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Comparison of Experimental Values with Theoritical Spectral Values of 1-Acetyl-3-ethyl-4-(3-acetoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

Şule Bahçeci
Fatih Education Faculty, Karadeniz Technical University, Trabzon, Turkey
E-mail: *sbahceci@gmail.com*

Haydar Yüksek
Department of Chemistry, Kafkas University, Kars, Turkey

Murat Beytur
Department of Chemistry, Kafkas University, Kars, Turkey

Nuri Yıldırım
Department of Chemistry, Karadeniz Technical University, Trabzon, Turkey

ABSTRACT

In this study, the 1-acetyl-3-ethyl-4-(3-hydroxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-onewas optimized by using the B3LYP/6311G (d, p) and HF/6311G (d, p) basis sets. Afterwards, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W. Experimental and theoretical values were inserted into the graphic according to equitation of δ exp$_{=}$a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of the molecule were calculated by two methods. Then, they were compared with experimental data and are shown to be accurate. The veda4f program, was used in defining IR data, which were calculated theoretically. Furthermore, theoretical bond lengths, bond angles, UV-Vis values, HOMO-LUMO energies and total energy of the molecule for both methods were calculated.

Key words: 4,5-dihydro-1H-1,2,4-triazol-5-one, 6311G, GIAO, total energy and veda4f

1. INTRODUCTION

Quantum chemical calculation methods have been widely used to predict as theoretical the structural, spectroscopic (IR, ^{1}H-NMR,^{13}C-NMR and UV spectroscopic parameters) of molecular systems. The quantum chemical calculation methods provide support for experimental structural and spectroscopic studies. Therefore, molecular geometry, vibrational spectra, ^{13}C and ^{1}H NMR chemical shifts, electronic properties and atomic charges of the corresponding molecule have been studied by using DFT/B3LYP/6–311G(d, p) and HF/6–311G(d, p) levels [1, 2]. The literature concerning the 1,2,4-triazole is rich and the papers published cover such subjects as vibrational properties, density functional theory(DFT) and Hartree-Fock (HF) calculations.Literature survey has revealed that the DFT and HF havea great accuracy in reproducing the experimental values in geometry,vibrational frequency, NMR chemical shifts etc. [3–7].

2. EXPERIMENTAL

2.1. Computational details

The optimized molecular structures, vibrational frequencies, ^{1}H and ^{13}C NMR chemical shifts, UV–vis spectroscopic parameters, atomic charges and frontier molecule orbitals of the compound **1**,have been calculated by using DFT/B3LYP and HF methods with 6–311G(d, p) basis set. In this study, all calculations were carried out with the Gauss–View molecular visualization program and Gaussian 09W program package on personal computer [1, 2].

For the vibrational computations, molecular structures of the compound **1**were calculated by using Becke–3–Lee Yang Parr (B3LYP) [8,9] of density functional method (DFT) and Hartree-Fock (HF)methods with 6–311G(d, p) basis set in ground state. The positive values of all calculated vibrational wavenumbers show that the optimized molecular structures are stable. Therefore, the calculated vibrational wavenumbers were scaled with 0.9614 ranges from 1700 to 4000 cm^{-1} for B3LYP/6–311G(d, p) and HF/6–311G(d, p)level [10]. The veda4f program, was used in defining IR data, which were calculated theoretically [11].

For the NMR calculations, the optimized molecular geometries of the compound **1**were firstly obtained at 6–311G(d, p) basis level in DMSO by using GIAO method. Then, ^{1}Hand ^{13}C NMR chemical shifts for the compound**1** were calculated at B3LYP/6–31G(d) and HF levels in solvent by using gauge invariant atomic orbital (GIAO) method [12–14]. The UV–vis spectroscopic calculations of the mentioned molecule were performed by using TD–SCF/B3LYP and TD–SCF/HF methos in ethanol [15]. In additional, HOMO and LUMO energy values and energy gaps for the compound **1**were calculated by using B3LYP and HF methods with 6–311G(d, p) basis set. Finally, mulliken atomic charges of the molecule were calculated by B3LYP and HF methods at the same level.

3. RESULTS AND DISCUSSION

3.1. Molecular Structure

The optimized molecular and chemical structure of the compound **1** were given in Fig. **1**. Similarly, the geometric parameters such as bond lenghts and bond angles of the compound **1**are listed in Tables**1** and **2**.

