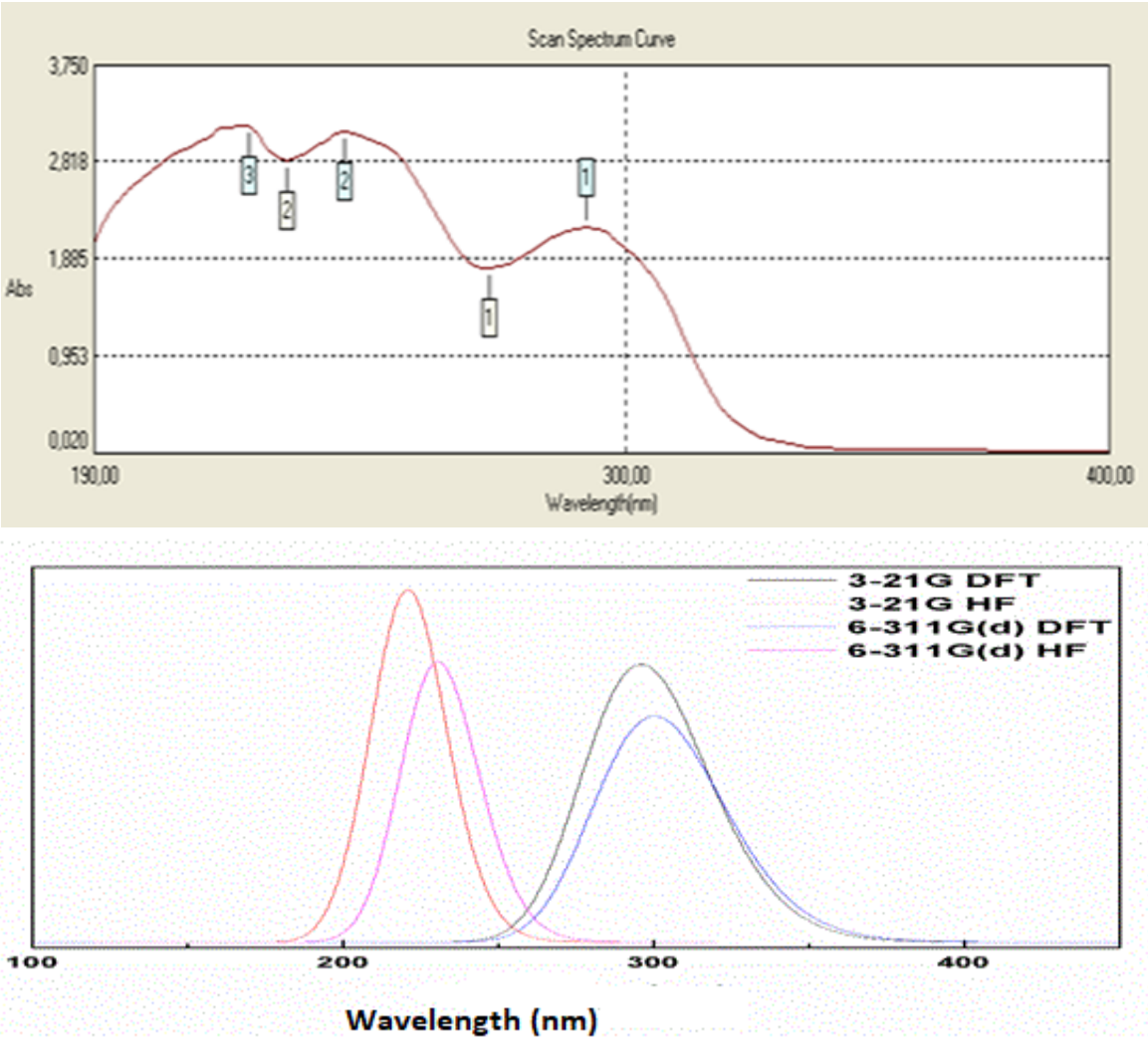


Figure 3. Experimental (a) and theoretical (6-311G(d)/3-21G DFT/HF) IR spectra of title compound



Experimental (nm)	**λ (nm) HF/B3LYP 6-311G(d)**	**λ (nm) HF/B3LYP 3-21G**	**Excitation Energy (eV) HF/B3LYP 6-311G(d)**	**Excitation Energy (eV) HF/B3LYP 3-21G**	***f* (osillatör strengths) HF/B3LYP 6-311G(d)**	***f* (osillatör strengths) HF/B3LYP 3-21G**
292.00	233.56/305.68	223.27/306.25	5.3086/4.0560	5.5532/4.0485	0.5635/0.0133	0.4944/0.0289
242.00	230.11/300.10	218.45/296.12	5.3881/4.1315	5.6756/4.1870	0.1160/0.6182	0.2256/0.4198
222.00	216.34/295.01	206.15/293.56	5.7311/4.2026	6.0143/4.2235	0.0905/0.0186	0.1064/0.1408

