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Research Article

INVESTIGATION OF THEORETICAL PROPERTIES OF NOVEL 1-(MORPHOLINE-4-YL-METHYL)-3-METHYL -4-(4-ETHOXYBENZYLIDENAMINO)-4,5-DIHYDRO -1*H*-1,2,4-TRIAZOL-5-ONE MOLECULE

Gül Kotan[1]* and Haydar Yüksek[2]

[1]Kafkas University, Kars Vocational School, Kars, Turkey.
[2]Kafkas University, Department of Chemistry, Kars, Turkey.

ABSTRACT

In this study, 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one was synthesized from the reaction of 3-methyl-4-(4-ethylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazole-5-one with morpholine and formaldehyde and characterized by IR, ^{1}H-NMR, ^{13}C-NMR spectral data. Then, the atomic structure of compound has been optimized using B3LYP/631G(d) and HF/631G(d) basis set. ^{1}H-NMR and ^{13}C-NMR isotropic shift values, IR absorption frequencies, bond angles, bond lengths, dipole moments, mulliken charges, HOMO-LUMO energies and total energy of the compound with both methods were calculated theoretically by using the program package Gaussian G09W. In addition, IR, ^{1}H-NMR, ^{13}C-NMR theoretical spectral data were compared with specific experimental data.

Keywords: 1,2,4-Triazol-5-one, 631G (d), mulliken charge, B3LYP and HF.

INTRODUCTION

Quantum chemical calculation methods have widely been used to theoretically predict the structural, spectroscopic, electronic and thermodynamic properties of molecular systems. The quantum chemical calculation methods ensure support for experimental structural and spectroscopic studies[1-6]. In this study, having a large number of theory and basic set options, including molecular mechanics, semi-empirical and ab-initio methods, Gaussian 09W[7] package is used. Hartree-Fock (HF) and Density Functional Theory (B3LYP) methods are used for the determination of the structure of compound and the investigated of spectroscopy, electronics, nonlinear optical properties. 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one was obtained according to the literature[8]. The compound was analyzed with IR, ^{1}H-NMR and ^{13}C-NMR spectral datas. In the present paper, theoretical values of compound were calculated theoretically on the computer. Firstly, the geometry structure of compound has been optimized using B3LYP/631G (d) and HF/631G (d) basis set[7,9]. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09[7]. Experimental[8] and theoretical values were inserted into the grafic according to equatation of $\delta_{exp=}a+b.\ \delta$ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. The correlation graphs for chemical shifts drawn with ^{1}H-NMR(DMSO) and ^{13}C-NMR(DMSO) spectral data of the molecule. IR absorption frequencies of analysed molecule were calculated by two methods. Theoretically calculated IR data are multiplied with appropriate adjustment factors 0,9613 for B3LYP/631G(d) and 0,8929 for HF/631G(d)[10] and the data obtained according to HF and DFT method program, was used in defining IR data, which were calculated theoretically[11]. Furthermore, molecule's theoretical bond angles, bond lengths, dipole moments, mulliken charges, the highest occupied molecular orbitals HOMO, lowest unoccupied molecular orbitals LUMO energys and total energy of the molecule for both methods were calculated.