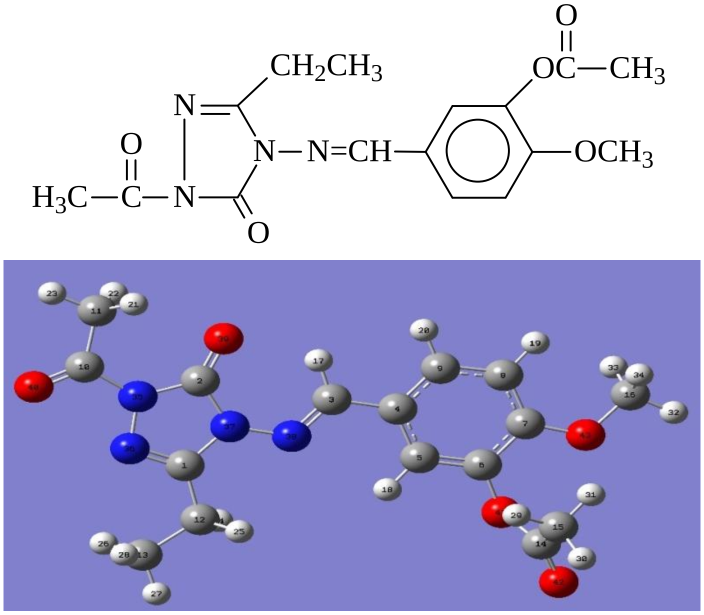


Fig. 1. The chemical structure and optimized molecular structure of compound**1.**

Table 1. The calculated bond lengths of compound **1**.

Bond Lengths		B3LYP	HF	Bond Lengths		B3LYP	HF
1	C(1)-N(36)	1.393	1.383	**23**	C(3)-C(4)	1.461	1.472
2	C(1)-N(37)	1.290	1.261	**24**	C(4)-C(5)	1.406	1.398
3	C(1)-C(12)	1.492	1.494	**25**	C(5)-H(18)	1.082	1.073
4	C(12)-H(24)	1.095	1.086	**26**	C(5)-C(6)	1.379	1.366
5	C(12)-H(25)	1.095	1.086	**27**	C(6)-O(41)	1.382	1.366
6	C(12)-C(13)	1.529	1.526	**28**	O(41)-C(14)	1.386	1.352
7	C(13)-H(26)	1.092	1.085	**29**	C(14)-O(42)	1.194	1.173
8	C(13)-H(27)	1.091	1.083	**30**	C(14)-C(15)	1.510	1.507
9	C(13)-H(28)	1.091	1.083	**31**	C(15)-H(29)	1.088	1.079
10	N(36)-N(35)	1.391	1.381	**32**	C(15)-H(30)	1.091	1.083
11	N(35)-C(10)	1.431	1.412	**33**	C(15)-H(31)	1.092	1.084
12	C(10)-O(40)	1.200	1.178	**34**	C(6)-C(7)	1.414	1.403
13	C(10)-C(11)	1.508	1.506	**35**	C(7)-O(43)	1.354	1.337
14	C(11)-H(21)	1.091	1.082	**36**	O(43)-C(16)	1.426	1.404
15	C(11)-H(22)	1.091	1.082	**37**	C(16)-H(32)	1.088	1.079
16	C(11)-H(23)	1.088	1.080	**38**	C(16)-H(33)	1.094	1.085
17	N(35)-C(2)	1.397	1.373	**39**	C(16)-H(34)	1.095	1.085
18	C(2)-O(39)	1.215	1.194	**40**	C(7)-C(8)	1.395	1.380
19	C(2)-N(37)	1.405	1.376	**41**	C(8)-H(19)	1.081	1.072
20	N(37)-N(38)	1.372	1.365	**42**	C(8)-C(9)	1.393	1.390
21	N(38)-C(3)	1.286	1.258	**43**	C(9)-H(20)	1.084	1.076
22	C(3)-H(17)	1.086	1.075	**44**	C(9)-C(4)	1.397	1.379

Table 2. The calculated bond angles of compound **1**.