Figure 4. The experimental and calculated UV-vis spectrums (B3LYP/HF 6-311G(d), 3-21G) of title compound

Table 5. The calculated bond angles (^{0}) of title compound (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)

	Bond Angels	**HF 6-311G(d)**	**B3LYP 6-311G(d)**	**HF 3-21G**	**B3LYP 3-21G**
1	C(1)-N(40)-N(39)	105.770	105.508	104.543	103.744
2	C(1)-N(41)-N(42)	120.975	121.129	120.272	120.488
3	C(1)-N(41)-C(2)	108.151	108.209	109.246	109.227
4	C(1)-C(18)-H(33)	110.538	110.982	110.099	110.302
5	C(1)-C(18)-H(34)	108.517	108.681	108.875	108.805
6	C(1)-C(18)-H(35)	110.542	110.980	110.099	110.302
7	H(33)-C(18)-H(35)	107.879	107.292	108.036	107.700
8	H(34)-C(18)-H(33)	109.678	109.435	109.862	109.861
9	H(34)-C(18)-H(35)	109.678	109.446	109.862	109.862
10	N(40)-C(1)-N(41)	111.683	111.914	112.041	112.710
11	N(40)-N(39)-C(19)	119.251	119.033	118.857	118.595
12	N(39)-C(19)-O(47)	119.737	119.732	120.513	120.642
13	N(39)-C(19)-C(20)	116.694	115.798	115.264	114.021
14	O(47)-C(19)-C(20)	123.569	124.470	124.223	125.337
15	C(19)-C(20)-H(36)	111.197	111.480	110.990	110.991
16	C(19)-C(20)-H(37)	107.039	107.378	107.237	107.378
17	C(19)-C(20)-H(38)	111.216	111.485	110.990	110.995
18	H(36)-C(20)-H(37)	110.194	110.173	110.299	110.523
19	H(36)-C(20)-H(38)	107.029	106.204	107.056	110.526
20	H(37)-C(20)-H(38)	110.197	110.151	110.299	106.468
21	O(47)-C(19)-N(39)	119.737	119.732	124.223	120.642
22	C(19)-N(39)-C(2)	128.974	128.716	129.765	129.251
23	N(39)-C(2)-N(41)	102.622	102.118	102.792	102.165
24	N(39)-C(2)-O(43)	129.540	129.924	129.598	129.891
25	O(43)-C(2)-N(41)	127.838	127.957	127.611	127.944
26	C(2)-N(41)-N(42)	130.865	130.654	130.483	130.284
27	N(41)-C(1)-C(18)	123.094	123.131	122.180	122.098
28	N(40)-C(1)-C(18)	125.223	124.955	125.779	125.192
29	N(41)-N(42)-C(3)	120.423	119.566	119.242	117.363
30	N(42)-C(3)-H(21)	122.541	122.228	122.716	122.661
31	N(42)-C(3)-C(4)	120.346	120.205	120.114	119.751
32	H(21)-C(3)-C(4)	117.113	117.567	117.170	117.588
33	C(3)-C(4)-C(5)	117.977	117.869	119.062	117.901
34	C(3)-C(4)-C(9)	122.434	122.452	121.682	121.666
35	C(4)-C(5)-H(22)	120.849	120.256	120.988	121.126
36	C(4)-C(5)-C(6)	119.732	119.536	119.062	119.170
37	H(22)-C(5)-C(6)	119.418	120.203	119.949	119.704
38	C(5)-C(6)-O(44)	119.960	122.614	124.875	125.412
39	C(5)-C(6)-C(7)	121.092	120.949	120.767	120.573
40	O(44)-C(6)-C(7)	118.872	116.320	114.357	114.016
41	C(6)-C(7)-H(23)	119.636	119.179	118.702	118.525
42	C(6)-C(7)-C(8)	119.145	119.372	119.741	119.877

