Kafkas Üniv Fen Bil Enst Derg.
6: 1-16, 2013

A Study on Theoretical and Experimentical Spectroscopic Properties 1-Methyl-3-benzyl-4-(3-ethoxy-4-methoxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one

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Yayın Kodu: 6-1A

ABSTRACT: In this study, theoretically spectral values of 1-methyl-3-benzyl-4-(3-ethoxy-4-methoxybenzylidenamino)-4,5-dihydro-*1H*-1,2,4-triazol-5-one were calculated and these values were compared with experimental values and obtained conclusions were evaluated. For this purpose, firstly, 1-methyl-3-benzyl-4-(3-ethoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one has been optimized using B3LYP/6-311G(d,p) and HF/6-311G(d,p) basis set. ^{1}H-NMR and ^{13}C-NMR spectral values according to GIAO method was calculated using Gaussian G09W program package in gas phase and in DMSO solvent. Theoretically and experimentally 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 Sigma plot program. Theoretically calculated IR values of this compound were calculated in gas phase by using of 6-311G(d,p) basis sets of B3LYP and HF methods and are multiplied with appropriate scale factors and the values obtained according to B3LYP and HF methods are formed using theoretical infrared spectrum. The identification of calculated IR values were used veda4f program. UV-vis values in ethanol were calculated. In addition, bond angles, bond lengths, dipole moments, the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) energy, mulliken charges and total energy of the molecule were calculated with both methods. The calculated and experimental results were exhibited a very good agreement.

Keywords: 1,2,4-triazol-5-on, Gaussian 09W, GIAO, B3LYP, HF, 6-311G(d,p) basic set

1-Metil-3-benzil-4-(3-etoksi-4-metoksibenzilidenamino)-4,5-dihidro-1H-1,2,4-triazol-5-on'un Teorik ve Deneysel Spektroskopik Özellikleri Üzerine Bir Çalışma

ÖZET: Bu çalışmada, 1-metil-3-benzil-4-(3-etoksi-4-metoksibenzilidenamino)-4,5-dihidro-1H-1,2,4-triazol-5-on'un teorik spektral verileri hesaplanmıştır. Bu değerler deneysel verilerle mukayese edilmiş ve elde edilen sonuçlar değerlendirilmiştir. Bu amaçla, öncelikle, 1-metil-3-benzil-4-(3-etoksi-4-metoksibenzilidenamino)-4,5-dihidro-1H-1,2,4-triazol-5-on B3LYP/6-311G(d,p) ve HF/6-311G(d,p) temel setleri kullanılarak optimize edilmiştir. GIAO metoduna göre ^{1}H-NMR ve ^{13}C-NMR spectral verileri DMSO çözücüsünde Gaussian G09W programı kullanılarak hesaplanmıştır. Deneysel ve teorik değerler δ exp=a+b. δ calc. eşitliğine göre grafiğe geçirilmiştir. Standart hata değerleri a ve b sabitlerinin regresyon katsayısı ile Sigmaplot programı kullanılarak bulunmuştur. Bu bileşiğin teorik olarak hesaplanmış IR değerleri basis sets of B3LYP ve HF metodlarının 6-311G(d,p) temel seti kullanılarak gaz fazda hesaplanmıştır. IR verilerini belirlenmesinde Veda 4f programı kullanılmıştır. İlaveten, molekülün bağ açıları, bağ uzunlukları, dipol momentleri, HOMO-LUMO enerjileri, mulliken yükleri ve molekülün toplam enerjileri her iki metodla hesaplanmıştır. Hesaplanan ve deney sonuçları çok iyi bir şekilde uyumlu olduğu görülmüştür.

Anahtar Kelimeler: 1,2,4-triazol-5-on, Gaussian 09W, GIAO, B3LYP, HF, 6-311G(d,p) basic set

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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 (Frisch et al., 2009; Wolinski, Hilton & Pulay, 1990). 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 have revealed that the DFT and HF have a great accuracy in reproducing the experimental values in geometry, vibrational frequency, NMR chemical shifts etc. (Yüksek et al., 2005a; 2005b; Yüksek et al., 2005).

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 **2**, were 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 (Frisch et al., 2009; Wolinski, Hilton & Pulay, 1990).

