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Experimental and theoretical values of novel 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule

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ABSTRACT

In this study, theoretical spectral values of 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule were calculated and these theoretical values were compared with experimental values. This purpose, the geometry of compound has been optimized using the B3LYP/631G(d,p) and HF/631G(d,p) basis sets (Fig. **1**) and ^{1}H-NMR and ^{13}C-NMR isotropic shift values, IR absorption frequencies, UV-vis values in ethanol, bond angles, bond lengths, the HOMO-LUMO energy and mulliken charges of the compound were calculated by using the program package Gaussian G09W.

Keywords : Mannich Bases, B3LYP/631G(d,p), HF/631G(d,p), HOMO-LUMO energy, Gaussian 09W.

1. INTRODUCTION

Mannich bases have applications the field medicinal chemistry, the product synthetic polymers, the petroleum industry, as products used in water treatment, cosmeticts, the dyes industry, etc [1]. In addition, Mannich bases have biological activity such as anticanser [2, 3], antibacterial [4-6], antimycobacterial [7-9], anti-inflammatory [10-12], analgesic [13, 14], antifungal [15, 16], antitumor [17, 18], antiviral [19-21], antidepressant [22, 23], antiulcer [24, 25], anticonvulsant [26, 27], antimalaria [28-30], antioxidant activities [31, 32].

On the other hand, quantum chemical calculation methods have widely been used to theoretically predict the structural, spectroscopic, thermodynamic and electronic properties of molecular systems. The quantum chemical calculation methods provide support for experimental structural and spectroscopic studies [33-38].

Finally, the compound was optimized by using the B3LYP/631G (d,p) and HF/631G (d,p) basis sets [39, 40]. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W [39]. Experimental [41] and theoretical values were inserted into the graphic according to equitation of δ exp $_{=}$ a+b. δ calc. The standard error values were found via Sigma Plot program with regression coefficient of a and b constants. IR absorption frequencies of analyzed molecule were calculated by B3LYP/HF631G (d,p) methods. The veda4f program was used in defining

IR data, which were calculated theoretically [42]. The experimental [41] and the obtained theoretical values were compared and found by regression analyses that are accurate. Experimentally [41] and theoretically UV-vis values in ethanol were calculated and compared. Additionally, this compound was found bond angles, bond lengths, the HOMO-LUMO energy and mulliken charges by using two basis sets.

2. THEORETICAL CALCULATIONS

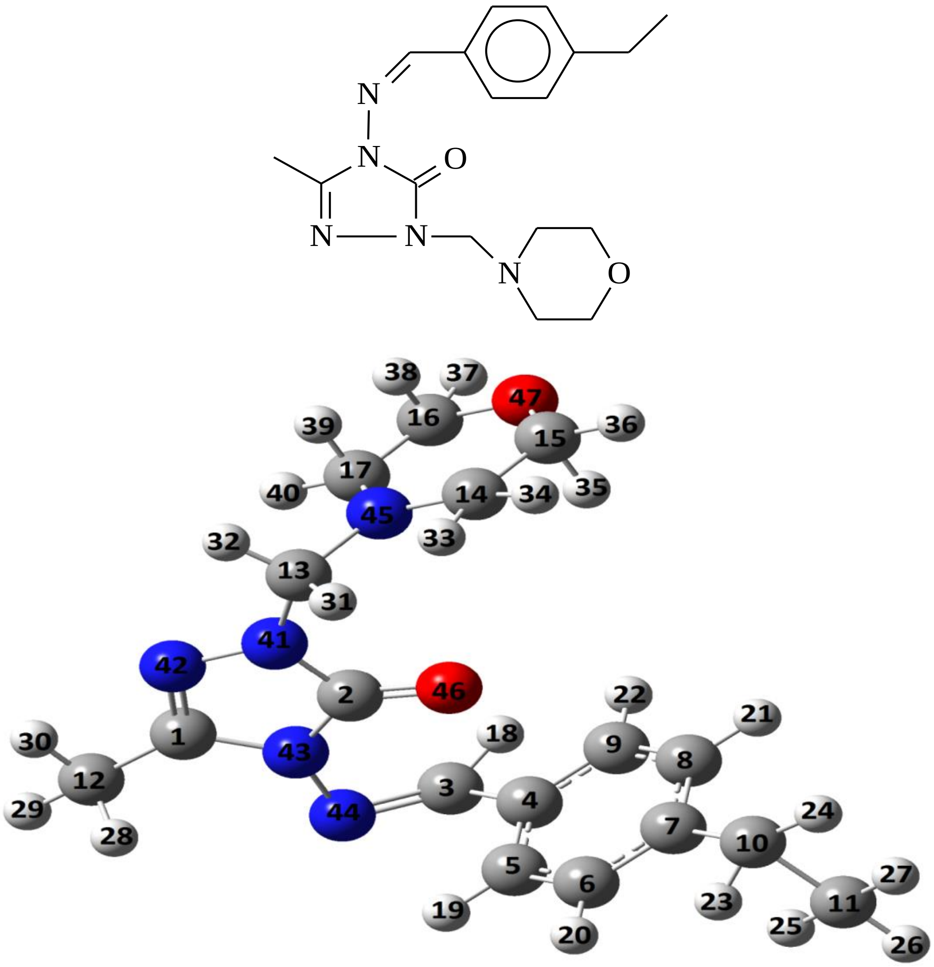


Figure 1. Gausview structure of the molecule 1-(Morpholine-4-yl-methyl)-3-methyl-4-(4-ethylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one.