43	H(23)-C(7)-C(8)	121.219	121.449	121.557	121.597
44	C(7)-C(8)-H(24)	119.521	119.482	119.587	119.508
45	C(7)-C(8)-C(9)	120.530	120.512	120.328	120.341
46	H(24)-C(8)-C(9)	119.949	120.006	120.085	120.150
47	C(8)-C(9)-H(25)	120.549	120.832	121.108	121.532
48	C(8)-C(9)-C(4)	119.911	119.952	119.517	119.605
49	H(25)-C(9)-C(4)	119.540	119.216	119.374	118.864
50	C(9)-C(4)-C(5)	119.589	119.678	120.584	120.434
51	C(6)-O(44)-C(10)	119.544	120.971	128.197	125.440
52	O(44)-C(10)-O(45)	123.206	123.551	123.387	124.068
53	O(44)-C(10)-C(11)	111.970	111.140	111.477	110.193
54	O(45)-C(10)-C(11)	124.824	125.308	125.136	125.739
55	C(10)-C(11)-C(16)	122.163	122.627	122.037	122.553
56	C(10)-C(11)-C(12)	117.234	117.038	116.957	116.611
57	C(11)-C(12)-H(26)	120.477	120.192	120.635	120.160
58	C(11)-C(12)-C(13)	120.278	120.321	120.064	120.238
59	H(26)-C(12)-C(13)	119.245	119.486	119.301	119.602
60	C(12)-C(13)-O(46)	115.786	115.730	116.040	115.833
61	C(12)-C(13)-C(14)	119.418	119.515	119.348	119.181
52	C(13)-O(46)-C(17)	119.962	118.632	120.977	118.208
63	O(46)-C(13)-C(14)	124.796	124.755	124.612	124.986
64	O(46)-C(17)-H(30)	111.452	111.517	111.298	111.584
65	O(46)-C(17)-H(31)	106.183	105.741	105.458	104.862
66	O(46)-C(17)-H(32)	111.454	111.538	111.298	111.584
67	H(30)-C(17)-H(31)	109.109	109.251	109.624	109.692
68	H(30)-C(17)-H(32)	109.442	109.447	109.459	109.335
69	H(31)-C(17)-H(32)	109.106	109.249	109.624	109.692
70	H(26)-C(12)-C(13)	119.245	119.486	119.301	119.602
71	C(13)-C(14)-C(15)	119.798	119.685	119.348	120.142
72	C(13)-C(14)-H(27)	121.107	121.011	120.690	120.613
73	H(27)-C(14)-C(15)	119.096	119.303	119.171	119.246
74	C(14)-C(15)-C(16)	121.130	121.135	120.796	120.904
75	C(14)-C(15)-H(28)	119.030	119.065	119.260	119.183
76	H(28)-C(15)-C(16)	119.839	119.800	119.944	119.913
77	C(15)-C(16)-H(29)	120.745	120.821	121.386	121.644
78	C(15)-C(16)-C(11)	118.773	119.007	118.647	118.700
79	H(29)-C(16)-C(11)	120.482	120.172	119.967	119.657
80	C(16)-C(11)-C(12)	120.603	120.336	121.006	120.836

Table 6. The calculated bond lengths (A^0) of title compound (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)

	Bond Lengths	**HF 6-311G(d)**	**HF 3-21G**	**B3LYP 6-311G**	**B3LYP 3-21G**
1	C(1)-N(41)	1.3843	1.3809	1.3907	1.3932
2	C(1)-N(40)	1.2751	1.2614	1.2898	1.3077
3	C(1)-C(18)	1.4836	1.4873	1.4849	1.4857
4	C(18)-H(33)	1.0823	1.0826	1.0925	1.0947
5	C(18)-H(34)	1.0792	1.0796	1.0889	1.0909
6	C(18)-H(35)	1.0823	1.0827	1.0926	1.0947
7	N(41)-C(2)	1.3847	1.3775	1.4070	1.4163
8	C(2)-O(43)	1.2166	1.1924	1.2137	1.2372
9	N(39)-C(2)	1.3762	1.3734	1.3978	1.4032