For the vibrational computations, molecular structures of the compound **2** were calculated by using Becke–3–Lee Yang Parr (B3LYP) (Becke, 1993; Lee, Yang & Parr, 1988) density functional 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 (Scott & Radom, 1996). The veda4f program, was used in defining IR data, which were calculated theoretically (Jamroz, 2004).

For the NMR calculations, the optimized molecular geometries of the compound were obtained at 6–311G(d, p) basis level in DMSO solvent by using GIAO method. Then, ^{1}H and ^{13}C NMR chemical shifts for the compound were calculated at B3LYP/6–31G(d) and HF levels in solvent by using gauge invariant atomic orbital (GIAO) method (Ditchfield, 1974; London, 1937; Wolinski, Hilton & Pulay, 1990). The UV–vis spectroscopic calculations of the mentioned molecule were performed by using TD–SCF/B3LYP and TD–SCF/HF method in ethanol solvent (Vlcek &Zalis, 2007). In additional, HOMO and LUMO energy values and energy gaps for the compound were calculated by using B3LYP and HF methods with 6–311G(d, p) basis set. Finally, mulliken atomic charges of the molecule under investigation were calculated by B3LYP and HF method at the same level.

RESULTS AND DISCUSSION

Molecular Structure

The optimized molecular structures and chemical structure of the compound were given in Figure **1**. Similarly, the optimized molecular geometric parameters such as bond angles bond and lenghts of the compound by using B3LYP/6–311G(d, p) and HF/6–311G(d, p) levels are listed in Table **1** and Table **2**.

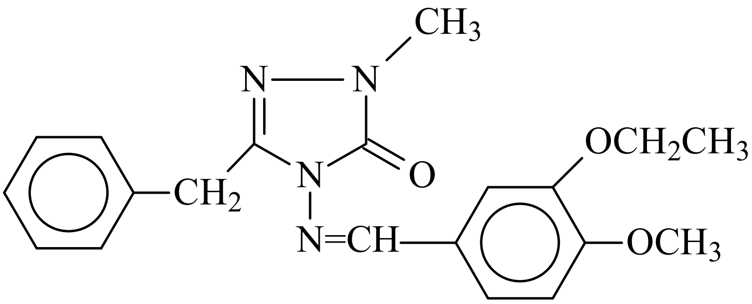


Figure 1. Structural formula of molecule

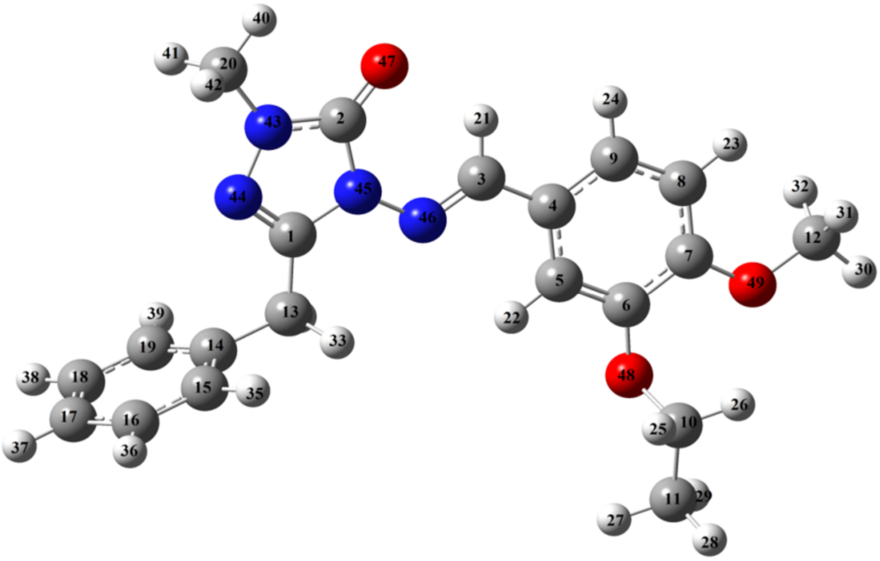


Figure 2. The optimized molecular structure of the molecule with DFT/B3LYP/6311G(d,p) level

