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Research Article

Investigation of theoretical properties of 1-Acetyl-3-(*p*-methylbenzyl)-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule

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ABSTRACT

In this study, firstly, 1-acetyl-3-(*p*-methylbenzyl)-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol -5-one molecule was optimized by using the B3LYP/DFT631G (d) and HF/631G (d) basis sets. Then, the veda4f program was used in defining of IR data theoretically. IR (infrared) vibrational frequencie values with two different basis sets of molecule was calculated in gas phase and multiplied by adjustment scale factors. Infrared spectra of molecule according to these values obtained were formed. Furthermore, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by GIAO method. Experimental and theoretical values of analyzed molecule were inserted into the graphic according to equation of δ exp = a + b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of *a* and *b* constants. Finally, bond angles, bond lengths, mulliken atomic charges, HOMO-LUMO energy, E_{LUMO}-E_{HOMO} energy gap (ΔE), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), total energy of the molecule, dipole moment and thermodynamic properties were calculated with Gaussian 09W program.

Keywords: Gaussian G09W, Veda4f, HOMO-LUMO, GIAO

1-Asetil-3-(*p*-metilbenzil)-4-(3-metil-2-thienilmetilenamino)-4,5-dihidro-1*H*-1,2,4-triazol-5-on molekülünün teorik özelliklerinin incelenmesi

ÖZ

Bu çalışmada, öncelikle, 1-Asetil-3-(*p*-metilbenzil)-4-(3-metil-2-thienilmetilenamino)-4,5-dihidro-1*H*-1,2,4-triazol-5-on molekülü B3LYP/DFT631G (d) and HF/631G (d) temel setleri kullanılarak optimize edilmiştir. Sonra, Veda 4f programı teorik olarak IR verilerini belirlemede kullanılmıştır. Molekülün iki farklı temel seti ile IR (infrared) titreşim frekans değerleri gaz fazında hesaplanmış ve uygun skala faktörleri ile çarpılmıştır. Elde edilen bu değerlere göre molekülün infrared spektrumları çizilmiştir. Ayrıca, ^{1}H- ve ^{13}C-NMR isotropik kayma değerleri GIAO metoduna ile hesaplanmıştır. Analiz edilen molekülün deneysel ve teorik değerleri δ exp = a + b. δ calc. eşitliğine göre grafiğe geçirilmiştir. Standart hata değerleri *a* ve *b* sabitlerinin regresyon katsayısı ile Sigmaplot programı kullanılarak bulunmuştur. Son olarak, bağ açıları, bağ uzunlukları, mulliken atomik yükleri, HOMO-LUMO enerjisi, E_{LUMO}-E_{HOMO} kapasitesi (ΔEg), elektronegatiflik (χ), elektron yoğunluğu (A), global sertlik (η), yumuşaklık (σ), iyonizasyon potansiyeli (I), molekülün toplam enerjisi, dipol moment ve termodinamik özellikleri Gaussian 09W programı ile hesaplanmıştır.

Anahtar Kelimeler: Gaussian G09W, Veda4f, HOMO-LUMO, GIAO.

1. INTRODUCTION

Schiff bases are of the fundamental compounds for organic chemistry. These compounds include -C=N- (azomethine group). They are, generally, synthesized by condensation of active -C=O- and -NH_2 containing compounds.[1] Their derivatives of 1,2,4-triazoles have also been found to possess pharmacological activities.[2-5] When heteroatoms such as sulfur, oxygen, nitrogen are added the structure of the Schiff base compounds, the biological activity increases.[6] The most known biological activities of them were anti-viral activity,[7] anti-fungal,[8] anti-oxidant,[9] anti-inflammmmatory,[10] anti-bacterial,[11] anti-tumor,[12] anti-cancer,[13,14] trypanosomal,[15] anti-proliferative [16] and antibiotics.[17] In the past years, by increases and trends in development of computational chemistry, theoretically properties of Schiff bases have been investigated. Quantum chemical calculations have been used commonly to theoretically estimate the structure, electronic properties, thermodynamics, spectroscopy of molecular systems. The aim of this study is to compare the calculated theoretical values with experimental values and to determine which of the DFT and HF methods close to experimental values.