	Bond Angles	B3LYP	HF		Bond Angles	B3LYP	HF
1	C(1)-N(36)-N(35)	105,647	105,938	**37**	C(3)-C(4)-C(5)	122,409	**122,288**
2	C(1)-N(37)-N(38)	121,258	121,148	**38**	C(3)-C(4)-C(9)	119,078	119,087
3	C(1)-N(37)-C(2)	108,272	108,219	**39**	C(4)-C(5)-H(18)	120,271	120,487
4	C(1)-C(12)-C(13)	113,085	112,973	**40**	C(4)-C(5)-C(6)	120,676	120,514
5	C(1)-C(12)-H(24)	108,112	107,872	**41**	H(18)-C(5)-C(6)	119,045	118,993
6	C(1)-C(12)-H(25)	108,107	107,861	**42**	C(5)-C(6)-O(41)	119,210	119,358
7	H(24)-C(12)-C(13)	110,953	105,997	**43**	C(5)-C(6)-C(7)	120,665	120,817
8	H(25)-C(12)-C(13)	110,978	110,908	**44**	C(6)-O(41)-C(14)	122,951	123,635
9	C(12)-C(13)-H(26)	109,831	110,919	**45**	O(41)-C(14)-C(15)	117,160	117,700
10	C(12)-C(13)-H(27)	111,206	109,468	**46**	O(41)-C(14)-O(42)	117,824	118,346
11	C(12)-C(13)-H(28)	111,216	111,215	**47**	O(42)-C(14)-C(15)	125,005	123,928
12	H(26)-C(12)-H(27)	108,528	111,198	**48**	C(14)-C(15)-H(29)	111,784	111,095
13	H(26)-C(12)-H(28)	108,505	108,544	**49**	C(14)-C(15)-H(30)	109,652	110,216
14	H(27)-C(12)-H(28)	107,457	108,561	**50**	C(14)-C(15)-H(31)	109,652	107,700
15	N(36)-C(1)- N(37)	111,710	107,771	**51**	H(29)-C(15)-H(30)	109,277	109,514
16	N(36)-N(35)- C(10)	119,032	119,218	**52**	H(29)-C(15)-H(31)	110,115	110,006
17	N(36)-N(35)- C(2)	112,187	111,713	**53**	H(30)-C(15)-H(31)	107,995	108,302
18	N(36)-C(1)-C(12)	125,439	105,938	**54**	O(41)-C(6)-C(7)	119,872	119,637
19	N(35)-C(10)-C(11)	115,828	116,738	**55**	C(6)-C(7)-O(43)	115,849	115,808
20	N(35)-C(10)-O(40)	119,719	116,695	**56**	C(6)-C(7)-C(8)	118,822	118,850
21	O(40)-C(10)-C(11)	124,453	126,567	**57**	C(7)-O(43)-C(16)	118,709	120,136
22	C(10)-C(11)-H(21)	111,155	110,912	**58**	O(43)-C(16)-H(32)	105,611	105,984
23	C(10)-C(11)-H(22)	111,185	110,919	**59**	O(43)-C(16)-H(33)	111,330	111,261
24	C(10)-C(11)-H(23)	107,256	106,939	**60**	O(43)-C(16)-H(34)	111,064	111,010
25	H(21)-C(11)-H(22)	106,342	107,178	**61**	H(32)-C(15)-H(33)	109,509	109,338
26	H(22)-C(11)-H(23)	110,68	110,465	**62**	H(32)-C(15)-H(34)	109,523	109,416
27	C(10)-N(35)-C(2)	110,487	110,465	**63**	H(33)-C(15)-H(34)	109,712	109,745
28	N(35)-C(2)-N(37)	102,183	102,689	**64**	O(43)-C(7)-C(8)	125,324	125,334
29	N(35)-C(2)-O(39)	129,858	129,480	**65**	C(7)-C(8)-H(19)	120,384	120,689
30	O(39)-C(2)-N(37)	127,958	127,831	**66**	C(7)-C(8)-C(9)	120,147	119,998
31	C(2)-N(37)-N(38)	130,469	130,630	**67**	H(19)-C(8)-C(9)	119,469	119,312
32	N(37)-C(1)-C(12)	122,851	122,695	**68**	C(8)-C(9)-H(20)	119,208	118,868
33	N(37)-N(38)-C(3)	119,466	120,387	**69**	C(8)-C(9)-C(4)	118,511	118,624
34	N(38)-C(3)-H(17)	122,222	122,616	**70**	H(20)-C(9)-C(4)	119,615	119,937
35	N(38)-C(3)-C(4)	120,284	120,395	**71**	C(9)-C(4)-C(5)	118,511	118,624
36	H(17)-C(3)-C(4)	117,493	116,989				

3.2. NMR spectral analysis

In nuclear magnetic resonance (NMR) spectroscopy, the isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties which provide the accurate predictions of molecular geometries [16–18]. In this study, the optimized molecular geometries of the compound **1**were obtained by using B3LYP and HF methods with 6–311G(d, p) basis level in DMSO solvent. Depending upon the optimized molecular geometries of the compound **1**the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital (GIAO) method. Theoretically and experimentally [19] values were plotted according to δ exp=a. δ calc.+ b, Eq. **a** and **b** constants regression coefficients with a standard error values were found using the SigmaPlot program. The correlation graphics are given Fig. **2** and the linear correlation data of the compound **1** by considering the results are given in Table **3**.

Table 3. The calculated and experimental [19] ^{13}C and ^{1}H NMR isotropic chemical shifts of compound**1**(with respect to TMS, all values in ppm).

No	Experimental	DFT/6311G(d.p)	Difference	HF/6311G(d.p)	Difference
H17	9,48	10,07	-0,59	9,99	-0,51
H18	7,73	8,02	-0,29	8,71	-0,98
H19	7,27	7,00	0,27	7,30	-0,03
H20	7,63	7,49	0,14	8,14	-0,51
H21	2,50	1,99	0,51	2,28	0,22
H22	2,50	2,61	-0,11	2,79	-0,29
H23	2,50	2,61	-0,11	2,79	-0,29
H24	2,74	2,82	-0,08	2,89	-0,15
H25	2,74	2,82	-0,08	2,90	-0,16
H26	1,23	1,24	-0,01	1,54	-0,31
H27	1,23	1,26	-0,03	1,56	-0,33
H28	1,23	1,26	-0,03	1,57	-0,34
H29	2,29	1,57	0,72	1,91	0,38
H30	2,29	1,86	0,43	1,92	0,37
H31	2,29	2,03	0,26	2,00	0,29
H32	3,86	3,65	0,21	3,69	0,17
H33	3,86	3,85	0,01	3,90	-0,04
H34	3,86	4,17	-0,31	4,23	-0,37