Table1. The calculated bond angles of the compound

	Bond Angles	B3LYP	HF		Bond Angles	B3LYP	HF
1	C(1)-N(44)-N(43)	105.34	105.66	36	N(45)-C(1)-C(13)	122.34	122.03
2	C(1)-N(45)-N(46)	121.41	121.23	37	N(45)-N(46)-C(3)	118.95	119.86
3	C(1)-N(45)-C(2)	108.00	107.83	38	N(46)-C(3)-H(21)	121.79	122.19
4	C(1)-C(13)-H(33)	108.16	107.88	39	N(46)-C(3)-C(4)	120.57	120.71
5	C(1)-C(13)-H(34)	108.15	107.87	40	H(21)-C(3)-C(4)	117.64	117.10
6	C(1)-C(13)-C(14)	113.70	113.79	41	C(3)-C(4)-C(5)	122.61	122.49
7	H(33)-C(13)-C(14)	110.56	110.55	42	C(3)-C(4)-C(9)	118.93	118.92
8	H(34)-C(13)-C(14)	110.54	110.54	43	C(4)-C(5)-H(22)	120.16	120.28
9	C(13)-C(14)-C(15)	120.60	120.63	44	C(4)-C(5)-C(6)	121.31	121.10
10	C(13)-C(14)-C(19)	120.69	120.61	45	H(22)-C(5)-C(6)	118.52	118.62
11	C(14)-C(15)-H(35)	119.50	119.67	46	C(5)-C(6)-O(48)	119.26	119.92
12	C(14)-C(15)-C(16)	120.76	120.72	47	C(5)-C(6)-C(7)	119.71	119.96

13	H(35)-C(15)-C(16)	119.74	119.61	48	O(48)-C(6)-C(7)	120.94	120.08
14	C(15)-C(16)-H(36)	119.82	119.78	49	C(6)-C(7)-O(49)	115.94	115.96
15	C(15)-C(16)-C(17)	120.07	120.12	50	C(6)-C(7)-C(8)	119.28	119.22
16	H(36)-C(16)-C(17)	120.11	120.10	51	O(49)-C(7)-C(8)	124.78	124.82
17	C(16)-C(17)-H(37)	120.20	120.21	52	C(7)-C(8)-H(23)	120.44	120.75
18	C(16)-C(17)-C(18)	119.62	119.57	53	C(7)-C(8)-C(9)	120.23	120.13
19	H(37)-C(17)-C(18)	120.18	120.22	54	H(23)-C(8)-C(9)	119.32	119.12
20	C(17)-C(18)-H(38)	120.09	120.11	55	C(8)-C(9)-H(24)	119.31	118.97
21	C(17)-C(18)-C(19)	120.11	120.12	56	C(8)-C(9)-C(4)	121.00	121.02
22	H(38)-C(18)-C(19)	119.80	119.78	57	H(24)-C(9)-C(4)	119.69	120.02
23	C(18)-C(19)-H(39)	119.76	119.61	58	C(9)-C(4)-C(5)	118.46	118.58
24	C(18)-C(19)-C(14)	120.72	120.72	59	C(6)-O(48)-C(10)	116.47	116.45
25	H(39)-C(18)-C(14)	119.52	119.68	60	O(48)-C(10)-H(25)	108.87	109.16
26	N(44)-N(43)-C(20)	121.07	120.80	61	O(48)-C(10)-H(26)	109.68	109.72
27	N(43)-C(20)-H(40)	107.26	107.75	62	H(25)-C(10)-C(11)	111.11	110.89
28	N(43)-C(20)-H(41)	110.41	110.23	63	H(26)-C(10)-C(11)	111.06	110.77
29	N(43)-C(20)-H(42)	110.42	110.23	64	C(10)-C(11)-H(27)	110.69	110.57
30	C(20)-N(43)-C(2)	125.47	126.36	65	C(10)-C(11)-H(28)	110.23	110.17
31	N(44)-C(1)-C(13)	125.34	126.88	66	C(10)-C(11)-H(29)	110.38	110.30
32	N(43)-C(2)-N(45)	101.94	102.58	67	C(7)-O(49)-C(12)	118.54	119.87
33	N(43)-C(2)-O(47)	129.45	129.19	68	O(49)-C(12)-H(30)	111.28	111.27
34	O(47)-C(2)-N(45)	128.62	128.22	69	O(49)-C(12)-H(31)	111.48	111.42
35	C(2)-N(45)-N(46)	130.60	130.94	70	O(49)-C(12)-H(32)	105.75	106.12