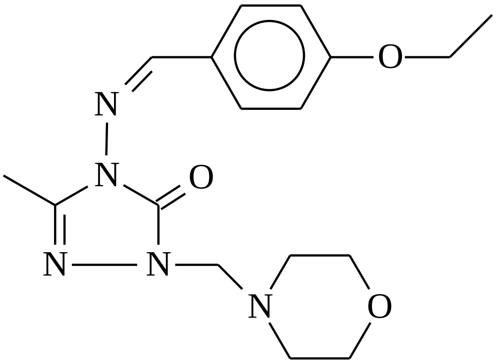


Fig. 1: 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

MATERIALS AND METHODS

EXPERİMENTAL

1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one was synthesized from the reaction of 3-methyl-4-(4-ethylbenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazole-5-one with morpholine and formaldehyde according to the literature [8]. 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. UV absorption spectra were measured in 10-mm quartz cells between 200 and 400 nm using a PG Instruments Ltd T80 UV/vis Spectrometer. Extinction coefficients (ε) are expressed in L·mol^{-1}·cm^{-1}. Yield 89%; m.p: 132 ^{0}C ; IR (υ): 1695 (C=O), 1601 (C=N), 824 (1,4-disubstituted benzenoid ring) cm^{-1}. ^{1}H-NMR (DMSO-d_6): 1.35 (t, 3H,OCH_2CH_3; J=7.20 Hz), 2.29 (s, 3H, CH_3), 2.56-2.59 (m, 4H, CH_2NCH_2), 3.55-3.57 (m, 4H, CH_2OCH_2), 4,10 (q, 2H,OCH_2CH3; J= 7.20 Hz), 4.52 (s, 2H, NCH_2), 7.04 (d, 2H, ArH; J= 8.80 Hz), 7.78 (d, 2H, ArH; J= 8.80 Hz), 9.58 (s, 1H, N=CH). ^{13}C-NMR (DMSO-d_6): 10.97 (CH_3), 14.49 (OCH_2CH_3), 49.97 (CH_2NCH_2), 63.40 (OCH_2CH_3), 65.87 (NCH_2N), 66.03 (CH_2OCH_2), 114.88 (2C), 125.65, 129.57 (2C), 161.29 (ArC), 143.03 (Triazole C_3), 150.34 (N=CH), 154.53 (Triazole C_5)

METHODS

The quantum chemical calculations were carried out with density functional theory (DFT) and Hartree-Fock (HF) methods using 631G (d) basis set at the Gaussian 09W program package on a computing system[7]. Firstly, the compound was optimized by using the B3LYP/631G (d) and HF/631G (d) basis sets[7,9]. Thus, the most stable geometrical comformer of compound was obtained. Then, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with method of GIAO[7]. The veda4f program was used in defining IR data[11]. Otherwise, bond angles, bond lengths, the HOMO-LUMO energy, electronegativity and mulliken charges of compound were calculated theoretically on the computer.

THEORETICAL CALCULATIONS

Fig. 2: Gausview structure of the molecule

Table 1: Data calculated ^{13}C and ^{1}H-NMR/DMSO(B3LYP/HF 631G(d) isotropic chemical shifts of the molecule (δ/ppm)

No	Experimental	DFT	Difference	DFT/DMSO	Differ./DMSO
C1	143,03	148,35	-5,32	143,75	-0,72
C2	150,34	155,13	-4,79	147,94	2,40
C3	154,53	155,25	-0,72	150,06	4,47
C4	125,65	129,75	-4,10	121,85	3,80
C5	129,57	130,24	-0,67	126,17	3,40
C6	114,88	115,48	-0,60	115,49	-0,61
C7	161,29	163,13	-1,84	156,00	5,29
C8	114,88	121,79	-6,91	117,53	-2,65
C9	129,57	138,51	-8,94	133,08	-3,51
C10	63,40	71,55	-8,15	58,83	4,57
C11	14,49	24,11	-9,62	13,44	1,05
C12	10,97	22,74	-11,77	11,70	-0,73
C13	65,87	74,48	-8,61	56,61	9,26
C14	49,97	57,09	-7,12	38,92	11,05
C15	66,03	69,99	-3,96	53,78	12,25
C16	66,03	75,08	-9,05	54,45	11,58
C17	49,97	53,15	-3,18	37,65	12,32
H18	9,58	10,04	-0,46	9,54	0,04
H19	7,78	8,52	-0,74	8,43	-0,65
H20	7,04	7,26	-0,22	7,21	-0,17
H21	7,04	7,14	-0,10	7,03	0,01
H22	7,78	7,64	0,14	7,62	0,16
H23	4,10	4,84	-0,74	3,71	0,39
H24	4,10	4,71	-0,61	3,94	0,16
H25	1,35	2,02	-0,67	0,85	0,50
H26	1,35	1,41	-0,06	1,04	0,31
H27	1,35	1,66	-0,31	0,50	0,85
H28	2,29	2,77	-0,48	2,17	0,12
H29	2,29	2,78	-0,49	2,20	0,09
H30	2,29	2,39	-0,10	1,86	0,43
H31	4,52	4,51	0,01	3,68	0,84
H32	4,52	5,17	-0,65	4,24	0,28
H33	2,58	3,67	-1,09	2,57	0,01
H34	2,58	3,77	-1,19	2,91	-0,33
H35	3,56	4,51	-0,95	3,21	0,35
H36	3,56	3,78	-0,22	3,03	0,53
H37	3,56	4,35	-0,79	3,49	0,07
H38	3,56	4,55	-0,99	3,34	0,22
H39	2,58	4,21	-1,63	2,93	-0,35
H40	2,58	2,83	-0,25	2,15	0,43