Molecule was optimized by using the B3LYP/631G (d,p) and HF/631G (d,p) basis sets [39, 40]. Starting from this optimized structure with ^{1}H-NMR and ^{13}C-NMR spectral data (Table **1**) and IR spectral values according to GIAO [40] method was calculated using the method of Gaussian G09W program package in gas phase. Theoretically and experimentally values were plotted according to exp =a +b. δ calc Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program (Table **2**). The correlation graphs for chemical shifts drawn with ^{1}H-NMR, ^{13}C-NMR and ^{1}H-NMR(DMSO), ^{13}C-NMR(DMSO) spectral data of the molecule (Fig. **2**) Theoretically calculated IR data are multiplied with appropriate adjustment factors and the data obtained according to HF and DFT method are formed using theoretical infrared spectrum (Fig. **3**). The identification of calculated IR data was used in veda4f program [42] (Table **3**). Experimentally and theoretically UV-vis values in ethanol were calculated and compared (Fig. **4**).The experimental absorption wavelength (λ), excitation energies of the molecule (Table **4**). Additionally, bond angles (Table **5**), bond lengths (Table **6**), the HOMO-LUMO energy (Fig. **5**) and mulliken charges (Table **7**) of this compound was found by using two basis sets.

Table 1. The calculated and experimental ^{13}C and ^{1}H-NMR (B3LYP/ HF 6-31G(d,p) NMR/NMR DMSO) isotropic chemical shifts of the molecule (δ/ppm)

No	Experimental	DFT	Difference	DFT/ DMSO	Differ./ DMSO	HF	Difference	HF/ DMSO	Differ./ DMSO
C1	147,80	146,58	1,22	148,34	-0,54	141,65	6,15	143,97	3,83
C2	154,39	153,77	0,62	154,23	0,16	147,49	6,90	147,81	6,58
C3	150,29	154,53	-4,24	155,25	-4,96	149,09	1,20	149,90	0,39
C4	130,80	136,80	-6,00	135,83	-5,03	126,24	4,56	125,32	5,48
C5	127,83	127,89	-0,06	127,38	0,45	123,36	4,47	122,79	5,04
C6	128,38	131,97	-3,59	132,41	-4,03	123,50	4,88	123,69	4,69
C7	143,06	151,10	-8,04	152,99	-9,93	144,66	-1,60	146,14	-3,08
C8	128,38	131,57	-3,19	132,11	-3,73	122,86	5,52	123,20	5,18
C9	127,83	136,21	-8,38	136,51	-8,68	130,27	-2,44	130,65	-2,82
C10	28,15	41,32	-13,17	40,99	-12,84	25,34	2,81	24,97	3,18
C11	15,19	27,93	-12,74	27,64	-12,45	15,82	-0,63	15,53	-0,34
C12	10,94	21,02	-10,08	20,82	-9,88	10,47	0,47	10,36	0,58
C13	65,89	72,19	-6,30	72,09	-6,20	55,83	10,06	54,33	11,56
C14	49,96	52,04	-2,08	51,76	-1,80	37,99	11,97	38,55	11,41
C15	66,03	73,84	-7,81	73,63	-7,60	53,12	12,91	49,39	16,64
C16	66,03	68,06	-2,03	67,64	-1,61	53,64	12,39	55,06	10,97
C17	49,96	55,75	-5,79	55,56	-5,60	37,32	12,64	35,85	14,11
H18	9,66	11,04	-1,38	10,98	-1,32	10,26	-0,60	10,22	-0,56
H19	7,75	9,12	-1,37	9,15	-1,40	8,90	-1,15	8,94	-1,19
H20	7,35	8,17	-0,82	8,36	-1,01	7,82	-0,47	8,03	-0,68
H21	7,35	8,13	-0,78	8,32	-0,97	7,77	-0,42	7,97	-0,62
H22	7,75	8,14	-0,39	8,27	-0,52	7,98	-0,23	8,16	-0,41
H23	2,66	3,37	-0,71	3,47	-0,81	2,73	-0,07	2,83	-0,17
H24	2,66	3,45	-0,79	3,55	-0,89	2,69	-0,03	2,79	-0,13
H25	1,21	1,95	-0,74	1,96	-0,75	1,41	-0,20	1,40	-0,19
H26	1,21	2,17	-0,96	2,24	-1,03	1,56	-0,35	1,63	-0,42
H27	1,21	1,95	-0,74	1,93	-0,72	1,38	-0,17	1,36	-0,15
H28	2,30	3,15	-0,85	3,27	-0,97	2,67	-0,37	2,78	-0,48
H29	2,30	3,17	-0,87	3,27	-0,97	2,64	-0,34	2,77	-0,47
H30	2,30	2,82	-0,52	2,91	-0,61	2,43	-0,13	2,47	-0,17
H31	4,53	5,72	-1,19	5,72	-1,19	4,77	-0,24	4,28	0,25
H32	4,53	5,04	-0,51	5,13	-0,60	4,05	0,48	4,71	-0,18
H33	2,59	3,85	-1,26	3,47	-0,88	3,19	-0,60	2,45	0,14
H34	2,59	3,51	-0,92	3,97	-1,38	3,39	-0,80	3,14	-0,55
H35	3,56	4,87	-1,31	4,66	-1,10	3,58	-0,02	3,46	0,10
H36	3,56	4,55	-0,99	4,85	-1,29	3,47	0,09	3,70	-0,14
H37	3,56	4,36	-0,80	4,47	-0,91	3,94	-0,38	3,69	-0,13
H38	3,56	4,33	-0,77	4,44	-0,88	3,74	-0,18	3,99	-0,43
H39	2,59	3,97	-1,38	3,99	-1,40	2,48	0,11	3,00	-0,41
H40	2,59	3,93	-1,34	3,98	-1,39	3,48	-0,89	2,65	-0,06

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

B3LYP/631G(d,p): ^{13}C: 0.9951, ^{1}H: 0.9854; HF/631G(d,p): ^{13}C: 0.9908, ^{1}H: 0.9819, B3LYP/631G(d,p) (DMSO): ^{13}C: 0.9947, ^{1}H: 0.9881; HF/631G(d,p) (DMSO): ^{13}C: 0.9889, ^{1}H: 0.9889. 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 formule exp =a +b. δ calc Eq. These values for compound were shown in the table **2**. Theoretical and experimental carbon and proton chemical shifts ratios between acording to a, b ve R^2 values, lineer a correlation were observed.