Table 2. The calculated bond lengths of the compound

	Bond Lenghts (A^{0})	**B3LYP**	**HF**		**Bond Lenghts (A^{0})**	**B3LYP**	**HF**
1	C(1)-N(44)	1.2957	1.2659	25	N(45)-C(2)	1.4168	1.3865
2	C(1)-N(45)	1.3870	1.3777	26	N(45)-N(46)	1.3720	1.3655
3	C(1)-C(13)	1.4982	1.4989	27	N(46)-C(3)	1.2863	1.2586
4	C(13)-H(33)	1.0950	1.0846	28	C(3)-H(21)	1.0869	1.0752
5	C(13)-H(34)	1.0944	1.0845	29	C(3)-C(4)	1.4608	1.4717
6	C(13)-C(14)	1.5127	1.5122	30	C(4)-C(5)	1.4064	1.3992
7	C(14)-C(15)	1.3966	1.3873	31	C(4)-C(9)	1.3963	1.3783
8	C(14)-C(19)	1.3969	1.3872	32	C(5)-H(22)	1.0823	1.0730
9	C(15)-H(35)	1.0852	1.0763	33	C(5)-C(6)	1.3814	1.3686
10	C(15)-C(16)	1.3928	1.3841	34	C(6)-O(48)	1.3699	1.3540
11	C(16)-H(36)	1.0844	1.0756	35	C(6)-C(7)	1.4180	1.4077
12	C(16)-C(17)	1.3929	1.3844	36	C(7)-O(49)	1.3590	1.3410
13	C(17)-H(37)	1.0842	1.0754	37	C(7)-C(8)	1.3948	1.3802
14	C(17)-C(18)	1.3932	1.3842	38	C(8)-H(23)	1.0815	1.0721
15	C(18)-H(38)	1.0844	1.0756	39	C(8)-C(9)	1.3936	1.3912
16	C(18)-C(19)	1.3924	1.3843	40	C(9)-H(24)	1.0845	1.0757
17	C(19)-H(39)	1.0851	1.0763	41	O(48)-C(10)	1.4414	1.4149
18	N(44)-N(43)	1.3805	1.3700	42	C(10)-C(11)	1.0931	1.5128
19	N(43)-C(20)	1.4454	1.4397	43	C(10)-H(25)	1.0972	1.0842
20	C(20)-H(40)	1.0894	1.0800	44	C(10)-H(26)	1.5156	1.0877
21	C(20)-H(41)	1.0922	1.0834	45	C(11)-H(27)	1.0921	1.0844
22	C(20)-H(42)	1.0922	1.0834	46	C(11)-H(28)	1.0922	1.0862
23	N(43)-C(2)	1.3695	1.3449	47	C(11)-H(29)	1.0933	1.0847
24	C(2)-O(47)	1.2202	1.2001				

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 (Rani et al., 2010; Subramanian, Sundaraganesan & Jayabharathi, 2010; Wade, 2006). In this framework, the optimized molecular geometry of the compound was obtained by using B3LYP and HF methods with 6–311G(d, p) basis level in DMSO solvent. By considering the optimized molecular geometry of the compound**.** the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital (GIAO) method. Theoretical and experimental (Yüksek et al., 2005) 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 Figure **2** and the linear correlation data of the compound by considering the results are given in Table **3**.

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

No	Experimental	DFT/631d/DMSO	Fark/DMSO	HF/631d/DMSO	Fark/DMSO
C1	148,40	169,12	-20,72	160,27	-11,87
C2	149,72	171,09	-21,37	160,59	-10,87
C3	153,88	170,75	-16,87	162,30	-8,42
C4	125,95	148,91	-22,96	133,20	-7,25
C5	111,64	139,33	-27,69	131,62	-19,98
C6	144,82	171,98	-27,16	154,71	-9,89
C7	152,05	180,50	-28,45	165,36	-13,31
C8	109,27	130,94	-21,67	117,51	-8,24
C9	126,94	151,29	-24,35	142,19	-15,25
C10	63,81	87,64	-23,83	67,31	-3,50