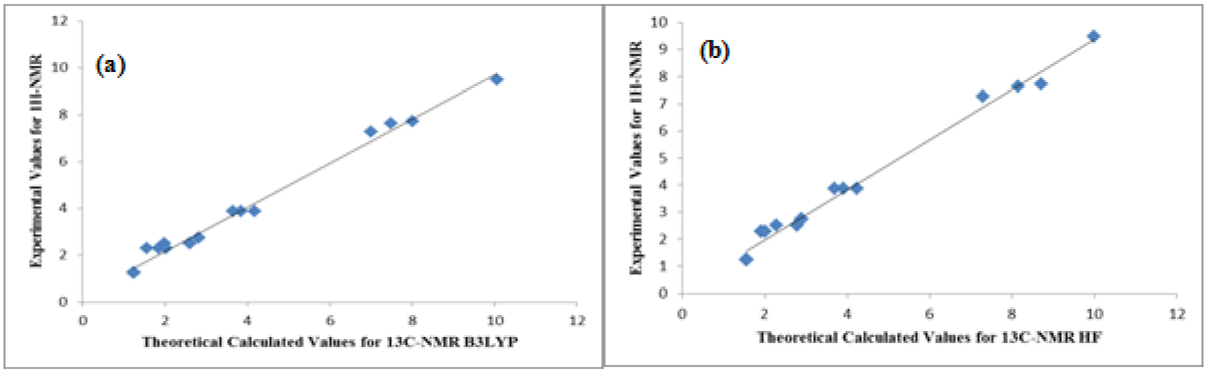


Fig. 2. The correlation graphics for and ^{1}H-NMR chemical shifts of compound 1 with DFT/B3LYP/6–311G(d, p) (a) and HF/B3LYP/6–311G(d, p) (b) levels.

3.3. Analysis of vibrational modes

The number of potentially active fundamentals of non-linear molecule which have N atoms is equal to (3N-6) apart from three translational and three rotational degrees of freedom[20]. The 1-acetyl-3-ethyl-4-(3-hydroxy-4-methoxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one molecule has 45atoms and therefore the normal vibration numbers are 123. The observed [19] and calculated vibrational frequenciesof compound **1**arelisted in Table **4**. Furthermore, the simulated spectra by using B3LYP/6–311G(d, p) and HF/6–311G(d, p) levels of the compound **1**under investigation are given in Fig. **3**.

Table 4. The calculated frequencies values of compound **1**.

Comp. 1	VibrationTypes	scaledDFT	scaledHF
1	τNCNN(25), τCCCN(12), τCNNC(17)	12	11
2	τNCNN(18), τ CCNN(14), τCOCC(11), τCCCN(18)	27	26
3	δCCN(17), τ CCOC(20)	34	33
4	τCCNC(37), τCOCC(10)	51	49
5	δCCN(10), τCCOC(39), τ CCNC(11)	53	52
6	τCCNN(10), τCCCN(39), τCCOC(14), τCCNC(11)	59	58
7	τCCOC(12), τCOCC(40),	67	65
8	τCCCN(25), τCCNC(25), τNCNN(11)	74	73
9	τCOCC(21), τCCCN(10)	97	90
10	δOCC(10), τOCCC(11)	110	106
11	τ CCNN(20), τ NCNN(11), τ CNNC(14)	122	122
12	δ CCN(15), δ NCN(10)	125	123
13	δ CCN(14), δ NNC(12)	133	134
14	τ HCCO(46)	143	146
15	τ CNNC(12), τ NCNN(18)	150	156
16	τ CCCN(32)	159	171
17	τ HCCN(64)	181	176
18	δ OCC(13), δ COC(14), δ NCN(10)	190	189
19	τ NCNN(12), τ CCCN(12), τ HCCN(10)	220	220
20	τ NCNN(12), τ HCCN(29)	233	234
21	δ OCC(10), δ NCN(11), τ HCCO(28)	237	239
22	τ HCCO(11)	247	252
23	δ CCC(21), δ OCC(11), δ NCN(10)	267	270
24	τ NCNN(12), τ CCNN(26)	319	320
25	δ COC(12), δ OCC(13)	325	326
26	τ CCNN(14), τ CNNC(36)	350	354
27	δ CCC(12), δ CCN(10), δ OCC(20)	361	365
28	δ CCN(15), δ NNC(11), δ OCN(35)	364	371
29	ν OC(14), δ CCO(18), δ COC(14)	374	379
30	δ CCO(10), δ CCC(21), δ CNN(10)	414	419
31	τ OCCC(16), τ CCNN(14), τ CCCN(25)	420	425
32	δ CCN(10), δ OCC(14)	436	442
33	ν NC(12), δ CCN(15)	444	449
34	δ OCC(26), τ OCCC(23), τ HCCC(10)	495	508
35	δ CNN(14)	535	540
36	δ COC(12), δ OCC(13)	552	564
37	τ HCCO(17)	562	575
38	τ ONNC(30), τ OCOC(34), τ HCCN(16)	567	580
39	ν CC(26), δ OCC(38)	594	601
40	τ CCCC(20), τ OCCC(14)	604	613
41	δ OCC(14)	628	635
42	δ CCC(10), τ NCNN(10), τ CNNC(20)	634	647
43	δ CCC(19), τ CCCC(11)	646	654
44	ν CC(12), δ CCN(17), δ NCN(13), δ OCN(15)	702	710
45	ν OC(12), CC(12), τ OCCC(10)	711	724
46	ν OC(10), δ CCC(17)	721	760
47	ν CC(11), τ OCCC(30), τ HCCC(10)	748	768
48	τ ONNC(34), τ HCCN(15)	755	771
49	τ ONNC(11), τ HCCN(32)	777	792
50	ν NC(17), ν NN(14), δ NNC(14)	785	799
51	τ OCCC(13), τ HCCC(68)	801	840
52	ν OC(10), ν CC(16)	833	847