2. MATERIALS AND METHODS

2.1. Computational Details

The quantum chemical calculations provide support for spectroscopic studies and experimental structers.[18-23] Firstly, the density functional theoretical (DFT) and Hatree Fock (HF) calculations of compounds were optimized at the Becke-Lee-Parr hybrid exchange correlation three-parameter functional (B3LYP) level with standard 6-31G(d) basis set.[24] All calculations reported in this work were carried out with the Gaussian 09 program.[25] Then, from the most stable structure of the optimized molecule, electronegativity (χ), mulliken charges, the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO), bond lengths, electron affinity (A), global hardness (η), softness (σ), ionization potential (I), chemical potential (Pi), Nucleophilic index (IP), electrophilic index(ω), total energy of the molecule, thermodynamics properties (thermal energies (E), thermal capacity (CV), entropy (S), dipole moments, E_{LUMO}-E_{HOMO} energy gap (ΔEg) were calculated with HF/631G (d) and DFT631G (d) basis sets. Moreover, IR data were calculated theoretically using the veda4f program.[26] Experimental data were obtained from the literature.[27] The calculated and the experimental data were compared with accuration of values found by regression analysis. Theoretical IR data are multiplied with chosen scala factors.[28] The data obtained according to DFT and HF method are formed using theoretical infrared spectrum. Finally, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with the method of gauge including atomic orbital GIAO[25] using the program package Gaussian G09. Experimental and theoretical parameters of investigated molecules were inserted into the graphic according to the equitation of $\delta_{exp} = a + b.\ \delta_{calc}$. The standard error and regression coefficient (a, b) were found by SigmaPlot program.

2.1.1. Optimized geometries

1-Acetyl-3-(*p*-methylbenzyl)-4-(3-methyl-2-thienylmet- hyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one was optimized by means of DFT(B3LYP)/HF methods with 6-31G(d) basis set. The chemical formula and the optimized geometric structure of molecule is shown in Figures 1 and 2.

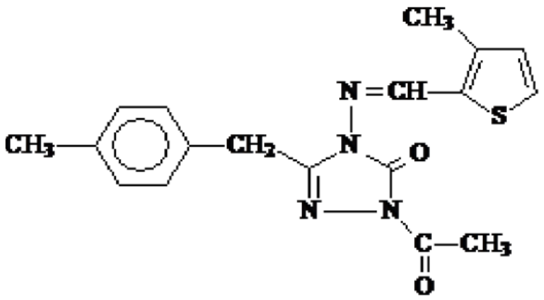

Figure 1. The chemical formula of the molecule.

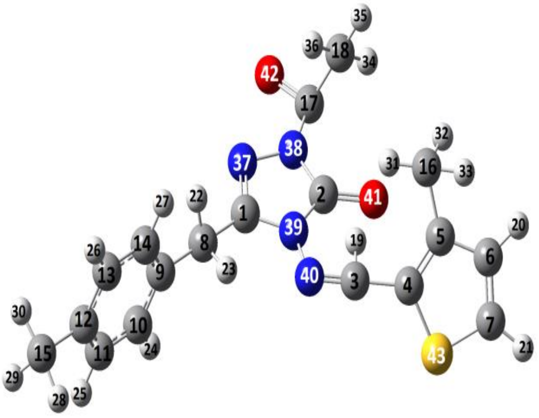

Figure 2. The optimized structure of the molecule.

2.2. The R^2 values of the compound

The experimental and calculated results are summarized in Table 1. A linear correlation in the experimental and theoretical values (proton and carbon chemical shifts ratios) was observed and shown in Figure 3. There is such a relationship between R-values of target compound: DFT 6-31G(d) DMSO ^{1}H: 0.9978, ^{13}C: 0,9974, HF 6-31G(d)DMSO: ^{1}H: 0,8212 ^{13}C: 0,8387 (Table 2).

2.3. FT-IR study of molecule

Theoretical IR data were calculated from veda4f programme, and scala vibration values were obtained. Theoretical IR data were multiplied with appropriate scala factors respectively 0.9613, 0.8929 for DFT/ HF 631G(d) basis sets. The data was found positively. The structure was stable according to the obtained result. IR spectra were drawn with data obtained according to HF and DFT methods. Theoretical IR values were compared with experimental IR values and listed in Table 3.