C11	14,81	33,16	-18,35	21,43	-6,62
C12	55,74	72,43	-16,69	54,17	1,57
C13	31,25	53,06	-21,81	35,73	-4,48
C14	135,90	157,88	-21,98	145,45	-9,55
C15	128,95	151,87	-22,92	140,80	-11,85
C16	128,65	149,85	-21,20	139,10	-10,45
C17	123,56	148,51	-24,95	137,53	-13,97
C18	128,65	149,78	-21,13	139,14	-10,49
C19	128,95	152,14	-23,19	140,76	-11,81
C20	32,12	47,38	-15,26	33,27	-1,15
H21	9,55	10,82	-1,27	10,05	-0,50
H22	7,58	8,73	-1,15	8,61	-1,03
H23	7,08	7,61	-0,53	7,21	-0,13
H24	7,20	8,05	-0,85	7,96	-0,76
H25	4,11	4,22	-0,11	3,46	0,65
H26	4,11	5,28	-1,17	3,94	0,17
H27	1,42	1,86	-0,44	1,35	0,07
H28	1,42	2,13	-0,71	1,72	-0,30
H29	1,42	2,13	-0,71	1,73	-0,31
H30	3,87	4,36	-0,49	3,66	0,21
H31	3,87	4,46	-0,59	3,78	0,09
H32	3,87	4,86	-0,99	4,21	-0,34
H33	4,11	4,74	-0,63	4,14	-0,03
H34	4,11	4,75	-0,64	4,15	-0,04
H35	7,35	8,23	-0,88	7,97	-0,62
H36	7,50	8,30	-0,80	8,01	-0,51
H37	7,30	8,24	-0,94	7,94	-0,64
H38	7,50	8,31	-0,81	8,01	-0,51
H39	7,35	8,24	-0,89	7,97	-0,62
H40	3,42	3,58	-0,16	3,03	0,39
H41	3,42	3,60	-0,18	3,03	0,39
H42	3,42	4,36	-0,94	3,78	-0,36

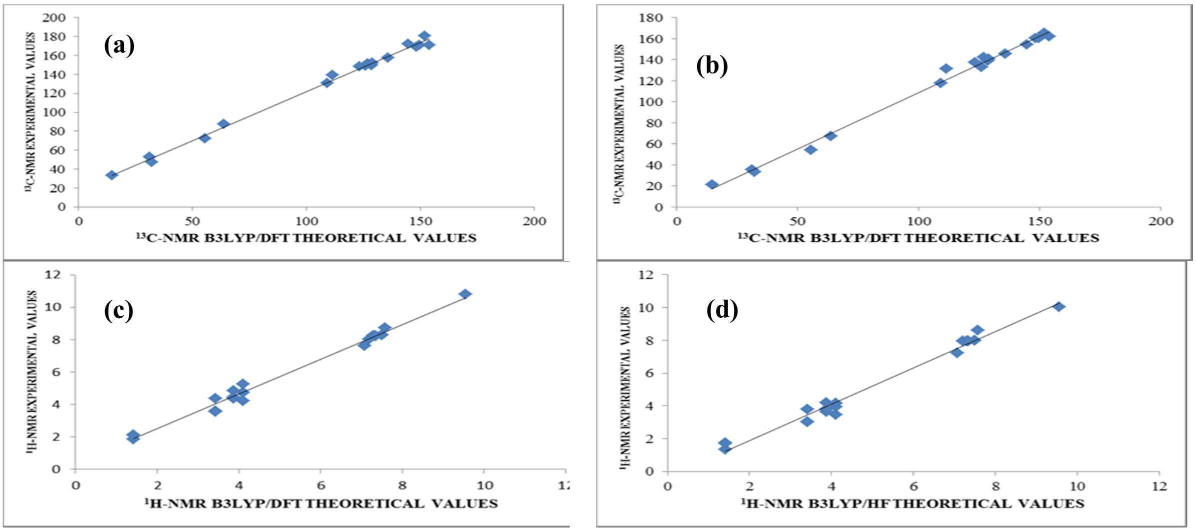


Figure 2. The correlation graphics for ^{1}H-NMR and ^{13}C-NMR chemical shifts of the compound with DFT/B3LYP/6–311G(d, p) (a, c) and HF/B3LYP/6–311G(d, p) (b, d) levels.