The relation between R^2 values of the compound

B3LYP/631G(d) (DMSO): ^{13}C: -10.1723, ^{1}H: 0.9644; HF/631G(d) (DMSO): ^{13}C: 8.3064, ^{1}H: 0.9824. 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

		C^{13}-NMR/DMSO		
	R^2	**S. error**	**a**	**b**
DFT	-10.1723	1.0454	1.6821	0.0152
HF	8.3064	0.9557	2.5024	0.0242
		H^1-NMR/DMSO		
	R^2	**S. error**	**a**	**b**
DFT	0.9644	0.4461	0.6002	1.0116
HF	0.9824	0.3129	0.4677	0.9262

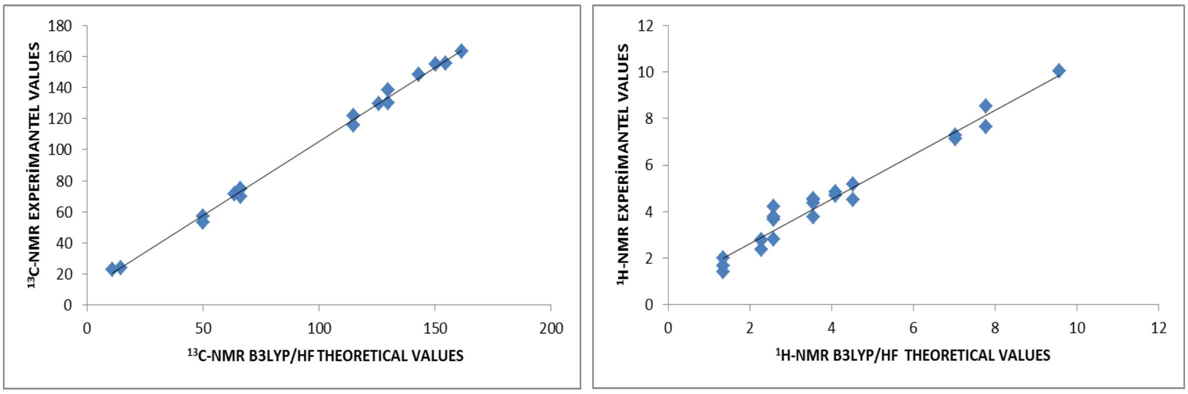


Fig. 3: The correlation graphs for chemical shifts of the molecule

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 1695 cm^{-1} and theoretically (C=O) peak in 1715 cm^{-1} were observed.

Table 3: The calculated frequencies values of the molecule

	Vibration Types	B3LYP	HF
1	τ NCNN(33)	13	12
2	τ NCNN(34), τ CCNN(12), τ CCCC(10)	15	13
3	τ NCCC(10), τ CNNC(14), τ CNCN(50)	23	24
4	τ NCCC(18), τ CNNC(17), τ CCNN(26)	34	29
5	τ NCCC(22)	43	33
6	τ NCCC(13), τ CCCC(13), τ COCC(16), τ CCNN(20)	44	43
7	τ HCCO(93), τ COCC(40), τ CCNN(12)	61	51
8	τ CNCN(37)	76	66
9	τ CNNC(15), τ COCC(20)	88	80
10	τ CNNC(11), τ CNCN(10), τ CCON(22)	115	97
11	τ CCNC(10)	136	136
12	δ CCC(11)	148	151
13	τ HCCN(53)	155	157
14	τ CNNC(23),τ NNCN(19)	170	168
15	τ NCCC(23), τ CCCC(13)	191	170
16	δ CCN(16)	195	199
17	δ CCN(14), τ HCOC(16), τ HCCO(15)	211	208
18	δ CNN(23), δ CNC(11)	217	222
19	δ CNN(10)	232	238
20	τ NCNN(20), τ NNCN(12), τ CCCC(17)	275	259
21	δ OCC(24), τ HCCO(10)	288	282
22	δ COC(18), τ COCC(18)	299	288
23	δ OCN(13), δ CCN(22)	320	327
24	τ CNNC(18)	328	334
25	δ CCO(17)	355	367
26	δ CCO(20), δ CNC(10)	370	375
27	δ CNC(11), τ CCCN(14)	392	398
28	τ CCCC(34)	400	401
29	τ HCCC(12), τ CCCC(28)	413	416
30	δ NNC(11), δ CCC(17)	423	443
31	δ COC(21)	460	447
32	δ COC(10)	486	461
33	δ CCN(14), δ COC(13)	505	495
34	τ HCCC(13), τ CCCC(16), τ OCCC(29)	526	521
35	δCOC(19), δ OCC(13), δ COC(20)	542	565
36	δ OCC(10)	584	576
37	ν CC(21), δ OCN(10), δ CNN(10)	600	600
38	τ NNCN(16)	615	618