Table 1. ^{13}C and ^{1}H-NMR (DMSO) isotropic chemical shifts (δ/ppm)

No	Exp.	DFT/dmso	Differ/DFT	HF/dmso	Differ/HF	No	Exp.	DFT/dmso	Differ/DFT	HF/dmso	Differ/HF
C1	148,59	154,34	-5,75	146,83	1,76	H19	9,73	10,34	-0,61	9,57	0,16
C2	149,21	156,68	-7,47	150,19	-0,98	H20	6,90	7,35	-0,45	6,84	0,06
C3	149,47	148,59	0,88	146,09	3,38	H21	7,42	7,73	-0,31	7,45	-0,03
C4	143,88	143,55	0,33	126,60	17,28	H22	4,05	4,37	-0,32	3,48	0,57
C5	148,87	150,89	-2,02	143,76	5,11	H23	4,05	4,27	-0,22	3,60	0,45
C6	132,07	133,76	-1,69	123,56	8,51	H24	7,11	7,59	-0,48	7,58	-0,47
C7	135,41	140,55	-5,14	133,51	1,90	H25	7,32	7,62	-0,30	7,11	0,21
C8	31,55	43,35	-11,80	27,56	3,99	H26	7,32	7,67	-0,35	7,34	-0,02
C9	126,25	133,66	-7,41	126,40	-0,15	H27	7,11	7,70	-0,59	7,58	-0,47
C10	131,02	134,25	-3,23	127,38	3,64	H28	2,29	2,93	-0,64	2,14	0,15
C11	129,25	132,85	-3,60	124,78	4,47	H29	2,29	2,48	-0,19	1,69	0,60
C12	137,04	141,85	-4,81	134,32	2,72	H30	2,29	2,75	-0,46	2,19	0,10
C13	129,36	132,97	-3,61	125,52	3,84	H31	2,37	2,69	-0,32	2,07	0,30
C14	129,79	133,96	-4,17	126,61	3,18	H32	2,37	2,76	-0,39	2,04	0,33
C15	21,04	31,80	-10,76	18,23	2,81	H33	2,37	2,75	-0,38	1,99	0,38
C16	14,13	24,96	-10,83	12,46	1,67	H34	2,62	3,03	-0,41	2,35	0,27
C17	166,46	167,50	-1,04	160,67	5,79	H35	2,62	3,05	-0,43	2,36	0,26
C18	23,55	35,12	-11,57	22,90	0,65	H36	2,62	2,31	0,31	1,82	0,80

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

	^{13}C				^{1}H			
	R	**S. error**	**a**	**b**	**R**	**S. error**	**a**	**b**
DFT	0.9974	3,0761	2,6820	0,01859	0,9978	2,6352	2,1076	0,0158
HF	0,8387	1,5023	0,9695	0,15994	0,8212	1,5816	0,9775	0,1756