Table 2. The correlation data for chemical shifts of the molecule.

	^{13}C				^{1}H			
	R^2	**S. error**	**a**	**b**	**R^2**	**S. error**	**a**	**b**
DFT	0.9951	3.6862	1.0504	-10.3802	0.9854	0.2963	0.9711	-0.7910
HF	0.9908	5.0605	0.9703	8.0371	0.9819	0.3309	0.9422	-0.0605
	^{13}C (DMSO)				**^{1}H(DMSO)**			
	R^2	**S. error**	**a**	**b**	**R^2**	**S. error**	**a**	**b**
DFT	0.9947	3.8180	1.0408	-9.5923	0.9881	0.2676	0.9703	-0.8548
HF	0.9889	5.5405	0.9586	9.1363	0.9889	0.2587	0.9279	-0.0044

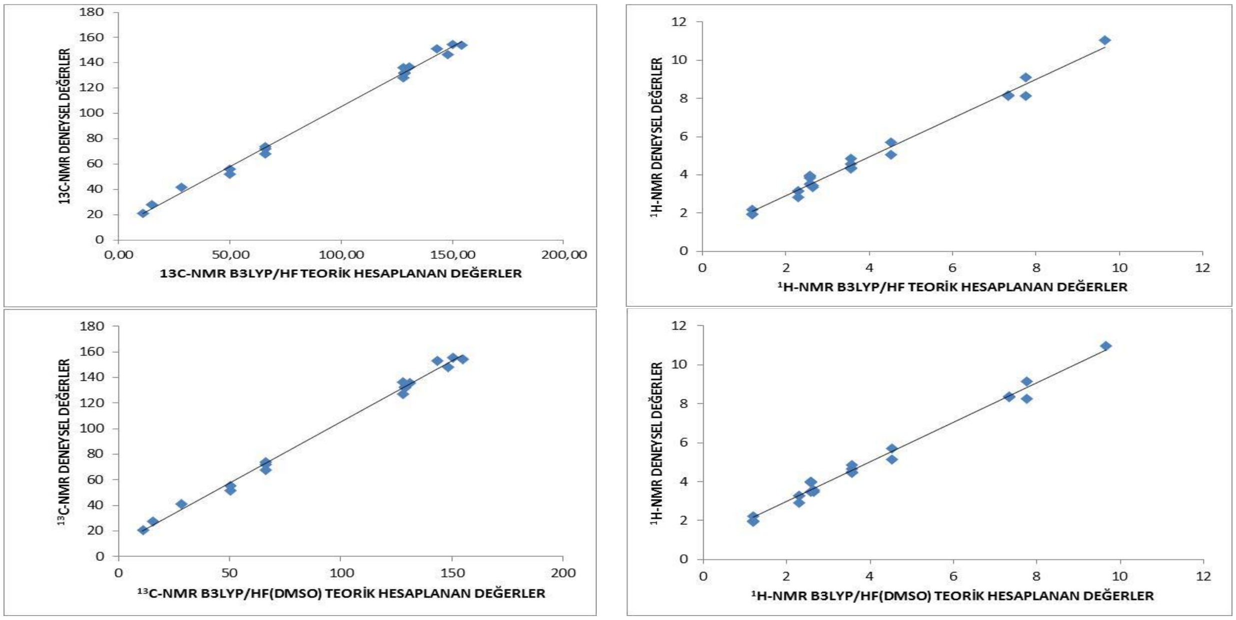


Figure 2. The correlation graphs for chemical shifts of the molecule.

2.2. The vibration frequency of the compound

Theoretically IR values were calculation veda 4f programme and scala values were obtain. The negative frequency in the data was not found. This result, structure of compound were shown stable. 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. Experimentally carbonyl peak (C=O) in 1690 cm^{-1} and theoretically (C=O) peak in 1721 cm^{-1} were observed.

Table 3. The calculated frequencies values of the molecule.