39	τ NNCN(13)	621	633
40	δ CCC(23)	632	640
	Vibration Types	**B3LYP**	**HF**
41	τ ONNC(58)	672	684
42	ν CC(16)	691	723
43	τ HCCC(20), τ CCCC(40), τ OCCC(18)	704	739
44	ν OC(14)	736	744
45	ν NC(45)	747	755
46	νNC(11), ν NN(15)	783	781
47	τ HCOC(25), τ HCCO(21)	797	795
48	τ HCCC(82)	799	838
49	τ HCCC(48), τ OCCC(12)	816	843
50	ν OC(54)	827	844
51	ν NC(10), τ HCNC(16)	845	851
52	ν CC(16)	848	856
53	δ CCN(14), τ COCC(10)	869	869
54	ν CC(37), ν OC(13), τ HCOC(17)	884	882
55	νNN(14), ν CC(10), δNNC(13)	916	928
56	τ HCCC(40), τ CCCC(13)	923	966
57	τ HCCC(43), τ CCCC(17)	930	972
58	ν NN(10), τ HCCN(17)	958	987
59	δ CCC(11)	984	991
60	ν CC(13),ν OC(16), τ HCNN(45)	984	992
61	δCCC(58)	989	1023
62	δ HCH(10), τ HCCN(26)	1003	1024
63	ν NC(12), τ HCOC(11)	1004	1029
64	ν CC(40), ν OC(42)	1028	1034
65	δ HCH(13), τ HCCN(52)	1039	1051
66	ν NC(22), δ CNN(10), δ NNC(13)	1054	1071
67	ν CC(12), τ HCNC(17)	1082	1080
68	ν OC(12), δ HCH(11), δ CCO(10), τ HCOC(42)	1084	1087
69	τ HCOC(16)	1086	1090
70	ν CC(14), δ HCC(59)	1103	1099
71	ν CC(13), δ HCC(70)	1106	1130
72	ν NC(10), ν OC(55)	1119	1143
73	ν NC(11)	1152	1152
74	δ HCC(50)	1156	1158
75	δ HCC(10), δ HCC(12), τ HCOC(33), τ CCOC(16)	1158	1165
76	ν CC(10), ν NN(13), δ NCN(14)	1191	1172
77	δ HCO(37)	1207	1200
78	δ HCC(13), δ HCO(15)	1227	1221
79	νOC(16), δ HCC(13)	1239	1240
80	δ HCO(44)	1242	1241
81	ν OC(13), δ HCO(13)	1243	1256
82	ν NN(15), δ HCO(10)	1256	1265
83	ν CC(13), δ HCC(38)	1281	1289
84	δ HCN(15)	1282	1297
85	ν NC(10), δ HCC(18)	1292	1304
86	δ HCC(68)	1295	1307
87	ν CC(45)	1311	1332
88	τ HCNC(16), τ HCOC(34)	1330	1347
89	νNC(10), δ HCN(34)	1347	1358
90	δ HCH(23), τ HCOC(15)	1352	1375
91	τ HCNC(11)	1367	1376
92	δ HCN(17), δ HCH(53)	1369	1391
93	τ HCNC(30), τ HCOC(11)	1381	1395
94	δ HCN(18), τ HCNC(20)	1386	1398
95	δ HCN(13), δ HCH(35)	1387	1402
96	δ HCH(18), τ HCOC(18)	1388	1405
97	τ HCOC(29)	1392	1410
98	ν CC(17), δ HCC(16)	1410	1420
99	ν CC(17), δ HCN(14), δ HCC(13)	1418	1432
100	δ HCH(22)	1430	1445
101	δ HCH(38), τ HCCN(15)	1443	1453
102	δ HCH(34), τ HCCN(10)	1455	1456
103	δ HCH(40), τ HCCO(18)	1458	1460
104	δ HCH(49)	1471	1466
105	δ HCH(61), τ HCOC(11)	1472	1486
106	δ HCH(42)	1483	1486
107	δ HCH(76)	1485	1487