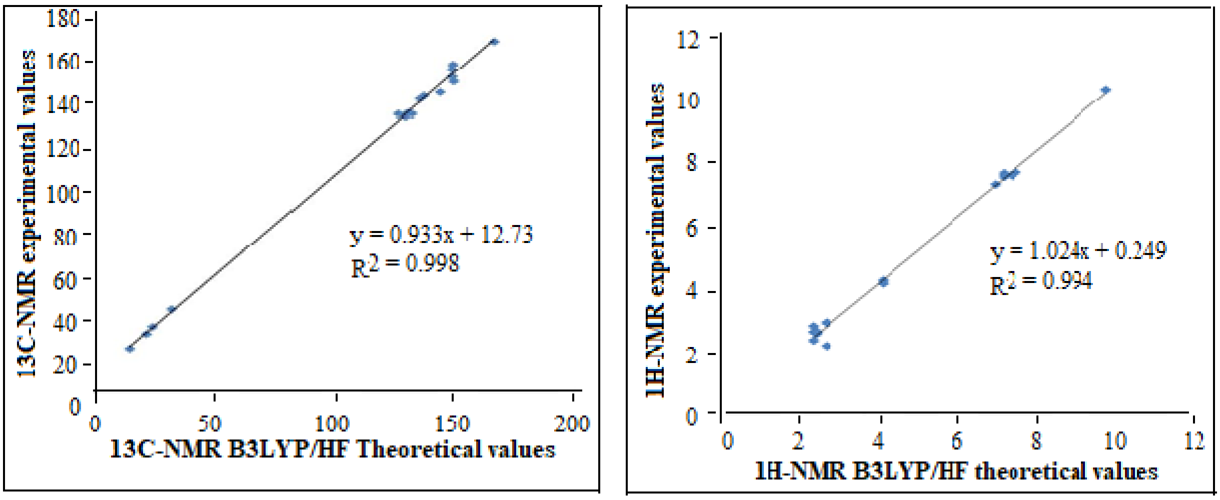

Figure 3. The correlation graphs for B3LYP/HF 631G(d) chemical shifts of the molecule.

2.4. Molecular geometry

The molecular geometric parameters such as bond lengths, bond angles, Mulliken atomic charges were calculated by using the HF and DFT/B3LYP methods with 6-31G(d) basis sets, dipole moments, total energies, and the obtained data are precondition in Tables 4-8. According to these results, the N37-N38, N37-C1, C2-O41, N38-C2, N39-C1, N39-C2 bond lengths in the triazole ring are calculated with DFT/HF 6-31G(d) methods 1.39/1.38, 1.29/1.26, 1.22/1.19, 1.39/1.37,1.39/1.38, 1.40/1.37 Å (Table 4). In the literature, the N=C, N-N, C=O bond lengths are measured as 1.280, 1.404, 1.212 Å.[29, 30] The calculated C9-C10, C10-C11, C11-C12, C12-C13, C13-C14 bond lengths of benzene rings in this compound are [1.39/1.38 Å], [1.39/1.38 Å], [1.40/1.38 Å], [1.39/1.39 Å] and [1.39/1.38 Å], respectively. The Ar(C)-Ar(C) bond lengths of benzene rings are generally observed at 1.34-1.53 Å in the literatüre.[31,32] The calculated C-H bond lengths of the compound are about 1.09, and the C-H bond lengths in the literature is 1.09 Å.[31,32] Also, the calculated N38-C2 bond length in 1,2,4-triazole-5-one ring is [1.39/1.37 Å]. It has been recorded to have bond

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length between single bonded N-N and double bonded N=N due to resonance. The same bond length in the literature is recorded between 1.29-1.47 Å.[31,32] When compared with the bond lengths in the literature, the results show that the molecular structure is very well. The Mulliken atomic charges[33] were calculated by using the Hartree Fock (HF) and DFT/B3LYP methods with 6-31G(d) basis sets. The electronegative oxygen (O) and nitrogen (N) atoms have negative atomic charge values. The carbon atoms surrounded by electronegative atoms have positive atomic charge values. The C1 atom surrounded by two electronegative atoms (N37, N39) and C2 atom which is surrounded by three electronegative atoms (N38, N39, O41) have the highest positive charges values. All hydrogen atoms of the compound have positive atomic charge values (Table 6).

Table 3. Significant vibrational frequencies (cm^{-1})