	Vibration Types	B3LYP	HF
1	τ NCNN(33), τ CNCN(14), τ CCNN(12)	19	13
2	τ NCCC(22), τ CNCN(20), τ CCCC(10)	24	16
3	τ CNCN(33), τ CCCC(11), τ CCNN(25)	33	28
4	τ CNNC(10), τ CCCC(16), τ CCNN(10)	38	33
5	τ NCCC(22)	42	37
6	τ CNCN(20), τ CCCC(14)	46	50
7	δ NCC(15), δ CCC(10), τ CCNC(11)	65	59
8	τ CNCN(15), τ CCNC(15)	79	77
9	τ NCNN(11), τ CNCN(11), τ CCNN(15)	94	96
10	δ CCC(11), τ CCCC(15), τ NNCN(11)	130	130
11	τ HCCN(35), τ COCC(10), τ CNNC(14)	145	140
12	τ HCCN(21)	155	156
13	τ COCC(17)	158	168
14	τ NCCC(11), τ CNNC(29), τ NNCN(10)	175	171
15	δ CCN(23)	196	196
16	δ CNN(16)	201	212
17	δ CCN(11), τ HCCC(19)	222	221
18	δ CNN(15)	233	231
19	τ CCCC(10)	242	246
20	δ COC(10), τ HCNC(13), τ HCOC(13), τ COCC(25)	269	284
21	δ CCC(11), τ NCNN(14), τ CCCC(14), τ NNCN(15)	300	305
22	δ CCN(13), δ CNC(10)	316	324
23	δ HCC(27), δ CCC(13), τ CNNC(13)	330	337
24	δ CCC(27)	347	350
25	δ CNC(17)	371	373
26	δ CNC(34)	387	402
27	τ HCCC(22), τ CCCC(55)	398	407
28	τ CCCC(14)	421	426
29	δ NNC(12), δ CCC(21)	430	432
30	δ COC(18)	478	460
31	δ COC(17), δ CCN(11)	511	498
32	δ COC(14)	520	524
33	δ CCC(13), τ CCCC(13), τ CCCC(13)	555	562
34	ν CC(31), δ NNC(12)	598	578
35	δ OCN(10)	608	603
36	τ NNCN(19)	621	624
37	δ CCC(29)	629	637
38	δ CNN(12)	638	644
39	τ ONNC(39)	677	688
40	δ CNN(13),τ ONNC(11)	697	727
41	τ HCCC(15), τ CCCC(32)	719	740
42	ν CC(16)	736	747
43	ν NC(39)	762	760
44	τ HCCC(45)	765	764
45	ν NC(13), ν NN(16), δ NCN(10), δ CNN(11)	783	794
46	τ HCCC(62)	818	846
47	ν OC(26), δ CNC(12),τ HCNC(11)	824	847
48	τ HCCC(81)	827	848
49	ν CC(17)	845	854
50	ν OC(27), τ HCNC(16)	854	858
51	ν CC(11), δ CCN(17)	878	873
52	ν NN(14), ν CC(10), δ NNC(12)	918	932

	Vibration Types	B3LYP	HF
53	**τ HCCC(40),τ CCCC(15)**	930	933
54	**ν CC(65), τ HCCC(17)**	938	975
55	**τ HCCC(42), τ CCCC(13)**	946	976
56	**τ HCCN(19)**	956	995
57	**ν NC(15), ν OC(16), τ HCNC(12)**	964	998
58	**τ HCNN(85)**	982	1002
59	**ν OC(16), ν CC(35)**	985	1025
60	**δ CCC(56)**	997	1028
61	**δ HCH(10), τ HCCN(27)**	998	1035
62	**δ HCH(14), τ HCCN(50)**	1029	1036
63	**τ HCCC(23), τ CCCC(12)**	1033	1051
64	**ν CC(17), CCC(11), τ HCCC(32)**	1043	1059
65	**ν NC(22), δ CNN(11),δ NNC(13)**	1052	1077
66	**τ HCNC(18)**	1058	1087
67	**ν NC(15), δ HCO(10)**	1095	1093
68	**ν NC(12), ν OC(12), δ HCC(17)**	1103	1101
69	**ν OC(11), δ HCC(38)**	1104	1135
70	**ν OC(50)**	1110	1163
71	**ν CC(13), δ HCC(70)**	1159	1166
72	**δ HCN(10), δ CNC(10), τ HCNC(14)**	1170	1169
73	**ν CC(33), δ HCC(13)**	1184	1177
74	**ν CC(12), ν NN(10), δ HCC(13), δ NCN(11)**	1188	1184
75	**ν NC(11), δ HCC(13), δ HCO(16)**	1208	1209
76	**δ HCC(11), δ HCO(29)**	1213	1223
77	**δ HCC(31), δ HCO(19)**	1226	1244
78	**δ HCC(49), τ HCCC(12)**	1228	1254
79	**ν CC(10), ν NN(13), δ NCN(13)**	1242	1258
80	**ν NN(10), δ HCO(28), τ HCNC(10)**	1262	1271
81	**ν NC(11), δ HCN(16), δ HCO(18)**	1279	1299
82	**ν NC(14), δ HCN(15)**	1290	1309
83	**δ HCC(61)**	1291	1314
84	**δ HCC(23), τ HCCC(36)**	1308	1336
85	**ν CC(11), δ HCC(12), τ HCCC(17)**	1314	1336
86	**τ HCNC(32)**	1320	1348
87	**δ HCN(31)**	1339	1362
88	**δ HCN(16), τ HCNC(20)**	1343	1378
89	**τ HCNC(18)**	1362	1390
90	**δ HCH(75)**	1368	1394
91	**δ HCN(14), τ HCNC(17)**	1369	1397
92	**δ HCN(17), δ HCH(53)**	1375	1399
93	**τ HCNC(24)**	1378	1405
94	**δ HCH(10), τ HCNC(24),τ HCOC(10)**	1379	1415
95	**ν CC(21), δ HCC(26)**	1402	1422
96	**δ HCN(14)**	1409	1433
97	**δ HCH(29)**	1414	1440
98	**δ HCH(39), τ HCCN(14)**	1427	1450
99	**δ HCH(29)**	1443	1456
100	**δ HCH(63), τ HCCC(16)**	1445	1460
101	**δ HCH(39), τ HCCC(16)**	1452	1462
102	**δ HCH(47)**	1456	1473
103	**δ HCH(68)**	1463	1481
104	**δ HCH(32), τ HCCC(19)**	1465	1483
105	**δ HCH(36), τ HCNC(12)**	1468	1490
106	**δ HCH(77)**	1479	1499