108	δ HCH(30), τ HCOC(14)	1489	1494
109	δ HCH(81)	1496	1503
110	ν CC(13), δ HCC(44)	1505	1517
111	ν CC(27), δ HCC(12)	1554	1579
112	ν NC(50)	1590	1620
113	ν NC(35), ν CC(18)	1594	1668
114	ν NC(31), ν CC(34)	1616	1699
	Vibration Types	**B3LYP**	**HF**
115	ν OC(74)	1715	1731
116	ν CH(21)	2866	2844
117	ν CH(20)	2886	2856
118	ν CH(40)	2907	2861
119	ν CH(58)	2909	2864
120	ν CH(40)	2937	2866
121	ν CH(44)	2943	2886
122	ν CH(31)	2944	2890
123	ν CH(72)	2947	2891
124	ν CH(28)	2954	2921
125	ν CH(53)	2960	2922
126	ν CH(29)	2968	2923
127	ν CH(34)	2987	2924
128	ν CH(71)	2993	2930
129	ν CH(50)	3002	2936
130	ν CH(54)	3009	2943
131	ν CH(81)	3023	2951
132	ν CH(16)	3024	2973
133	ν CH(57)	3043	2979
134	ν CH(37)	3059	3003
135	ν CH(35)	3066	3019

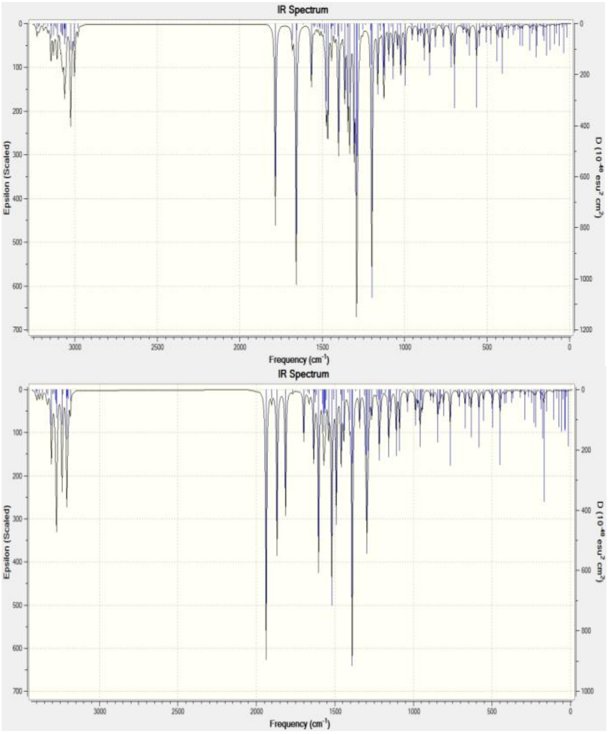
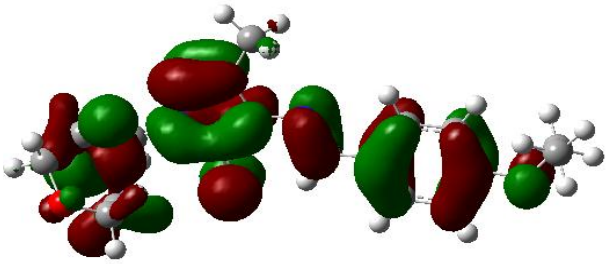
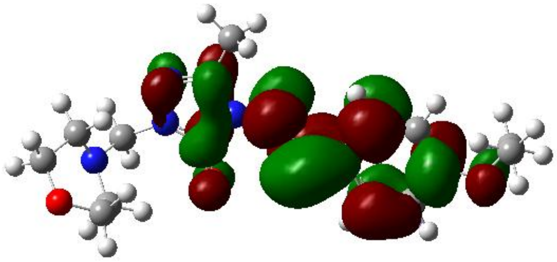