10	N(39)-N(40)	1.4353	1.3806	1.3917	1.4506
11	N(39)-C(19)	1.4046	1.4122	1.4314	1.4265
12	C(19)-C(20)	1.5080	1.5061	1.5081	1.5149
13	C(19)-O(47)	1.2017	1.1775	1.2000	1.2234
14	C(20)-H(36)	1.0809	1.0813	1.0913	1.0934
15	C(20)-H(37)	1.0784	1.0792	1.0884	1.0901
16	C(20)-H(38)	1.0809	1.0813	1.0914	1.0934
17	N(41)-N(42)	1.4008	1.3642	1.3716	1.4143
18	N(42)-C(3)	1.2670	1.2574	1.2845	1.2969
19	C(3)-H(21)	1.0699	1.0737	1.0863	1.0846
20	C(3)-C(4)	1.4709	1.4763	1.4661	1.4648
21	C(4)-C(5)	1.3883	1.3854	1.4006	1.4033
22	C(4)-C(9)	1.3864	1.3937	1.4036	1.4035
23	C(5)-H(22)	1.0656	1.0746	1.0820	1.0778
24	C(5)-C(6)	1.3807	1.3815	1.3909	1.3949
25	C(6)-O(44)	1.3949	1.3782	1.3922	1.4087
26	C(6)-C(7)	1.3816	1.3746	1.3897	1.3975
27	C(7)-H(23)	1.0693	1.0741	1.0840	1.0817
28	C(7)-C(8)	1.3817	1.3895	1.3955	1.3949
29	C(8)-H(24)	1.0712	1.0746	1.0848	1.0833
30	C(8)-C(9)	1.3811	1.3777	1.3868	1.3917
31	C(9)-H(25)	1.0695	1.0726	1.0829	1.0819
32	O(44)-C(10)	1.3579	1.3782	1.3739	1.3955
33	C(10)-O(45)	1.2049	1.1781	1.2019	1.2276
34	C(10)-C(11)	1.4782	1.4916	1.4885	1.4800
35	C(11)-C(12)	1.3773	1.3802	1.3927	1.3925
36	C(11)-C(16)	1.3885	1.3934	1.4027	1.4029
37	C(12)-H(26)	1.0687	1.0722	1.0828	1.0812
38	C(12)-C(13)	1.3859	1.3903	1.3973	1.3986
39	C(13)-O(46)	1.3686	1.3452	1.3608	1.3822
40	C(13)-C(14)	1.3821	1.3851	1.3988	1.4000
41	C(14)-H(27)	1.0695	1.0726	1.0827	1.0815
42	C(14)-C(15)	1.3879	1.3902	1.3965	1.3990

43	C(15)-H(28)	1.0714	1.0749	1.0850	1.0836
44	C(15)-C(16)	1.3769	1.3770	1.3871	1.3901
45	C(16)-H(29)	1.0673	1.0713	1.0815	1.0793
46	O(46)-C(17)	1.4370	1.3979	1.4195	1.4604
47	C(17)-H(30)	1.0830	1.0849	1.0953	1.0967
48	C(17)-H(31)	1.0772	1.0784	1.0881	1.0900
49	C(17)-H(32)	1.0830	1.0849	1.0954	1.0967

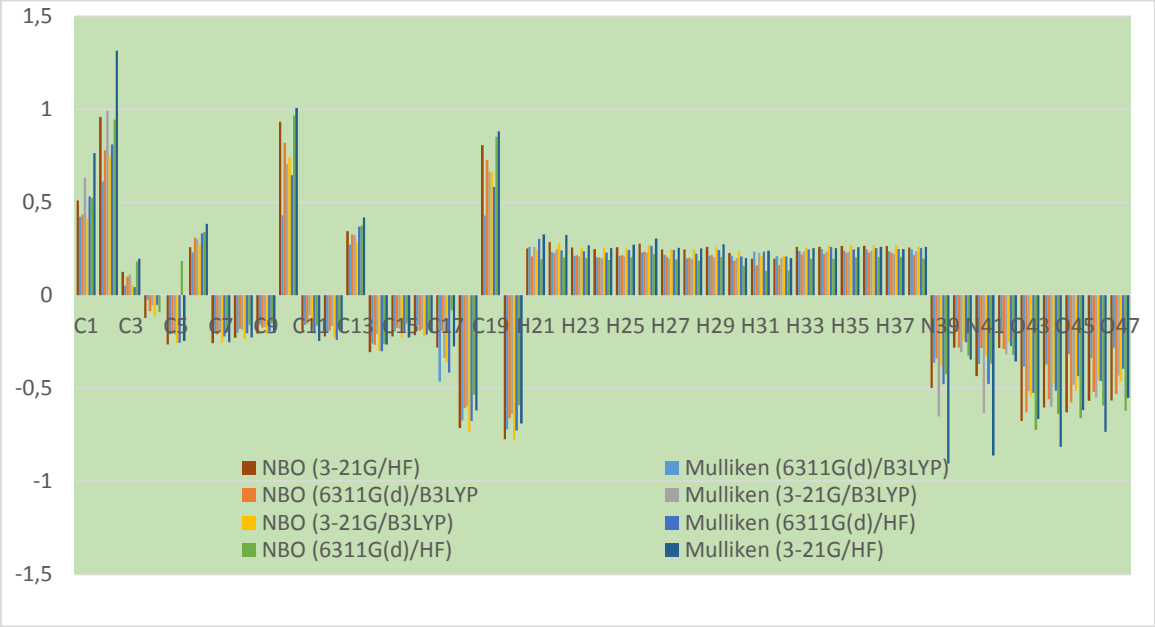
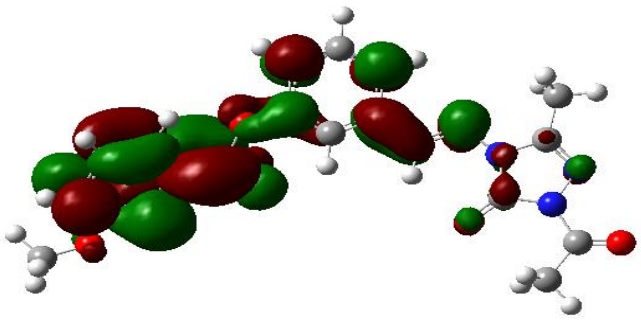
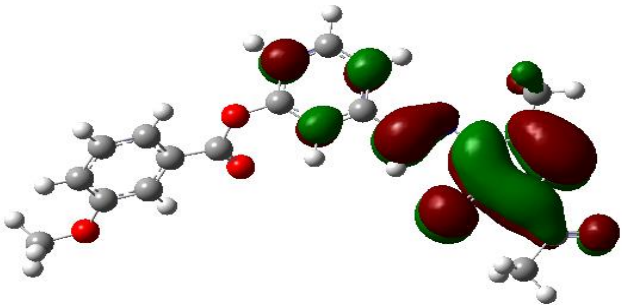