Analysis of vibrational modes

Investigation of vibrational wavenumbers of the chemical compounds plays a primary role in the spectral analysis. In spectroscopic field, the vibrational spectra of substituted benzene derivatives have been greatly investigated by various spectroscopic, since the single substitution can have a tendency to put greater changes in vibrational wavenumbers of benzene (Tereci et al., 2012; Pir et al., 2013a; 2013b). 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. The 1-methyl-3-benzyl-4-(3-ethoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule has 49 atoms and therefore the normal vibration numbers are 141. The experimental (Yüksek et al., 2005) and calculated vibrational frequencies of the compound were summarized in Table **4**. Furthermore, the simulated spectra by using B3LYP/6–311G(d, p) and HF/6–311G(d, p) levels of the compound under investigation were given in Figure **3**.

Table 4. The calculated frequencies values of the compound

Selected Vibration Types	Exp.	scaled DFT	scaled HF
τ HCCC (19), τ OCNN (54), τ COCC (19)	712	731	765
ν CC (28), τ HCCC (87)	756	768	799
τ HCCC (39)		797	839
τ HCCC (91)		855	909
τ COCC (35)		1012	1187
ν OC (42), ν CC (18), δ COC (24)		1287	1358
ν OC (49), δ OCC (32)		1362	1423
ν CN (76), δ CNC (10)		1467	1538
ν CN (19), ν CC (45)		1585	1678
ν NC (52)	1576	1642	1765
ν NC (58)	1624	1667	1792
ν OC (67), ν NC (14)		1772	1864
ν OC (85)	1703	1826	1897
ν CH (54)		2907	2860
ν CH(62)		2930	2886
ν CH (41)		3067	3012

ν, gerilme; δ, bükülme; δ_s, makaslama; ρ, sallanma; γ, düzlem dışı bükülme τ, dönme

Figure 3. IR spectra of simulated (a and b) with DFT/B3LYP/6–311G(d,p) and HF/B3LYP/6–311G(d, p) levels of the compound

UV–visible Spectroscopy and HOMO–LUMO Analyses

The theoretical absorption wavelengths of the compound in ethanol solvent are given in Table 5 and the graphics of this UV-vis are given in Figure 4. The excitation energies, oscillator strengths (*f*) and absorption wavelengths (λ) of UV–vis absorption spectroscopy of the compound have been calculated by using TD–SCF/B3LYP and TD–SCF/HF methods.

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). 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 (Silverstein, Bassler & Morrill, 1991). In our study, HOMO, LUMO values and 3D plots of this HOMOs and LUMOs are given in Figures 5.