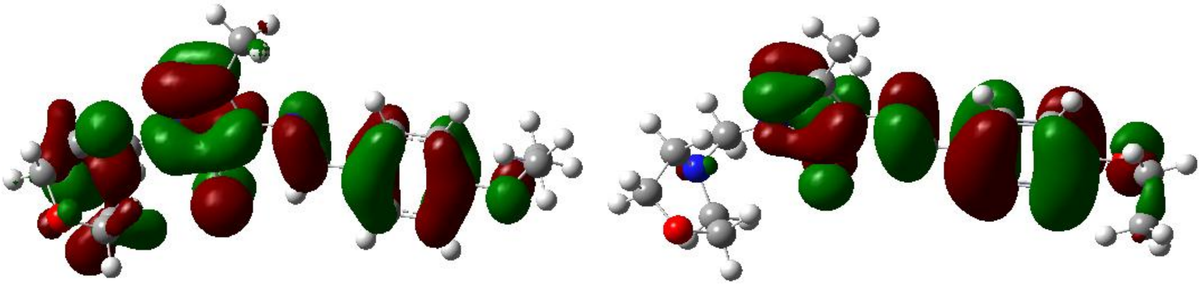
Fig. 4: IR spectra experimental and simulated with DFT/B3LYP/631G(d) and HF/B3LYP/631G(d) levels of the molecule



E_{HOMO} **(B3LYP) : -0.22409 Hatree**



E_{LUMO} **(B3LYP) : -0.06789 Hatree**



E_{HOMO} **(HF) : -0.31919Hatree** E_{LUMO} **(HF) : 0.08127Hatree**

Fig. 5: HOMO-LUMO energy calculated with DFT/B3LYP/HF 631G(d) levels of the molecule

Table 4: The calculated bond angles of the molecule

	Bond Angles	B3LYP	HF		Bond Angles	B3LYP	HF
1	N(41)-C(1)-N(43)	111.372	111.186	**37**	H(23)-C(10)-H(24)	107.467	107.877
2	N(41)-N(42)-C(2)	113.062	112.326	**38**	H(23)-C(10)-C(11)	111.854	110.733
3	N(42)-N(41)-C(13)	121.082	121.264	**39**	C(10)-C(11)-H(25)	111.828	110.025
4	C(13)-N(42)-C(2)	125.809	126.237	**40**	C(10)-C(11)-H(26)	109.936	110.429
5	N(42)-C(2)-O(46)	129.064	128.814	**41**	C(10)-C(11)-H(27)	110.213	111.315
6	O(46)-C(2)-N(43)	128.638	128.210	**42**	H(30)-C(12)-H(29)	109.351	108.464
7	N(43)-C(1)-C(12)	123.396	123.304	**43**	H(30)-C(12)-H(28)	109.366	108.109
8	N(41)-C(1)-C(12)	125.233	125.510	**44**	H(29)-C(12)-H(28)	107.270	108.415
9	C(1)-C(12)-H(28)	108.720	108.644	**45**	N(42)-C(13)-H(31)	105.565	105.862
10	C(1)-C(12)-H(29)	111.031	110.600	**46**	N(42)-C(13)-H(32)	105.461	106.144
11	C(1)-C(12)-H(30)	111.075	110.602	**47**	N(42)-C(13)-N(45)	117.150	117.066
12	H(28)-C(12)-H(29)	109.366	109.591	**48**	C(13)-N(45)-C(14)	116.070	117.013
13	H(28)-C(12)-H(30)	109.351	109.568	**49**	C(13)-N(45)-C(17)	115.852	115.843
14	H(29)-C(12)-H(30)	107.270	107.823	**50**	N(45)-C(14)-H(33)	110.985	109.457
15	N(42)-C(2)-N(43)	102.298	102.975	**51**	N(45)-C(14)-H(34)	109.198	110.241
16	N(42)-N(41)-C(1)	105.210	105.647	**52**	N(45)-C(14)-C(15)	110.975	111.562
17	C(2)-N(43)-N(44)	130.910	131.192	**53**	H(33)-C(14)-H(34)	107.535	107.504
18	N(43)-N(44)-C(3)	118.522	119.751	**54**	H(33)-C(14)-C(15)	109.064	109.197
19	N(44)-C(3)-H(18)	121.788	122.184	**55**	H(34)-C(14)-C(15)	109.001	108.781
20	H(18)-C(3)-C(4)	117.638	117.176	**56**	C(14)-C(15)-H(35)	109.975	110.003
21	C(3)-C(4)-C(5)	122.928	122.631	**57**	C(14)-C(15)-H(36)	110.132	110.232
22	C(3)-C(4)-C(9)	118.957	118.736	**58**	H(35)-C(15)-H(36)	107.423	107.731
23	C(4)-C(5)-C(6)	121.313	120.013	**59**	C(14)-C(15)-O(47)	112.216	111.991
24	C(4)-C(5)-H(19)	119.376	119.331	**60**	H(35)-C(15)-O(47)	110.879	109.850
25	H(19)-C(5)-C(6)	119.819	119.947	**61**	H(36)-C(15)-O(47)	106.028	106.902
26	C(5)-C(6)-H(20)	119.151	120.222	**62**	C(15)-O(47)-C(16)	114.436	115.698