Figure 5. Graphics of the calculated Mulliken atomic charges and NBO values of title compound



E_{LUMO}

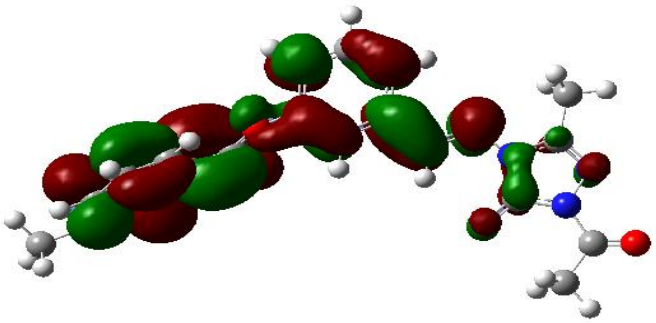


E_{HOMO}

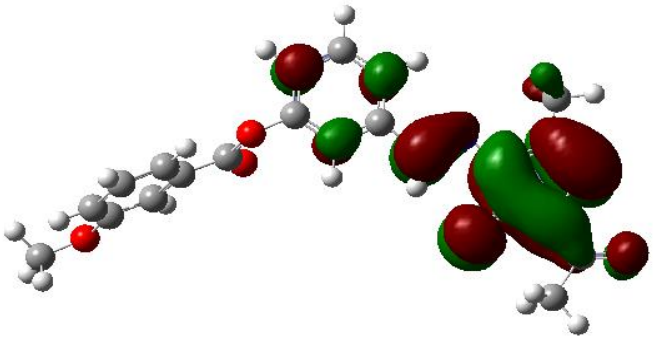
LUMO: -2,03318 eV

ΔE:4,48677 eV

HOMO: -6,51996 eV



E_{LUMO}



E_{HOMO}

LUMO: -1,89359 eV

ΔE:6,96967 eV

HOMO: -8,85627 eV

B3LYP (3-21G)