Comp. 1	VibrationTypes	scaled DFT	scaled HF
53	ν CC(11), δ OCN(12)	880	895
54	τ HCCC(43)	894	934
55	ν CC(35)	919	950
56	ν CC(10), τ HCCN(16)	940	968
57	ν CC(15)	960	974
58	ν CC(15), τ HCCO(14)	973	981
59	ν CC(10), δ CCC(12)	977	1010
60	τ HCNN(88)	986	1033
61	ν OC(45), τ HCCO(11)	1019	1050
62	δ HCH(19), τ HCCN(52), τ ONNC(10)	1026	1053
63	ν OC(16), δ HCH(14), τ HCCO(24), τ OCOC(17)	1029	1058
64	ν NC(11), δ HCH(11), τ HCCN(15), τ HCCC(16)	1037	1063
65	ν NC(14), ν CC(13)	1061	1079
66	δ HCC(37), τ HCCN(19), τ HCCC(11)	1079	1098
67	ν CC(23), δ HCC(11)	1107	1115
68	ν NN(21), τ HCCN(22)	1120	1141
69	ν OC(12), ν CC(13), δ HCC(15)	1136	1152
70	δ HCH(13), τ HCOC(50)	1145	1162
71	ν CC(20), δ HCC(11)	1157	1168
72	τ HCOC(18), τ HCOC(22)	1170	1198
73	ν OC(12), ν CC(13), δ OCC(12)	1173	1220
74	ν NC(16), ν NN(18)	1206	1235
75	ν OC(17), δ HCC(32)	1224	1237
76	δ HCC(37)	1243	1262
77	δ HCC(48), τ HCCN(16)	1257	1262
78	ν (16)	1258	1287
79	ν CC(18), ν OC(28), δ HCC(16)	1269	1305
80	ν NC(23), ν NN(12)	1285	1313
81	ν NC(23), ν NN(10), δ NNC(12)	1307	1357
82	δ HCN(15), δ HCH(15)	1350	1386
83	δ HCN(10), δ HCH(28)	1361	1387
84	δ HCH(75)	1365	1397
85	δ HCN(18), δ HCH(34)	1379	1404
86	δ HCH(72), τ HCCN(23)	1495	1428
87	ν CC(12), δ HCC(11)	1409	1432
88	δ HCH(16)	1413	1439
89	δ HCN(11), δ HCH(35)	1426	1440
90	δ HCH(76), τ HCCN(23)	1427	1445
91	δ HCH(39)	1430	1452
92	δ HCH(62), HCCO(20)	1433	1454
93	δ HCH(52)	1439	1459
94	δ HCH(38)	1448	1459
95	δ HCH(51), τ HCOC(13)	1449	1470
96	δ HCH(26)	1457	1473
97	τ HCOC(12)	1461	1476
98	ν OC(11), δ HCC(32), δ CCC(10)	1493	1524
99	ν CC(35)	1554	1600
100	ν CC(56), δ HCC(16)	1589	1632
101	ν NC(48)	1604	1701
102	ν NC(45)	1617	1710
103	ν OC(39)	1727	1764
104	ν OC(49)	1769	1827
105	ν OC(89)	1608	1846

Comp. 1	VibrationTypes	scaled DFT	scaled HF
106	ν CH(68)	2919	2874
107	ν CH(59)	2939	2883
108	ν CH(68)	2952	2892
109	ν CH(50)	2960	2901
110	ν CH(97)	2960	2905
111	ν CH(60)	2961	2917
112	ν CH(53)	2981	2934
113	ν CH(36)	3017	2943
114	ν CH(45)	3021	2955
115	ν CH(35)	3022	2963
116	ν CH(100)	3023	2969
117	ν CH(48)	3048	2990
118	ν CH(79)	3058	2993
119	ν CH(97)	3058	2993
120	ν CH(26)	3058	3020
121	ν CH(33)	3076	3041
122	ν CH(52)	3108	3058
123	ν NH(100)	3109	3059

ν, stretching; δ, bending; δ_s, scissoring; ρ, rocking; γ, out-of-plane bending; τ, torsion