Vibration Types	scaled dft	scaled hf
τ CCCN(19), τ NCCN(15), τ CNNC(39)	10	4
τ HCCC(70)	15	7
τ CCCC(17), τ CCNN(31), τ NCCN(29)	21	18
δ CCN(41), δ CNN(30), δ CCC(12)	28	24
τ HCCN(68), τ CNNC(17)	37	25
τ CNCN(20), τ CCCC(14)	40	34
τ CNNC(11), τ CCCN(17), τ CNNC(24)	56	53
δ CNN(12), δ CCC(17), δ NNC(22)	71	66
δ CCN(16), δ CCC(19)	77	87
δ CCC(11), τ CCCC(15), τ NNCN(11)	96	108
τ CCCN(12), τ CCCC(19), τ NCCN(30)	120	125
τ HNNC(20), τ CNNC(17), τ NCNN(16)	133	143
δ CCN(38), δ CCC(34)	134	167
τ CCCC(10), τ CCNN(29), τ SCCC(21),	145	174
δ OCN(18), δ CNN(10), δ NNC(13), δ CCC(15)	188	197
δ CCC(24)	193	202
τ HNNC(59), τ ONNC(10)	200	210
τ CCCC(17), τ CCNN(12), τ SCCC(49)	219	215
ν CC(21), δ SCC(29)	230	231
ν NC(12), δ OCN(37), δ NNC(10), δ CCN(13)	244	250
ν NN(10), ν CC(21), δ CNN(29)	252	256
τ HCCS(15), τ CCCN(30), τ SCCC(10)	305	303
τ HNNC(12), τ NCNN(54), τ CNNC(11)	312	304
ν SC(22), δ CCC(17)	328	327
ν CC(10), ν SC(14), δ CCC(24), δSCC(16)	337	349
τ HCCS(80)	358	379
τ ONNC(81)	386	382
ν NN(18), δ NNC(10)	397	405
ν OC(10), ν NC(21), ν CC(10), δ CNN(27)	407	429
ν SC(44), δ SCC(26)	428	431
τ HCCS(82), τ SCCC(10)	432	434
ν CC(12), δ HCS(10),δ CCC(17), τ HCCC(17)	446	449
τ HCNN(93)	453	461
δ HCH(12), δ NNC(15), τ HCCN(36)	458	469
ν CC(10), τ HCCC(35)	479	484
δ HCH(11), τ HCCC(51), τ CCCC(10)	497	493
δ HCH(21), τ HCCN(59)	512	522
ν NN(12), ν NC(15), δ NNC(19)	528	543
ν NN(27), δ HNN(10), τ HCCN(28)	554	567
ν CC(16), δ HCS(34), δ HCC(31)	591	591
ν CC(11), ν NC(20), ν NN(16), δ CNN(15)	601	601
δ HCS(13), δ HCC(14), δ CCC(13)	608	617
ν NC(39)	635	643
ν NN(22), δ CNN(24)	638	663
δ HNN(65)	672	686
τ HCCC(62)	674	691
ν CC(12), δ HCS(14),δ HCC(10), δ HCH(23)	678	701
ν CC(14), δ HCH(56)	695	717
δ HCH(56)	699	734
ν CC(16), ν NC(12), δ HCH(12)	707	742
δ HCH(77), τ HCCN(22)	711	745
ν CC(25), δ HCH(19)	726	760
ν SC(44), δ SCC(26)	745	774
τ HCCS(82), τ SCCC(10)	751	776
ν CC(12), δ HCS(10),δ CCC(17), τ HCCC(17)	771	792
τ HCNN(93)	775	802
δ HCH(12), δ NNC(15), τ HCCN(36)	792	806
ν CC(10), τ HCCC(35)	793	835
δ HCH(11), τ HCCC(51), τ CCCC(10)	835	854
δ HCH(21), τ HCCN(59)	845	887
ν NN(12), ν NC(15), δ NNC(19)	855	892
ν NN(27), δ HNN(10), τ HCCN(28)	960	1005
ν CC(16), δ HCS(34), δ HCC(31)	976	1012
ν CC(11), ν NC(20), ν NN(16), δ CNN(15)	977	1016
δ HCS(13), δ HCC(14), δ CCC(13)	980	1022
ν NC(39)	1011	1029
ν NN(22), δ CNN(24)	1022	1038
δ HNN(65)	1024	1048
τ HCCC(62)	1034	1049
ν CC(12), δ HCS(14),δ HCC(10), δ HCH(23)	1040	1052
ν CC(14), δ HCH(56)	1063	1071
δ HCH(56)	1075	1080
ν CC(16), ν NC(12), δ HCH(12)	1111	1086
δ HCH(77), τ HCCN(22)	1115	1099
ν CC(25), δ HCH(19)	1129	1105
ν NN(18), δ NNC(10)	1131	1119
ν OC(10), ν CC(10), δ CNN(27,)ν NC(21)	1147	140
ν SC(44), δ SCC(26)	1149	1146
τ HCCS(82), τ SCCC(10)	1152	1155
ν CC(12), δ HCS(10),δ CCC(17), τ HCCC(17)	1177	1178
τ HCNN(93)	1179	1189
δ HCH(12), δ NNC(15), τ HCCN(36)	1201	1197
ν CC(10), τ HCCC(35)	1236	1203
δ HCH(11), τ HCCC(51), τ CCCC(10)	1244	1210
δ HCH(21), τ HCCN(59)	1265	1254
ν NN(12), ν NC(15), δ NNC(19)	1269	1256
ν NN(27), δ HNN(10), τ HCCN(28)	1273	1265
ν CC(12), δ HCS(10),δ CCC(17), τ HCCC(17)	1280	1282
τ HCNN(93)	1251	1298
δ HCH(12), δ NNC(15), τ HCCN(36)	1313	1326
ν CC(10), τ HCCC(35)	1331	1368
δ HCH(11), τ HCCC(51), τ CCCC(10)	1352	1395
τ HCCN(22)	1377	1400
δ HCH(24), τ HCCC(28)	1388	1414
δ HCH(58), τ HCCC(14)	1415	1437
δ HCH(75), τ HCCC(22)	1420	1441
δ HCH(79), τ HCCC(22)	1423	1451
δ HCC(10), δ HCC(10)	1436	1453
δ HCH(38)	1448	1460
ν CC(65), δ HCC(10)	1467	1488
ν NC(11), δ HCN(17)	1469	1490
ν NC(52)	1473	1495
ν CC(53), δ HCC(10)	1555	1590
ν OC(10)	1564	1590
ν NC(10,)ν OC(72)	1566	1610
ν CH(83)	1570	1617
ν CH(92)	1591	1623
ν CH(100)	1593	1632
ν CH(100)	1595	1679
ν CH(82)	1612	1716
ν CH(92)	1754	1774
ν CH(54)	1760	1803
ν CH(50)	2941	2886
ν CH(83)	3004	2951
ν CH(92)	3016	2956
ν CH(100)	3056	3006