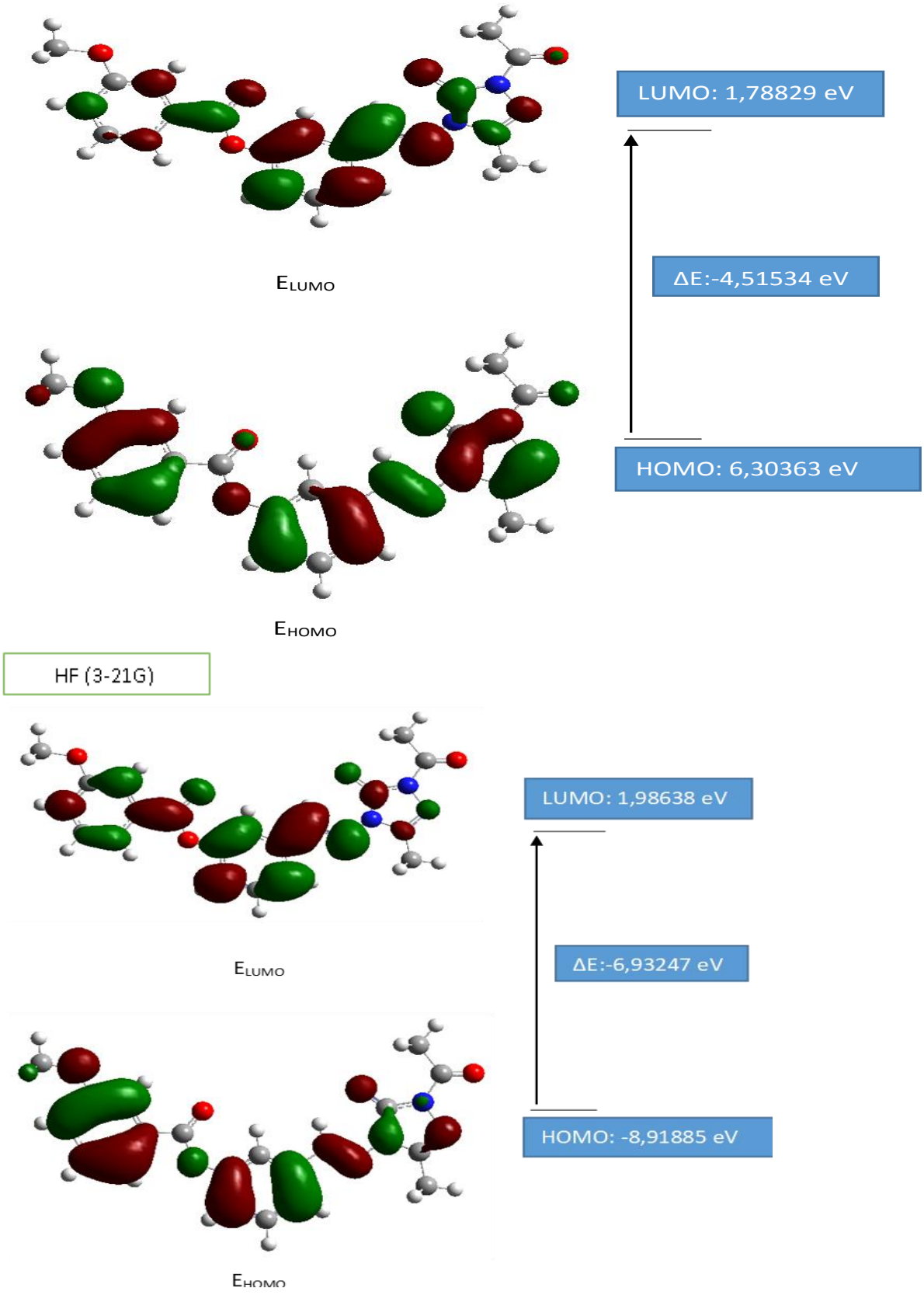


Figure 6. 3D plots of HOMO-LUMO energies of title compound at the HF/B3LYP 6-311G(d) and 3-21G levels

Table 7. The calculated electronic properties of title compound (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)

	B3LYP (6-311G(d))	**Hartree**	**Ev**	**Kcal/mol**	**Kj/mol**
	LUMO	-0,07472	-2,03318	-46,887	-196,177
	HOMO	-0,23961	-6,51996	-150,356	-629,096
A	**Electron Affinity**	0,07472	2,03318	46,887	196,177
I	**Ionization Potential**	0,23961	6,51996	150,356	629,096
ΔE	**Energy Gap**	0,16489	4,48677	103,469	432,919
χ	**Electronegativity**	0,157165	4,27657	98,6215	412,637
Pi	**Chemical Potential**	-0,157165	-4,27657	-98,6215	-412,637
ω	**Electrophilic Index**	0,00101823	0,02771	0,63894	2,67336
IP	**Nucleophilic Index**	-0,01295747	-0,35258	-8,13085	-34,0198
S	**Molecular Softness**	12,1293	330,047	7611,17	31845,5
η	**Molecular Hardness**	0,082445	2,24339	51,7345	216,459
	HF (6-311G(d))	**Hartree**	**Ev**	**Kcal/mol**	**Kj/mol**
	LUMO	-0,06959	-1,89359	-43,6679	-182,709
	HOMO	-0,32547	-8,85627	-204,233	-854,521
A	**Electron Affinity**	0,06959	1,89359	43,6679	182,709
I	**Ionization Potential**	0,32547	8,85627	204,233	854,521
ΔE	**Energy Gap**	0,25588	6,96267	160,565	671,813
χ	**Electronegativity**	0,19753	5,37493	123,951	518,615
Pi	**Chemical Potential**	-0,19753	-5,37493	-123,951	-518,615
ω	**Electrophilic Index**	0,002495988	0,06792	1,56624	6,55322
IP	**Nucleophilic Index**	-0,02527199	-0,68767	-15,8582	-66,3516
S	**Molecular Softness**	7,8162	212,683	4904,67	20521,3
η	**Molecular Hardness**	0,12794	3,48134	80,2827	335,906