27	C(5)-C(6)-C(7)	119.857	120.013	**63**	O(47)-C(16)-H(37)	108.250	109.696
28	H(20)-C(6)-C(7)	120.992	119.755	**64**	O(47)-C(16)-H(38)	108.078	107.145
29	C(6)-C(7)-C(8)	119.387	119.845	**65**	H(37)-C(16)-H(38)	108.128	108.084
30	C(7)-C(8)-H(21)	118.453	119.071	**66**	O(47)-C(16)-C(17)	113.361	112.127
31	C(7)-C(8)-C(9)	120.160	119.764	**67**	H(37)-C(16)-C(17)	109.164	109.433
32	C(8)-C(9)-H(22)	119.457	119.270	**68**	H(38)-C(16)-C(17)	109.721	110.254
33	C(8)-C(9)-C(4)	121.167	121.022	**69**	H(39)-C(17)-N(45)	108.683	109.133
34	C(7)-O(47)-C(10)	120.355	118.548	**70**	H(40)-C(17)-N(45)	113.225	112.746
35	O(47)-C(10)-H(23)	110.143	110.238	**71**	C(16)-C(17)-N(45)	109.291	109.073
36	O(47)-C(10)-H(24)	104.116	105.020				

Table 5: The calculated bond lengths of the molecule

Bond lengths		**B3LYP**	**HF**	**Bond lengths**		**B3LYP**	**HF**
1	C(1)-C(12)	1.487	1.489	**27**	C(10)-H(23)	1.097	1.084
2	C(1)-N(41)	1.300	1.268	**28**	C(10)-H(24)	1.093	1.080
3	C(1)-N(43)	1.386	1.376	**29**	C(10)-C(11)	1.524	1.519
4	N(42)-N(41)	1.386	1.376	**30**	C(11)-H(25)	1.094	1.085
5	N(42)-C(2)	1.373	1.348	**31**	C(11)-H(26)	1.096	1.084
6	C(2)-N(43)	1.413	1.383	**32**	C(11)-H(27)	1.094	1.084
7	C(2)-O(46)	1.228	1.207	**33**	N(41)-C(13)	1.475	1.460
8	N(43)-N(44)	1.376	1.368	**34**	C(13)-H(31)	1.093	1.080
9	C(12)-H(28)	1.091	1.080	**35**	C(13)-H(32)	1.092	1.079
10	C(12)-H(29)	1.095	1.083	**36**	C(13)-N(45)	1.431	1.424
11	C(12)-H(30)	1.095	1.083	**37**	N(45)-C(14)	1.479	1.464
12	N(44)-C(3)	1.291	1.261	**38**	C(14)-H(33)	1.097	1.082
13	C(3)-H(18)	1.088	1.074	**39**	C(14)-H(34)	1.099	1.086
14	C(3)-C(4)	1.460	1.472	**40**	C(14)-C(15)	1.528	1.521
15	C(4)-C(5)	1.404	1.394	**41**	C(15)-H(35)	1.101	1.087
16	C(5)-H(19)	1.085	1.073	**42**	C(15)-H(36)	1.094	1.082
17	C(5)-C(6)	1.390	1.378	**43**	C(15)-O(47)	1.420	1.404
18	C(6)-H(20)	1.083	1.074	**44**	O(47)-C(16)	1.431	1.405
19	C(6)-C(7)	1.405	1.392	**45**	C(16)-H(37)	1.098	1.086
20	C(7)-C(8)	1.403	1.383	**46**	C(16)-H(38)	1.098	1.082
21	C(8)-H(21)	1.085	1.073	**47**	C(16)-C(17)	1.526	1.518
22	C(8)-C(9)	1.386	1.384	**48**	C(17)-H(39)	1.097	1.086
23	C(9)-H(22)	1.087	1.076	**49**	C(17)-H(40)	1.102	1.088
24	C(4)-C(9)	1.407	1.388	**50**	C(17)-N(45)	1.461	1.454
25	C(7)-O(47)	1.360	1.355	**51**			
26	C(47)-C(10)	1.432	1.415	**52**			