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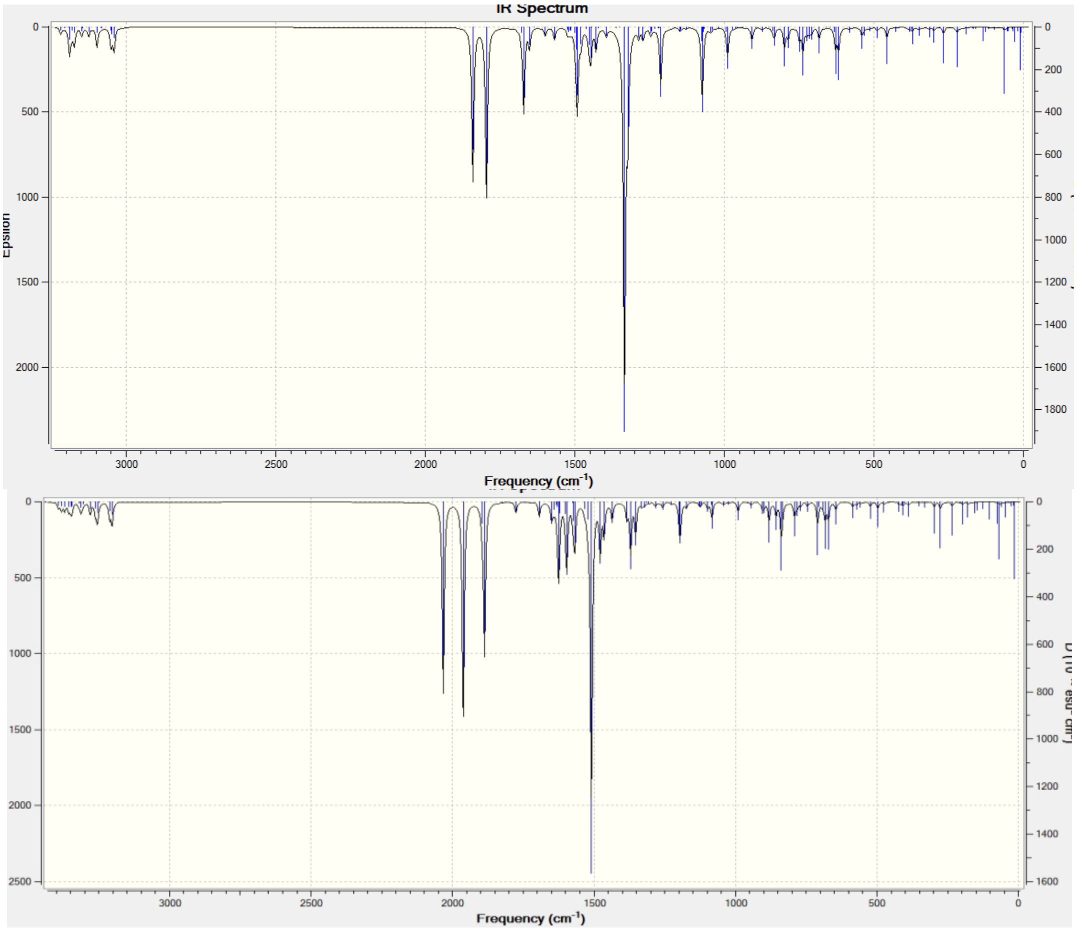