	B3LYP (3-21G)	**Hartree**	**Ev**	**Kcal/mol**	**Kj/mol**
	LUMO	0,06572	1,78829	41,2395	172,548
	HOMO	0,23166	6,30363	145,367	608,223
A	**Electron Affinity**	-0,06572	-1,78829	-41,2395	-172,548
I	**Ionization Potential**	-0,23166	-6,30363	-145,367	-608,223
ΔE	**Energy Gap**	-0,16594	-4,51534	-104,128	-435,675
χ	**Electronegativity**	-0,14869	-4,04596	-93,3034	-390,386
Pi	**Chemical Potential**	0,14869	4,04596	93,3034	390,386
ω	**Electrophilic İndex**	-0,00091718	-0,02496	-0,57553	-2,40806
IP	**Nucleophilic İndex**	-0,01233681	-0,33569	-7,74138	-32,3903
S	**Molecular Softness**	-12,0525	-327,958	-7563,01	-31644
η	**Molecular Hardness**	-0,08297	-2,25767	-52,0639	-217,838
	HF (3-21G)	**Hartree**	**Ev**	**Kcal/mol**	**Kj/mol**
	LUMO	0,073	1,98638	45,8077	191,662
	HOMO	0,32777	8,91885	205,677	860,56
A	**Electron Affinity**	-0,073	-1,98638	-45,8077	-191,662
I	**Ionization Potential**	-0,32777	-8,91885	-205,677	-860,56

ΔE	**Energy Gap**	-0,25477	-6,93247	-159,869	-668,899
χ	**Electronegativity**	-0,200385	-5,45262	-125,742	-526,111
Pi	**Chemical Potential**	0,200385	5,45262	125,742	526,111
ω	**Electrophilic İndex**	-0,00255752	-0,06959	-1,60485	-6,71476
IP	**Nucleophilic İndex**	-0,02552604	-0,69458	-16,0177	-67,0186
S	**Molecular Softness**	-7,8502	-213,61	-4926,04	-20610,7
η	**Molecular Hardness**	-0,127385	-3,46624	-79,9345	-334,449

Table 8. The mean polizability (<α>), the anisotropy of the polarizability (Δα), the mean first-order hyperpolarizability (<β>) values of title compound

	B3LYP (6-311G(d))	**B3LYP(3-21G)**	**HF(6-311G(d))**	**HF(3-21G)**
μ_x	5.990 Debye	5.1631 Debye	7.0546 Debye	6.3365 Debye
μ_y	-4.973 Debye	-4.2226 Debye	-6.5512 Debye	-6.0344 Debye
μ_z	-1.143 Debye	-1.0421 Debye	-1.4866 Debye	-1.5253 Debye
μ_{Toplam}	7.869 Debye	6.7508 Debye	9.7414 Debye	8.8821 Debye
α_{xx}	62,93 a.u.	62,00 a.u.	51,04 a.u.	49,55 a.u.
α_{yy}	42,44 a.u.	25,78 a.u.	34,08 a.u.	36,49 a.u.
α_{zz}	21,95 a.u.	15,69 a.u.	24,02 a.u.	11,60 a.u.
α	42,440x10^{-24} esu	42,176x10^{-24} esu	36,389x10^{-24} esu	33,394x10^{-24} esu
Δα	35,489x10^{-24} esu	34,491x10^{-24} esu	23,648x10^{-24} esu	32,547x10^{-24} esu
βx	667 a.u.	20608 a.u.	739 a.u.	-2094 a.u.
βy	2036 a.u.	-2544 a.u.	1181 a.u.	-794 a.u.
βz	-170 a.u.	1310 a.u.	369 a.u.	-0,0948 a.u.
βxxx	48,83 a.u.	-2361,57 a.u.	31,97 a.u.	-249,90 a.u.
βxxy	243,85 a.u.	-125,85 a.u.	130,25 a.u.	-52,66 a.u.
βxyy	67,75 a.u.	-9,83 a.u.	90,77 a.u.	-81,40 a.u.
βyyy	-40,59 a.u.	-137,91 a.u.	-26,40 a.u	-14,45 a.u.
βxxz	-145,33 a.u.	76,32 a.u.	-43,56 a.u.	0,000193 a.u.
βxyz	-44,33 a.u.	-13,01 a.u.	-34,44 a.u.	-0,00221 a.u.
βyyz	71,44 a.u.	17,38 a.u.	38,91 a.u.	-0,00985 a.u.
βxzz	-36,87 a.u.	-90,96 a.u.	-21,68 a.u.	81,02 a.u.
βyzz	40,03 a.u.	-40,21 a.u.	37,25 a.u.	-27,86 a.u.
βzzz	53,50 a.u.	62,80 a.u.	48,73 a.u.	-0,00166 a.u.
β	2,149x10^{-30} esu	20,806x10^{-30} esu	1,441x10^{-30} esu	2,241x10^{-30} esu