Table 6: The calculated mulliken charges of the molecule

	DFT	**HF**		**DFT**	**HF**
C1	0.542	0.609	**H26**	0.152	0.177
C2	0.845	1.098	**H27**	0.167	0.176
C3	0.028	0.094	**H28**	0.180	0.210
C4	0.135	-0.048	**H29**	0.181	0.202
C5	-0.174	-0.178	**H30**	0.182	0.202
C6	-0.193	-0.255	**H31**	0.169	0.204
C7	0.387	0.426	**H32**	0.184	0.220
C8	-0.182	-0.253	**H33**	0.171	0.212
C9	-0.189	-0.208	**H34**	0.148	0.175
C10	-0.464	-0.001	**H35**	0.128	0.148
C11	-0.041	-0.505	**H36**	0.158	0.173
C12	-0.507	-0.522	**H37**	0.138	0.157
C13	-0.032	0.073	**H38**	0.132	0.170
C14	-0.156	-0.172	**H39**	0.147	0.177
C15	-0.040	0.011	**H40**	0.145	0.171
C16	-0.006	0.018	**N41**	-0.345	-0.343
C17	-0.161	-0.154	**N42**	-0.373	-0.586
H18	0.206	0.286	**N43**	-0.423	-0.631
H19	0.152	0.235	**N44**	-0.322	-0.322
H20	0.137	0.215	**N45**	-0.385	-0.602
H21	0.144	0.221	**O46**	-0.488	-0.682
H22	0.143	0.222	**O47**	-0.568	-0.677
H23	0.146	0.154	**O48**	-0.516	-0.645
H24	0.161	0.181			
H25	0.164	0.164			

Table 7: The calculated dipole moments values of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
Dft	-4.3640	-2.0179	-0.9473	4.9004
Hf	1.5556	2.5689	1.3428	3.2897

Table 8: The calculated total energy values of the molecule

Enerji (a.u.)	**B3LYP**	**HF**
	-1161.0312	-1153.9185

RESULTS AND DISCUSSION

In this work, geometrical parameters and spectroscopic parameters such as IR, ^{1}H-NMR and ^{13}C-NMR spectra of 1-(morpholine-4-yl-methyl)-3-methyl-4-(4-ethoxybenzylidenamino) -4,5-dihydro-1*H*-1,2,4-triazol-5-one are calculated by density functional theory (DFT) and Hartree-Fock (HF) methods with the 631G(d) basis set. Obtained spectroscopic parameters are compared with experimental data. 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 acording to a, b ve R^2 values, lineer a correlation were observed. Furthermore, IR vibrational frequencies experimentally carbonyl peak (C=O) in 1695 cm^{-1} and theoretically (C=O) peak in 1715 cm^{-1} were observed. The negative frequency in the IR data was not found. This result, structure of compound were shown stable.

In addition, bond angles, bond lengths, the HOMO-LUMO energy, electronegativity and mulliken charges are calculated theoretically by using the B3LYP/631G (d) and HF/631G (d) basis sets.

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