	Vibration Types	B3LYP	HF
107	**δ HCC(50), δ CCC(13)**	1498	1519
108	**ν CC(30), δ HCC(11), δ CCC(12)**	1552	1586
109	**ν NC(55)**	1589	1636
110	**ν NC(27), ν CC(32), δ HCC(11)**	1597	1679
111	**ν NC(33), ν CC(23)**	1615	1711
112	**ν OC(75), ν NC(11)**	1721	1742
113	**ν CH(30)**	2838	2843
114	**ν CH(62)**	2868	2855
115	**ν CH(73)**	2876	2859
116	**ν CH(53)**	2883	2862
117	**ν CH(73)**	2926	2863
118	**ν CH(50)**	2929	2872
119	**ν CH(39)**	2934	2888
120	**ν CH(72)**	2944	2893
121	**ν CH(16)**	2960	2902
122	**ν CH(77)**	2963	2919
123	**ν CH(31)**	2968	2921
124	**ν CH(53)**	2986	2925
125	**ν CH(47)**	2988	2932
126	**ν CH(63)**	3000	2937
127	**ν CH(51)**	3002	2949
128	**ν CH(76)**	3003	2979
129	**ν CH(14)**	3017	2980
130	**ν CH(58)**	3043	3000
131	**ν CH(47)**	3049	3003
132	**ν CH(45)**	3052	3017
133	**ν CH(95)**	3053	3035
134	**ν CH(51)**	3069	3043

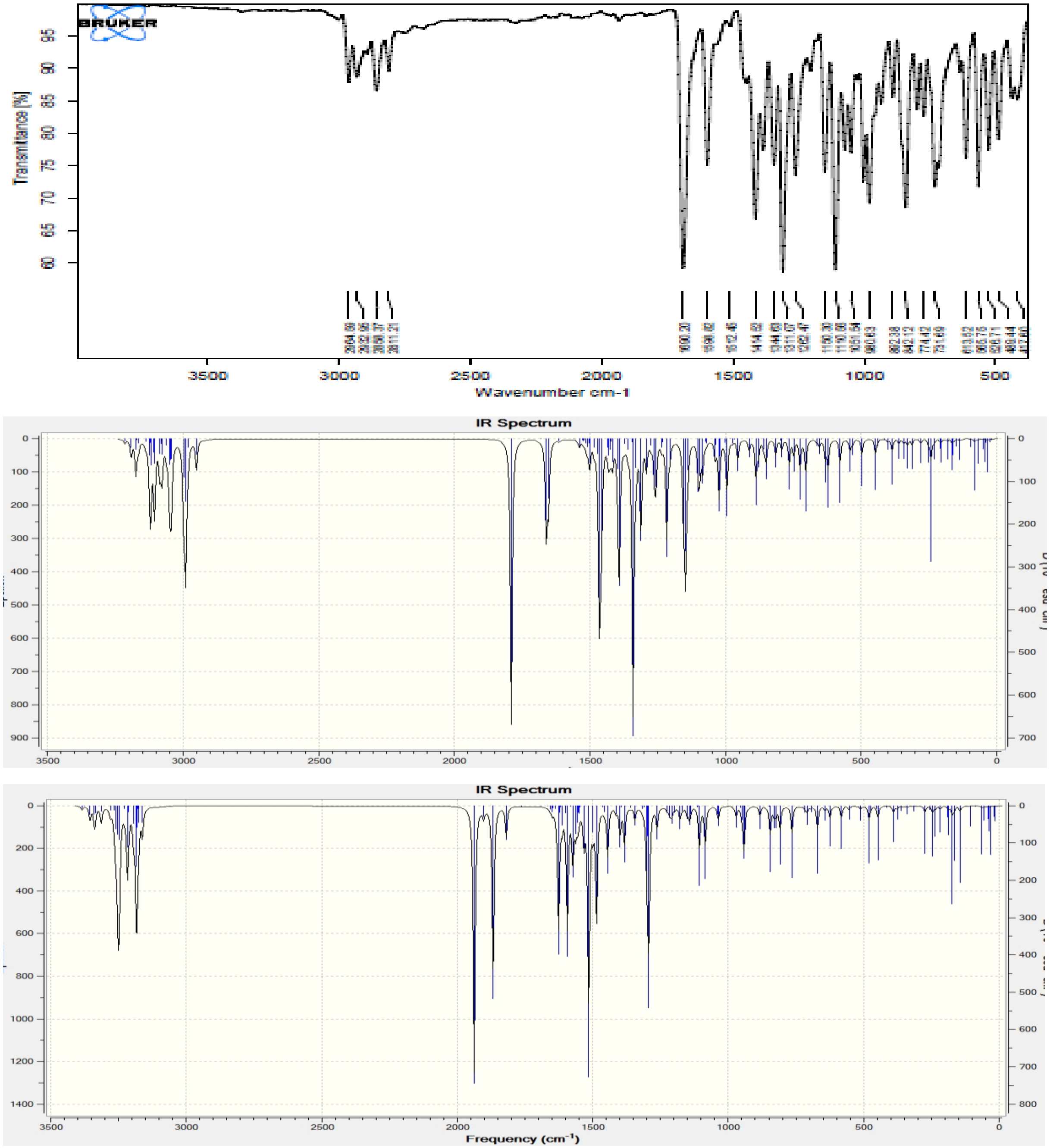


Figure 3. Experimental and theoretical IR spectrums and simulated with DFT/B3LYP/6-31G(d,p) and HF/B3LYP/6-31G(d,p) levels of the molecule.