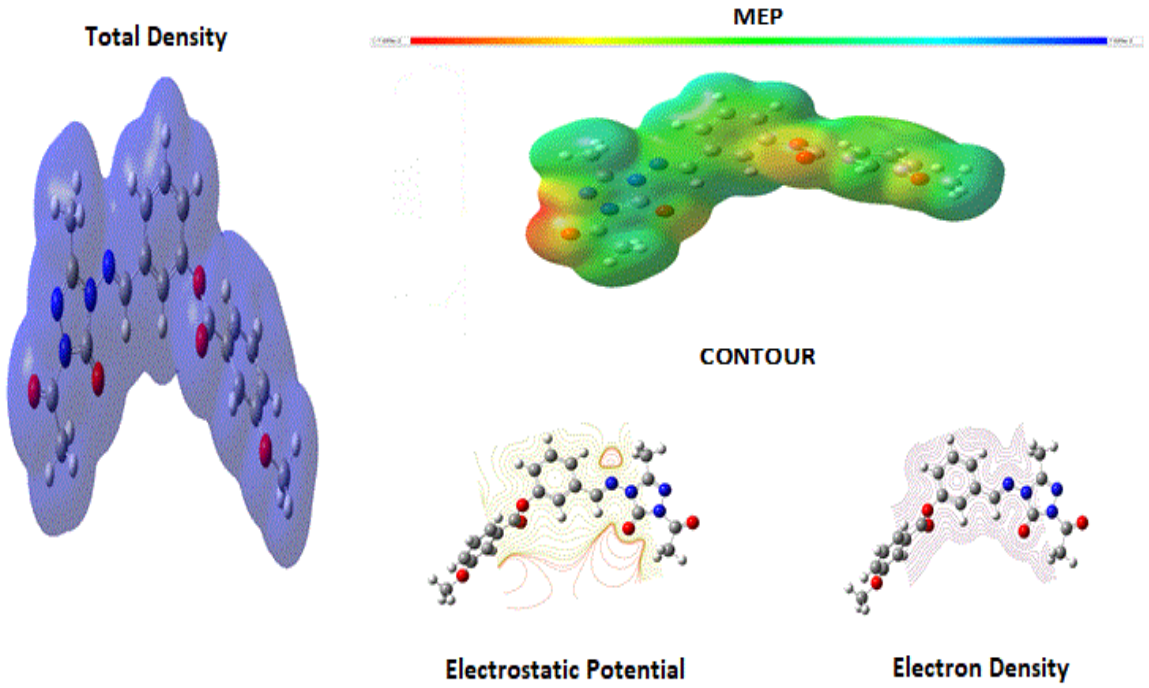


Figure 7. The calculated molecular surfaces of title compound

Table 9. The calculated dipole moment values of title compound (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)

Dipole Moment	HF 6-311G(d)	HF 3-21G	B3LYP 6-311G(d)	B3LYP 3-21G
μ_x	7.0546	6.3365	5.9903	5.1631
μ_y	-6.5512	-6.0344	-4.9729	-4.2226
μ_z	-1.4866	-1.5253	-1.1429	-1.0421
μ_{Toplam}	9.7414	8.8821	7.8689	6.7508

Conclusion

In this paper, the spectroscopic, geometric and electronic parameters of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy)benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one have been calculated by using DFT (B3LYP) and HF methods with the 6-311G(d) and 3-21G basis sets and compared with the experimental parameters. The IR, ^{1}H- and ^{13}C- NMR spectra have been recorded and analyzed. The theoretically computed spectra were found good agreement with experimental IR, UV-vis, ^{1}H- and ^{13}C- NMR spectra. The Mulliken atomic charges, NBO, HOMO and LUMO energy of 1-acetyl-3-methyl-4-[3-(3-methoxybenzoxy) benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one in the ground state have been calculated by using DFT/6-311G(d) and DFT/3-21G, HF/6-311G(d) and HF/3-21G levels. The value of the energy gap between the HOMO-LUMO energies were determined. Geometric parameters; bond angels and bond lengths were compared with experimental values obtained from literature. All results showed that the calculated spectroscopic, geometric and electronic parameters obtained by B3LYP/6-311G(d) method had a better agreement with the experimental values than 3-21G and HF method.

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