Figure 4. Theoretical IR spectrums simulated with DFT/631G(d)**(a)** ,HF/ 631G(d)**(b).**

Table 4. Bond legths (A^0) theoretical data

Bond Lengths	B3LYP	HF	Bond Lengths	B3LYP	HF
C(1)-C(8)	1,500	1,496	C(12)-C(15)	1,511	1,511
C(1)-N(37)	1,294	1,265	C(15)-H(28)	1,098	1,083
C(1)-N(39)	1,392	1,380	C(15)-H(29)	1,095	1,086
N(37)-N(38)	1,393	1,382	C(15)-H(30)	1,094	1,085
N(38)-C(2)	1,398	1,373	C(17)-O(42)	1,207	1,183
N(38)-C(17)	1,428	1,408	C(17)-C(18)	1,510	1,506
C(2)-N(39)	1,402	1,375	C(18)-H(34)	1,093	1,081
C(2)-O(41)	1,223	1,199	C(18)-H(35)	1,093	1,081
N(39)-N(40)	1,374	1,368	C(18)-H(36)	1,090	1,079
N(40)-C(3)	1,293	1,261	C(3)-H(19)	1,086	1,071
C(8)-H(22)	1,096	1,082	C(3)-C(4)	1,442	1,457
C(8)-H(23)	1,097	1,081	C(4)-C(5)	1,387	1,358
C(8)-C(9)	1,513	1,520	C(5)-C(6)	1,429	1,438
C(9)-C(10)	1,399	1,383	C(5)-C(16)	1,505	1,506
C(10)-H(24)	1,087	1,075	C(6)-H(20)	1,085	1,085
C(10)-C(11)	1,392	1,388	C(6)-C(7)	1,367	1,343
C(10)-H(25)	1,087	1,076	C(7)-H(21)	1,082	1,071
C(11)-C(12)	1,401	1,385	C(7)-S(43)	1,729	1,719
C(12)-C(13)	1,399	1,393	C(4)-S(43)	1,755	1,741
C(13)-H(26)	1,087	1,076	C(16)-H(31)	1,092	1,080
C(13)-C(14)	1,394	1,380	C(16)-H(32)	1,097	1,085
C(14)-H(27)	1,087	1,076	C(16)-H(33)	1,096	1,085