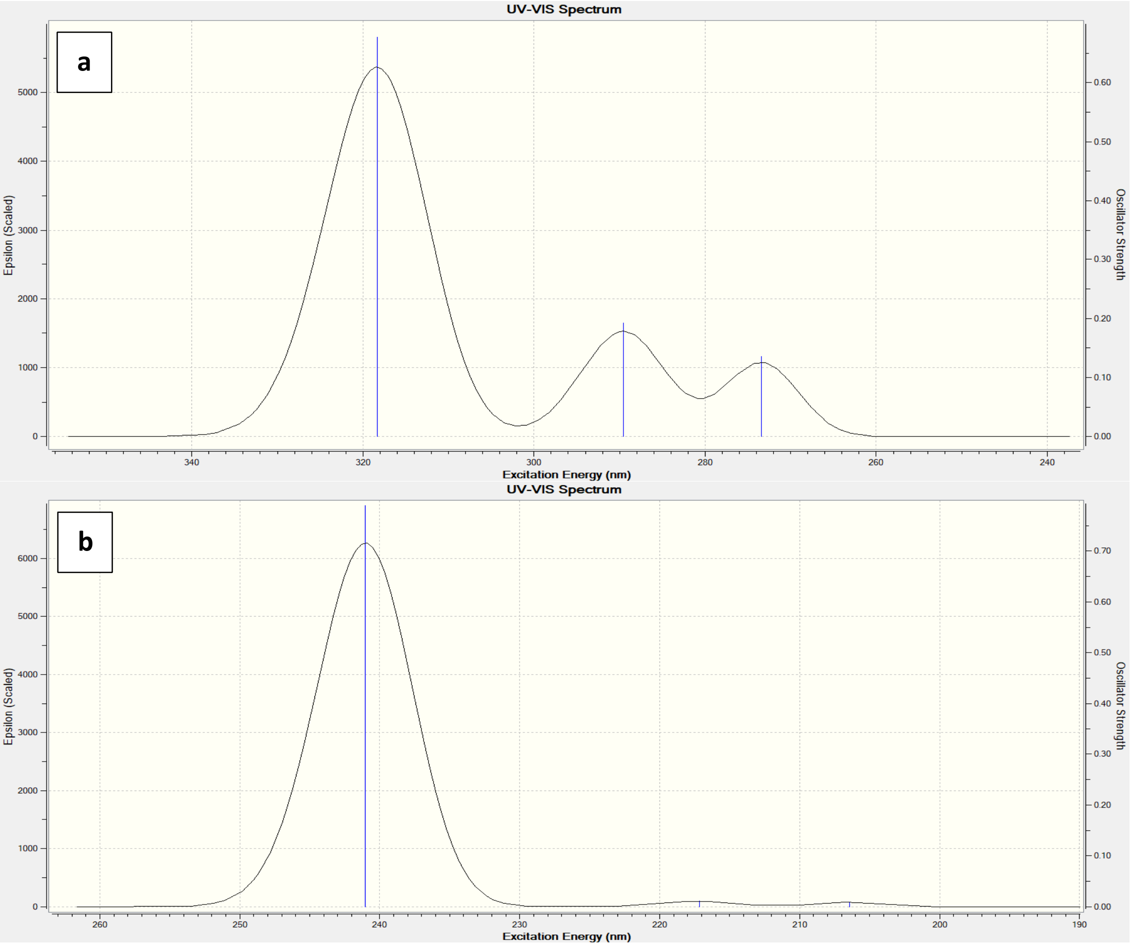
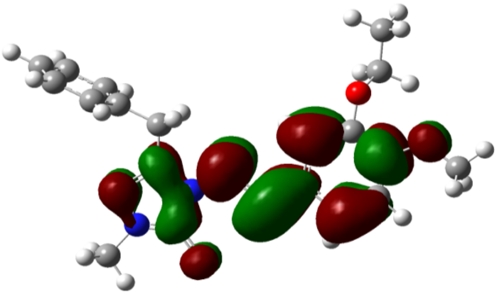


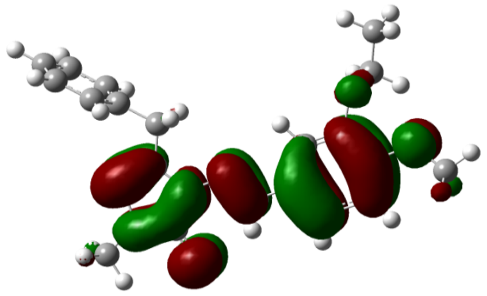
Figure 4. UV-Visible spectra (a and b) simulated with DFT/B3LYP/6–311G(d, p) and HF/B3LYP/6–311G(d, p) levels of the compound

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

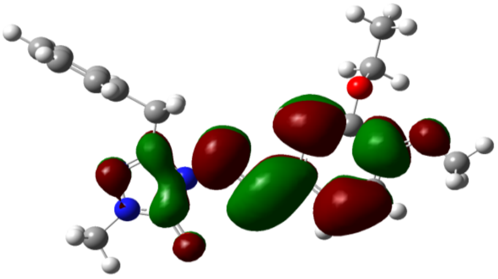
λ (nm) **Exp/DFT/HF**	**Excitation energy (eV)** **DFT/HF**	***f*** **(oscillator strength)** **DFT/HF**
323.00/318.36/241.03	3.8945/5.1439	0.6769/0.7900
215.00/289.57/217.14	4.2817/5.7098	0.1924/0.0117
/273.42/206.43	4.5345/6.0061	0.1354/0.0098