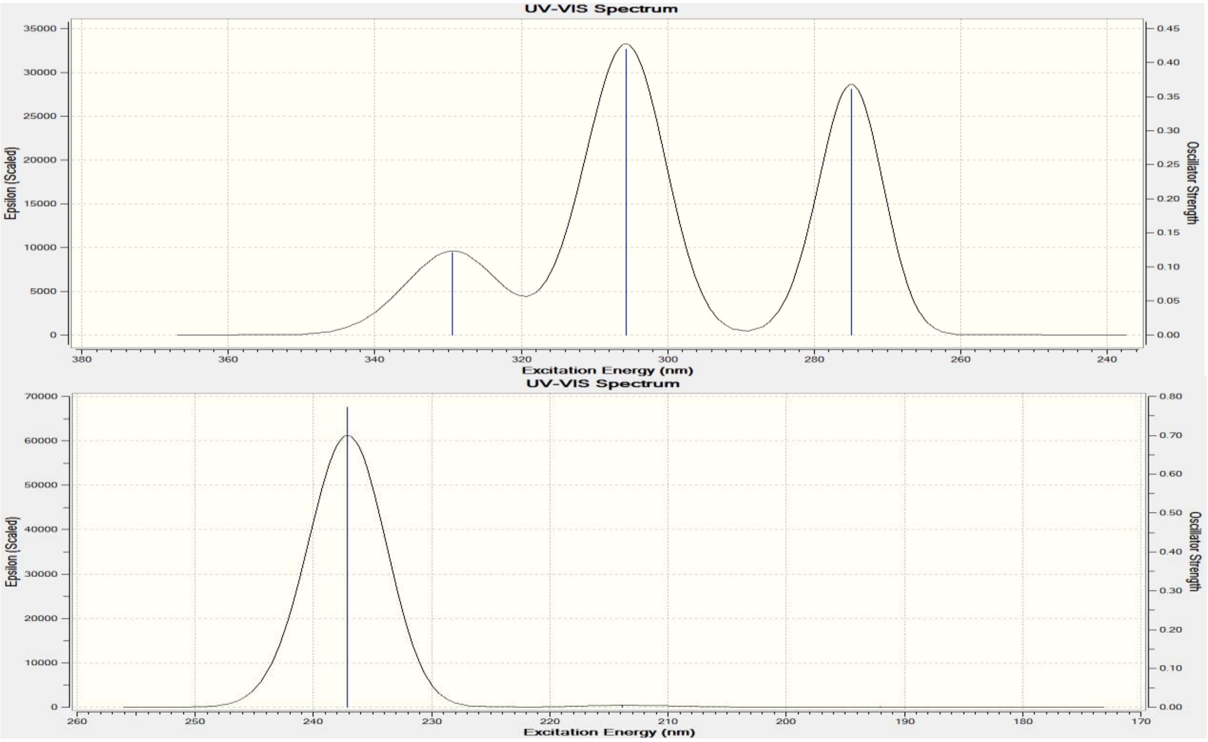


Figure 4. UV-Visible spectra simulated with DFT/B3LYP/6-31G(d,p) and HF/B3LYP/6-31G(d,p) levels of the molecule.

Table 4. The experimental and calculated absorption wavelength (λ) B3LYP/HF 6-31G(d,p) excitation energies of the molecule.

λ (nm)B3LYP/HF	Excitation energy (eV) B3LYP/HF
329.37/237.10	3.7642/5.2292
305.70/213.85	4.0557/5.7978
274.91/192.05	4.5100/6.4559

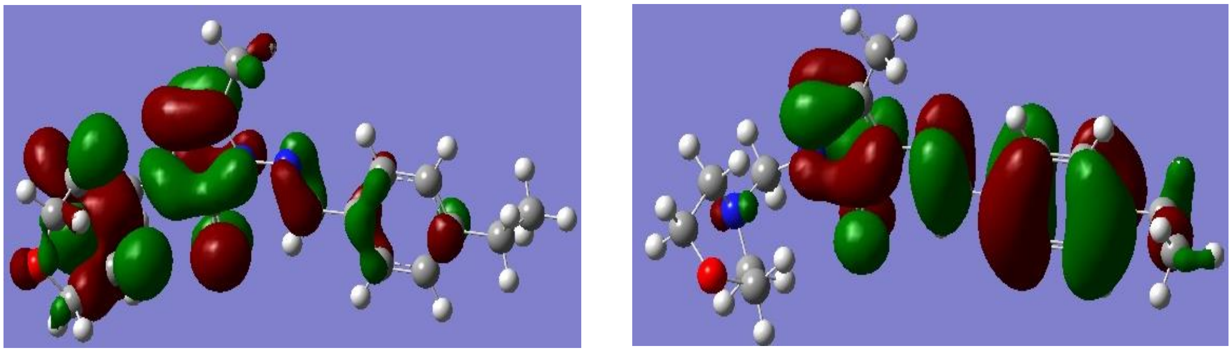
Table 5. The calculated bond angles B3LYP/HF 6-31G(d,p) of the molecule.