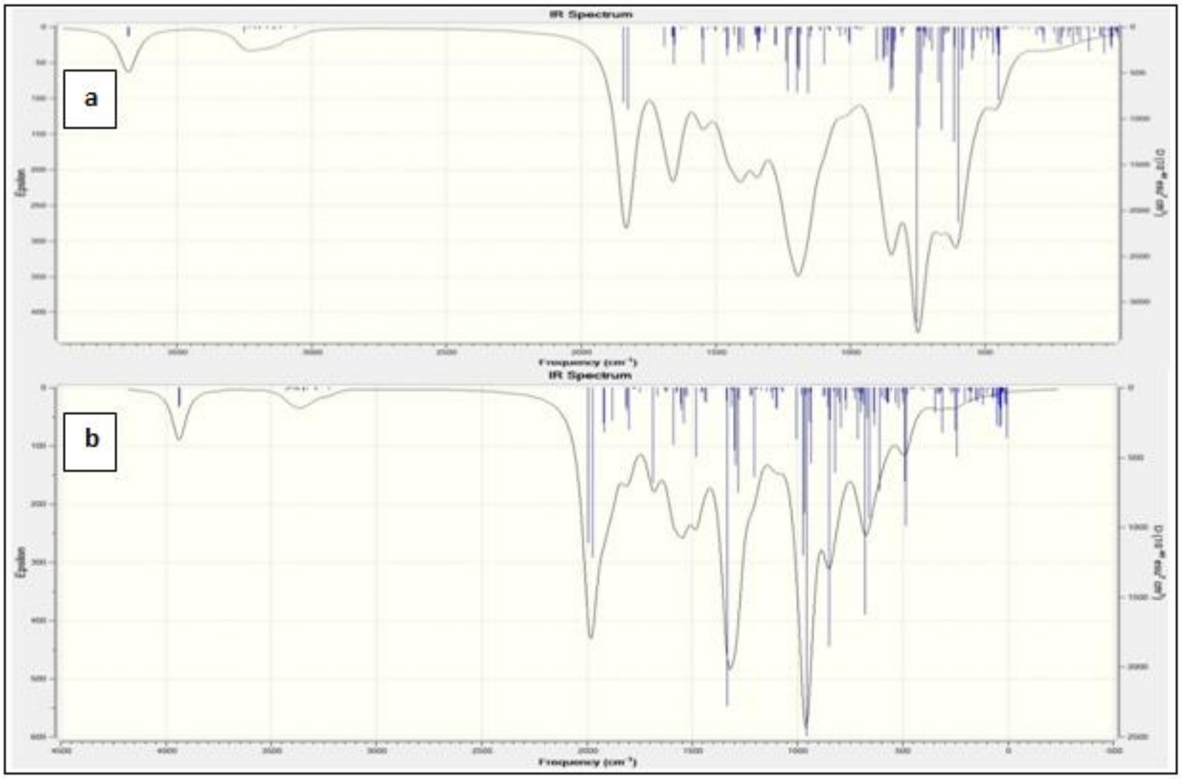


Fig. 3. IR spectra of compound **1** (**a:** DFT/B3LYP/6–311G(d, p)and **b:** HF/B3LYP/6–311G(d, p)).

3.4. UV–visible Spectroscopy and HOMO–LUMO Analyses

The theoretical absorption wavelengths of the compound **1**in ethanol are given in Table **5** and the graphics are given in Fig.**4**. The excitation energies, oscillator strengths (*f*) and absorption wavelengths (λ) of UV–vis absorption spectra of the compound **1**have been calculated by using TD–SCF/B3LYP and TD–SCF/HF methods. The calculated absorption wavelengths for the compound **1**were found as 310.60/239.74, 275.14/216.93, 267.76/193.23 nm in ethanol, respectively.

It is well known that the highest occupied molecular orbital (HOMO) which implies the outermost orbital filled by electrons and behaves as an electron donor and lowest unoccupied molecular orbital (LUMO) which can be thought as the first empty innermost orbital unfilled by electron and behaves as an electron acceptor are called as the frontier molecule orbitals (FMOs) [21]. Therefore, the energy of the HOMO is directly related to the ionization potential and represents the ability of electron giving. But, LUMO energy is directly related to the electron affinity and represents the ability of electron accepting. The formed energy gap between HOMO and LUMO indicates the molecular chemical stability and is a critical parameter to determine molecular electrical transport properties [21]. In our study, HOMO, LUMO values and 3D plots of this HOMOs and LUMOswere given in Fig.**5**.