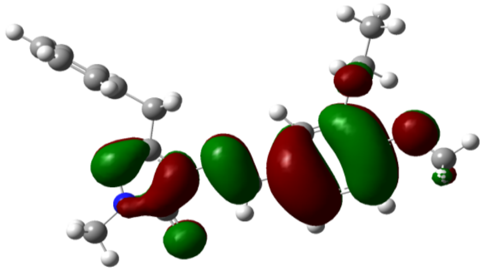
ELUMO (B3LYP) : -0.05535 Hatree



E_{HOMO} (B3LYP) : -0.21312 Hatree



E_{LUMO} (HF) : 0.09085 Hatree



E_{HOMO} (B3LYP) : -0.30016 Hatree

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

Mulliken's atomic charges

The Mulliken atomic charges at the HF/6-31 G(d) and B3LYP/6-31 G(d) level of compound **2** in gas phase are given in Table 6 (Mulliken, 1955). The electronegative N43, N44, N45, N46, O47, O48 and O49 atoms of the compound have negative atomic charge values. The Mulliken atomic charges (B3LYP/HF) of the mentioned atoms were calculated as -0.333/-0.436, -0.213/-0.274, -0.372/-0.477, -0.216/-0.281, -0.409/-0.551, -0.375/-0.499 and -0.345/-0.461 a.u., respectively. The C1, C2, C3, C6 and C7 carbon atoms bounded to the mentioned electronegative atoms in the molecule under study have positive atomic charge values. The values of the positive charges of the mentioned carbon atoms were found as 0.355/0.470, 0.570/0.768, 0.131/0.242, 0.144/0.230 and 0.177/0.258 a.u., respectively. Therefore the C1 atom surrounded with two electronegative N44 and N45 atoms and the C2 atom surrounded with the electronegative N43, N45 and O47 atoms have the highest positive charge values. Because the carbon atoms π bonding have more positive charge density compared to ones having only σ bonding. In other words, the charge density of the carbon atoms with sp^2 hybrids is greater than those of the carbon atoms with sp^3 hybrids. Therefore the title molecule shows strong delocalization energy. In the the compound the atomic charges of all hydrogen atoms have positive values.

Table 6. Mulliken atomic charges of the compound

	DFT	HF		DFT	HF		DFT	HF
C1	0.355	0.470	**C18**	-0.093	-0.078	**H34**	0.146	0.145
C2	0.570	0.768	**C19**	-0.047	-0.079	**H35**	0.083	0.085
C3	0.131	0.242	**C20**	-0.124	-0.032	**H36**	0.092	0.097
C4	-0.163	-0.189	**H21**	0.139	0.163	**H37**	0.093	0.097
C5	-0.012	-0.042	**H22**	0.104	0.116	**H38**	0.093	0.097
C6	0.144	0.230	**H23**	0.109	0.113	**H39**	0.083	0.086
C7	0.177	0.258	**H24**	0.095	0.098	**H40**	0.126	0.107
C8	-0.117	-0.125	**H25**	0.093	0.071	**H41**	0.126	0.108
C9	-0.060	-0.075	**H26**	0.113	0.091	**H42**	0.133	0.125
C10	-0.014	0.083	**H27**	0.103	0.084	**N43**	-0.333	-0.436
C11	-0.347	-0.256	**H28**	0.114	0.097	**N44**	-0.213	-0.274
C12	-0.134	-0.031	**H29**	0.116	0.101	**N45**	-0.372	-0.477
C13	-0.182	-0.133	**H30**	0.114	0.090	**N46**	-0.216	-0.281
C14	-0.096	-0.095	**H31**	0.117	0.094	**O47**	-0.409	-0.551
C15	-0.053	-0.078	**H32**	0.133	0.116	**O48**	-0.375	-0.499
C16	-0.092	-0.078	**H33**	0.144	0.143	**O49**	-0.345	-0.461
C17	-0.089	-0.106						

Total energy

The energetic behavior of title molecule was investigated in vacum. Total energy values of title molecule were calculated by using B3LYP/6-311G(d, p) and HF/6-

311G(d, p) level. The calculated total energy values are given in Table 7.

Table 7. The total energy of the of the compound

Energy	B3LYP	HF
(a.u.)	-1220.32	-1212.79

4. Conclusion

The vibrational frequencies, ^{1}H and ^{13}C-NMR chemicals shifts, UV–vis spectroscopies, HOMO and LUMO analyses of 1-methyl-3-benzyl-4-(3-ethoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-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 ^{13}C and ^{1}H NMR chemical shifts spectroscopic parameters obtained theoretically are in a very good agreement with the experimental data.

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