No	Bond Angles	B3LYP	HF	No	Bond Angles	B3LYP	HF
1	N(42)-C(1)-N(43)	111.32	111.16	**37**	H(23)-C(10)-C(11)	109.22	109.30
2	N(42)-N(41)-C(2)	113.12	112.41	**38**	C(10)-C(11)-H(25)	111.03	111.05
3	N(42)-N(41)-C(13)	121.87	121.00	**39**	C(10)-C(11)-H(26)	110.87	110.71
4	C(13)-N(41)-C(2)	124.99	126.47	**40**	C(10)-C(11)-H(27)	110.98	110.97
5	N(41)-C(2)-O(46)	129.09	128.88	**41**	H(23)-C(10)-C(11)	109.16	109.30
6	O(46)-C(2)-N(43)	128.68	128.24	**42**	H(25)-C(11)-H(26)	108.08	108.08
7	N(43)-C(1)-C(12)	123.39	123.28	**43**	H(26)-C(11)-H(27)	108.12	108.13
8	N(42)-C(1)-C(12)	125.28	125.52	**44**	H(25)-C(11)-H(27)	107.61	107.75
9	C(1)-C(12)-H(28)	110.97	110.55	**45**	N(41)-C(13)-H(31)	106.00	106.06
10	C(1)-C(12)-H(29)	111.02	110.53	**46**	N(41)-C(13)-H(32)	105.22	105.32
11	C(1)-C(12)-H(30)	108.69	108.60	**47**	N(41)-C(13)-N(45)	117.12	117.01
12	H(28)-C(12)-H(29)	107.26	107.80	**48**	C(13)-N(45)-C(14)	116.65	116.93
13	H(28)-C(12)-H(30)	109.41	109.66	**49**	C(13)-N(45)-C(17)	115.53	115.84
14	H(29)-C(12)-H(30)	109.43	109.67	**50**	N(45)-C(14)-H(33)	112.50	111.26

No	Bond Angles	B3LYP	HF	No	Bond Angles	B3LYP	HF
15	N(41)-C(2)-N(43)	102.22	102.87	**51**	N(45)-C(14)-H(34)	109.27	109.50
16	N(41)-N(42)-C(1)	105.24	105.63	**52**	N(45)-C(14)-C(15)	108.32	111.56
17	C(2)-N(43)-N(44)	130.81	131.13	**53**	H(33)-C(14)-H(34)	106.11	107.52
18	N(43)-N(44)-C(3)	118.63	119.71	**54**	H(33)-C(14)-C(15)	110.58	109.10
19	N(44)-C(3)-H(18)	121.90	122.14	**55**	H(34)-C(14)-C(15)	110.01	108.77
20	H(18)-C(3)-C(4)	117.86	117.32	**56**	C(14)-C(15)-H(35)	110.23	110.15
21	C(3)-C(4)-C(5)	122.73	122.66	**57**	C(14)-C(15)-H(36)	109.65	109.95
22	C(3)-C(4)-C(9)	118.71	118.64	**58**	H(35)-C(15)-H(36)	108.26	107.69
23	C(4)-C(5)-C(6)	120.35	120.31	**59**	C(14)-C(15)-O(47)	112.49	112.00
24	C(4)-C(5)-H(19)	118.95	119.37	**60**	H(35)-C(15)-O(47)	105.75	106.99
25	H(19)-C(5)-C(6)	120.69	120.31	**61**	H(36)-C(15)-O(47)	110.28	109.36
26	C(5)-C(6)-H(20)	119.45	119.34	**62**	C(15)-O(47)-C(16)	112.24	115.70
27	C(5)-C(6)-C(7)	121.34	121.24	**63**	O(47)-C(16)-H(37)	106.84	107.24
28	H(20)-C(6)-C(7)	119.20	119.41	**64**	O(47)-C(16)-H(38)	110.78	109.73
29	C(6)-C(7)-C(8)	118.07	118.18	**65**	H(37)-C(16)-H(38)	107.26	108.06
30	C(7)-C(8)-H(21)	119.47	119.75	**66**	O(47)-C(16)-C(17)	111.16	112.14
31	C(7)-C(8)-C(9)	120.96	120.81	**67**	H(37)-C(16)-C(17)	110.38	109.36
32	C(8)-C(9)-H(22)	119.89	119.52	**68**	H(38)-C(16)-C(17)	110.26	110.17
33	C(8)-C(9)-C(4)	120.71	120.74	**69**	H(39)-C(17)-N(45)	108.11	109.18
34	C(7)-C(10)-C(11)	112.80	112.72	**70**	H(40)-C(17)-N(45)	112.61	112.75
35	C(7)-C(10)-H(23)	109.42	109.35	**71**	C(16)-C(17)-N(45)	109.41	109.09
36	C(7)-C(10)-H(24)	109.46	109.36				

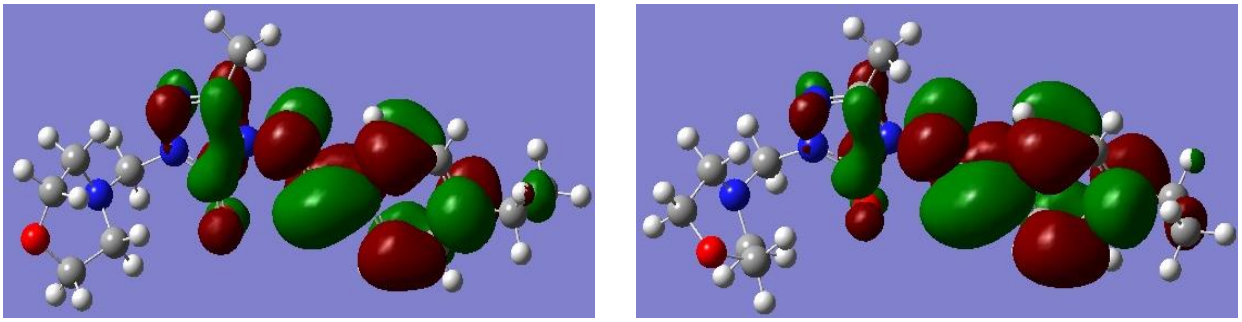
Table 6. The calculated bond lengths B3LYP/HF 6-31G(d,p) of the molecule.