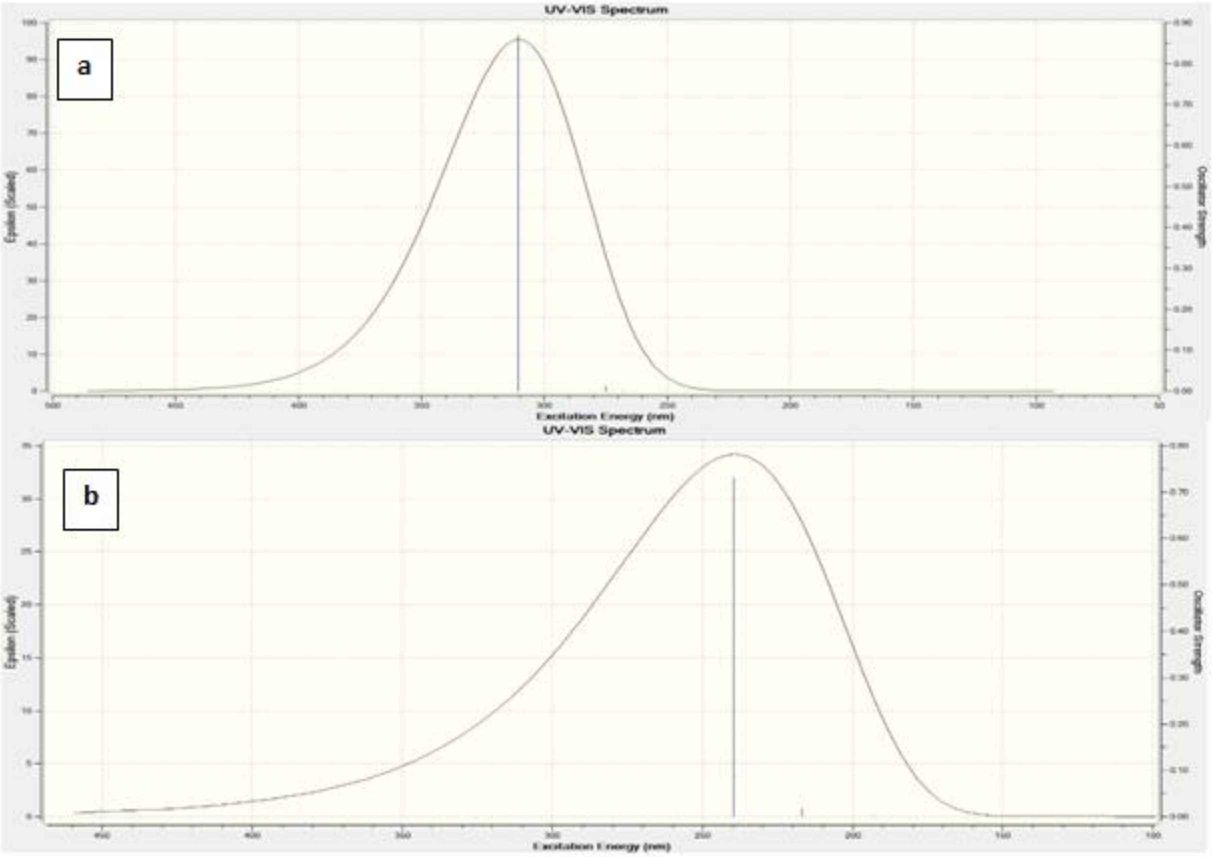
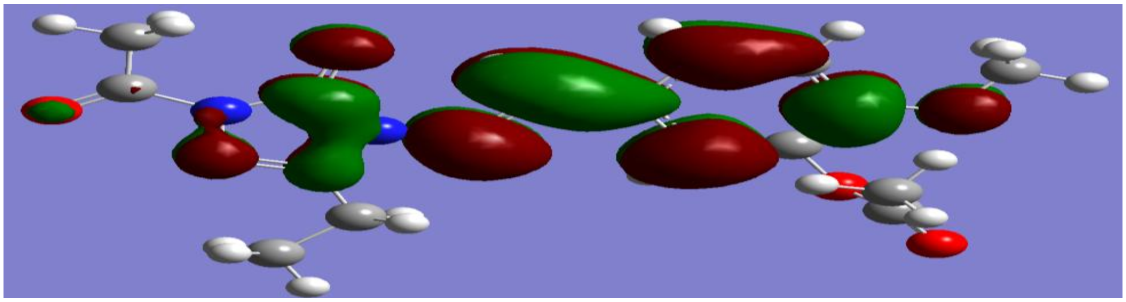


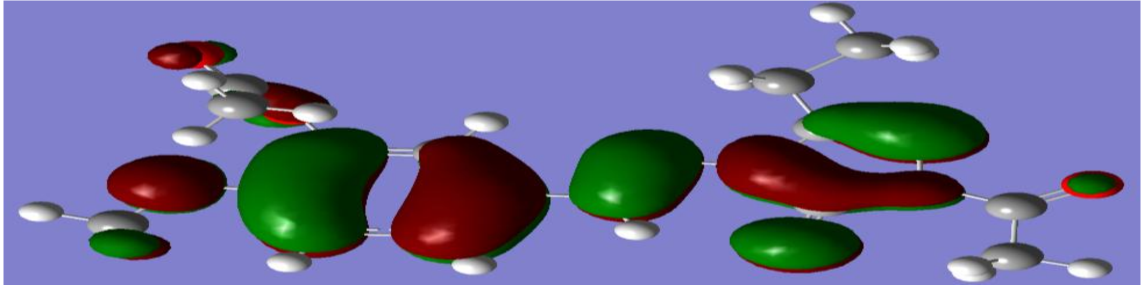
Fig. 4. UV-Visible spectra (a and b) simulated with DFT/B3LYP/6–311G(d, p) and HF/B3LYP/6–311G(d, p) levels of compound **1**.