No	Bond Lengths	B3LYP	HF		Bond Lengths	B3LYP	HF
1	C(1)-C(12)	1.487	1.488	**26**	C(10)-H(23)	1.096	1.086
2	C(1)-N(42)	1.304	1.268	**27**	C(10)-H(24)	1.096	1.085
3	C(1)-N(43)	1.383	1.376	**28**	C(10)-C(11)	1.539	1.533
4	N(42)-N(41)	1.387	1.376	**29**	C(11)-H(25)	1.094	1.085
5	N(41)-C(2)	1.374	1.347	**30**	C(11)-H(26)	1.094	1.085
6	C(2)-N(43)	1.412	1.383	**31**	C(11)-H(27)	1.094	1.085
7	C(2)-O(46)	1.226	1.207	**32**	N(41)-C(13)	1.472	1.460
8	N(43)-N(44)	1.378	1.367	**33**	C(13)-H(31)	1.093	1.080
9	C(12)-H(28)	1.097	1.083	**34**	C(13)-H(32)	1.092	1.081
10	C(12)-H(29)	1.094	1.083	**35**	C(13)-N(45)	1.432	1.424
11	C(12)-H(30)	1.092	1.080	**36**	N(45)-C(14)	1.458	1.464
12	N(44)-C(3)	1.290	1.261	**37**	C(14)-H(33)	1.093	1.083
13	C(3)-H(18)	1.088	1.075	**38**	C(14)-H(34)	1.104	1.087
14	C(3)-C(4)	1.463	1.473	**39**	C(14)-C(15)	1.539	1.520
15	C(4)-C(5)	1.406	1.394	**40**	C(15)-H(35)	1.094	1.083
16	C(5)-H(19)	1.084	1.073	**41**	C(15)-H(36)	1.101	1.088
17	C(5)-C(6)	1.388	1.378	**42**	C(15)-O(47)	1.428	1.404
18	C(6)-H(20)	1.087	1.076	**43**	O(47)-C(16)	1.415	1.406
19	C(6)-C(7)	1.405	1.395	**44**	C(16)-H(37)	1.101	1.083
20	C(7)-C(8)	1.400	1.513	**45**	C(16)-H(38)	1.093	1.087
21	C(8)-H(21)	1.087	1.076	**46**	C(16)-C(17)	1.539	1.517
22	C(8)-C(9)	1.392	1.385	**47**	C(17)-H(39)	1.097	1.089
23	C(9)-H(22)	1.086	1.076	**48**	C(17)-H(40)	1.101	1.086
24	C(4)-C(9)	1.403	1.387	**49**	C(17)-N(45)	1.470	1.454
25	C(7)-C(10)	1.512	1.513				



E_{HOMO} (B3LYP) : -0.20927 Hatree

E_{HOMO} (HF) : -0.30934 Hatree



E_{LUMO} (B3LYP) : -0.05574 Hatree

E_{LUMO} (HF) : 0.08801 Hatree

Fig. 5. HOMO-LUMO energy calculated with DFT/B3LYP/6-31G(d,p) and HF/B3LYP/6-31G(d,p) levels of the molecule.

Table 7. The calculated mulliken charges datas B3LYP/HF 6-31G(d,p) of the molecule.

	DFT	HF		DFT	HF
C1	0.521	0.593	**H25**	0.112	0.111
C2	0.844	1.100	**H26**	0.106	0.116
C3	0.113	0.179	**H27**	0.112	0.120
C4	0.083	-0.086	**H28**	0.140	0.155
C5	-0.097	-0.111	**H29**	0.142	0.155
C6	-0.126	-0.162	**H30**	0.139	0.159
C7	0.134	0.006	**H31**	0.138	0.153
C8	-0.129	-0.165	**H32**	0.128	0.168
C9	-0.124	-0.142	**H33**	0.126	0.158
C10	-0.246	-0.235	**H34**	0.091	0.128
C11	-0.308	-0.324	**H35**	0.107	0.123
C12	-0.359	-0.358	**H36**	0.081	0.101
C13	0.082	0.193	**H37**	0.087	0.110
C14	-0.091	-0.059	**H38**	0.107	0.120
C15	0.092	0.115	**H39**	0.104	0.122
C16	0.028	0.122	**H40**	0.105	0.129
C17	0.028	-0.045	**N41**	-0.386	-0.596
H18	0.156	0.226	**N42**	-0.343	-0.343
H19	0.104	0.177	**N43**	-0.425	-0.631
H20	0.083	0.150	**N44**	-0.327	-0.330
H21	0.084	0.151	**N45**	-0.409	-0.631
H22	0.095	0.164	**O46**	-0.565	-0.683
H23	0.104	0.126	**O47**	-0.489	-0.661
H24	0.105	0.126			

3. CONCLUSIONS

Quantum-chemical methods such as DFT and HF methods are used to obtain geometrical parameters and calculate the IR, ^{1}H-NMR and ^{13}C-NMR spectra of the compound. The calculated the chemical shifts are compared with the experimental observations. The chemical shifts calculated by B3LYP/6-31G(d,p) and HF/6-31G(d,p) methods are in a very good agreement are in a very good agreement with the experimental data. The normal mode vibrational frequencies calculated at the B3LYP and HF methods of theory are in accordance with the recorded IR spectrum. In addition, vibrational bands assignments and analysis of the fundamental modes of the compound are performed.

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