Tablo 5. The calculated UV-vis values with B3LYP/6–311G(d, p) and HF/6–311G(d, p) level in ethanol

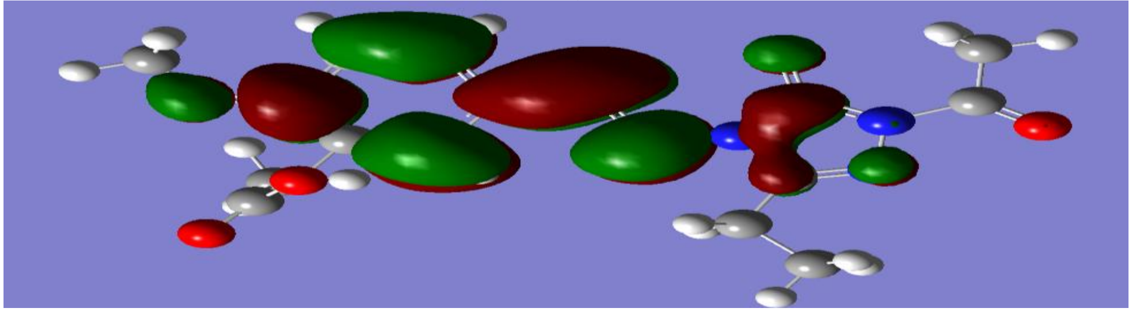
λ (nm)	Excitation energy (eV)	*f* (oscillator strength)
310.60/239.74	3.9917/5.1716	0.8699/0.7310
275.14/216.93	4.5062/5.7153	0.0116/0.0163
267.76/193.23	4.6305/6.4163	0.0002/0.0011



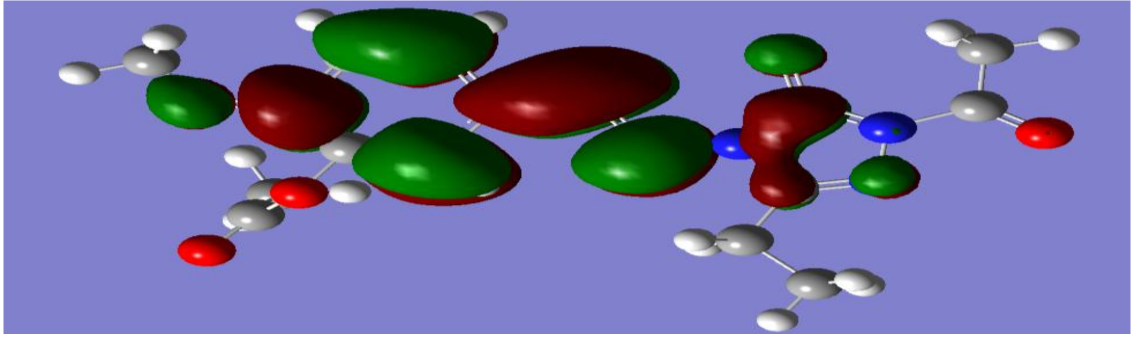
E_{LUMO} (B3LYP) : -0,07505 Hatree



E_{HOMO} (B3LYP) : -0,23506 Hatree



E_{LUMO} (HF) : 0,07025 Hatree



E_{HOMO} (HF) : -0,32231 Hatree

Fig. 5. The calculated HOMO-LUMO energies of compound **1** according to DFT/B3LYP/6–311G(d, p) and HF /6–311G(d, p) levels

3.5. Dipole moment and total energy

The energetic behavior of title molecule was investigated in vacum. Dipol moments and total energy values of title molecule were calculated by using B3LYP/6-311G(d, p) and HF/6-311G(d, p) level. The calculated dipole moments and total energy values are given in Table 6 and 7.

Table 6. The calculated dipole moment values of compound **1**.

Dipole Moment	**B3LYP**	**HF**
μ_x	-1.8364	-5.7657
μ_y	3.0225	-2.2041
μ_z	2.313	-2.9049
μ_{Toplam}	4.2263	6.8220

Table 7. The total energy of the of compound **1**.

Energy	**B3LYP**	**HF**
(a.u.)	-1215.962	-1208.746

4.CONCLUSION

The molecular structures, vibrational frequencies, ^{1}H and ^{13}C-NMR chemicals shifts, UV–vis spectra, HOMO and LUMO analyses of 1-acetyl-3-ethyl-4-(3-hydroxy-4-methoxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one molecule have been calculated by using DFT/B3LYP and HF methods. By considering the results of experimental works it can be easily stated that the vibrational frequencies and 13C and 1H NMR chemical shifts spectroscopic parameters obtained theoretically are in a very good agreement with the experimental data.

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