Table 5. Bond angles (^{0}) theoretical data

bond angles	B3LYP	HF	bond angles	B3LYP	HF
N(37)-C(1)-N(39)	111,89	111,65	C(12)-C(15)-H(29)	111,43	111,10
N(37)-N(38)-C(2)	112,37	111,69	C(12)-C(15)-H(30)	111,42	111,15
N(37)-N(38)-C(17)	119,03	119,29	H(28)-C(15)-H(29)	107,12	107,81
C(17)-N(38)-C(2)	128,58	129,01	H(28)-C(15)-H(30)	107,35	107,85
N(38)-C(2)-O(41)	129,81	129,35	H(29)-C(15)-H(30)	107,93	107,41
O(41)-C(2)-N(39)	127,99	127,85	N(38)-C(2)-N(39)	102,18	102,79
N(37)-C(1)-C(8)	126,34	124,46	N(38)-N(37)-C(1)	105,21	105,66
N(39)-C(1)-C(8)	121,76	123,85	C(2)-N(39)-N(40)	130,57	130,07
C(1)-C(8)-H(22)	107,90	106,26	C(1)-N(39)-N(40)	121,08	121,29
C(1)-C(8)-H(23)	107,78	109,11	N(39)-N(40)-C(3)	118,94	119,69
C(1)-C(8)-C(9)	113,96	112,53	N(40)-C(3)-H(19)	122,03	122,53
H(22)-C(8)-H(23)	105,15	108,17	H(19)-C(3)-C(4)	118,17	117,65
H(22)-C(8)-C(9)	110,75	110,31	C(3)-C(4)-C(5)	127,41	126,86
H(23)-C(8)-C(9)	110,84	110,27	C(3)-C(4)-S(43)	120,97	121,21
C(9)-C(10)-H(24)	119,62	119,88	C(4)-C(5)-C(6)	111,71	111,64
C(9)-C(10)-C(11)	120,79	120,70	C(4)-C(5)-C(16)	125,96	127,17
H(24)-C(10)-C(11)	119,58	119,41	H(31)-C(16)-H(32)	107,62	107,86
C(10)-C(11)-H(25)	119,43	119,14	H(31)-C(16)-H(33)	107,63	107,75
H(25)-C(11)-C(12)	119,46	119,74	H(32)-C(16)-H(33)	107,05	107,46
C(10)-C(11)-C(12)	121,10	121,11	C(16)-C(5)-C(6)	122,32	121,17
C(11)-C(12)-C(13)	117,88	117,94	C(5)-C(6)-C(7)	113,401	113,09
C(12)-C(13)-H(26)	119,47	119,57	H(20)-C(6)-C(7)	123,46	123,82
C(12)-C(13)-C(14)	121,08	121,09	C(6)-C(7)-S(43)	112,31	112,40
H(26)-C(13)-C(14)	119,43	119,32	C(6)-C(7)-H(21)	127,73	127,31
C(13)-C(14)-H(27)	119,54	119,68	H(21)-C(7)-S(43)	119,95	120,28
H(27)-C(14)-C(9)	119,63	119,62	C(4)-S(43)-C(7)	90,97	90,93
C(12)-C(15)-H(28)	111,35	111,31			

Table 6. The calculated mulliken charges data of the molecule

	DFT	HF		DFT	HF
C1	0,566	0,657	H23	0,187	0,225
C2	0,860	1,116	H24	0,125	0,219
C3	0,085	0,130	H25	0,123	0,198
C4	-0,230	-0,327	H26	0,122	0,200
C5	0,172	0,077	H27	0,124	0,225
C6	0,130	-0,183	H28	0,163	0,174
C7	-0,337	-0,407	H29	0,161	0,179
C8	-0,441	-0,405	H30	0,157	0,178
C9	0,184	0,003	H31	0,175	0,190
C10	-0,160	-0,212	H32	0,173	0,190
C11	-0,177	-0,232	H33	0,172	0,191
C12	0,181	0,042	H34	0,191	0,211
C13	-0,179	-0,219	H35	0,191	0,213
C14	-0,169	-0,205	H36	0,180	0,210
C15	-0,531	-0,508	N37	-0,310	-0,302
C16	-0,535	-0,514	N38	-0,445	-0,684
C17	0,579	0,753	N39	-0,437	-0,650
C18	-0,521	-0,571	N40	-0,318	-0,312
H19	0,218	0,290	O41	-0,542	-0,514
H20	0,144	0,214	O42	-0,421	-0,649
H21	0,180	0,240	S43	0,283	0,337
H22	0,187	0,232			

Table 7. The calculated dipole moments data of the molecule

Dipol Moment	B3LYP	HF
μ_x	0.4376	0.4753
μ_y	-2.9185	-3.3217
μ_z	2.1723	0.1502
μ_{Toplam}	3.6644	3.3589

Table 8. The calculated total energy data B3LYP/HF of the molecule

Enerji	B3LYP	HF
(a.u.)	-1464.3804	-1457.1220

2.5. Electronic properties of molecule

The HOMO-LUMO energy gap in compound is 4.21; 10.68 e.v. All these parameters such as global chemical potential (μ), global hardness (η), the electronegativity (χ), ionization potential (I), chemical potential (Pi), Nucleophilic index (IP), electrophilic index (ω) have been determined for the target compound using 6-31G (d) basis set (Table 9).

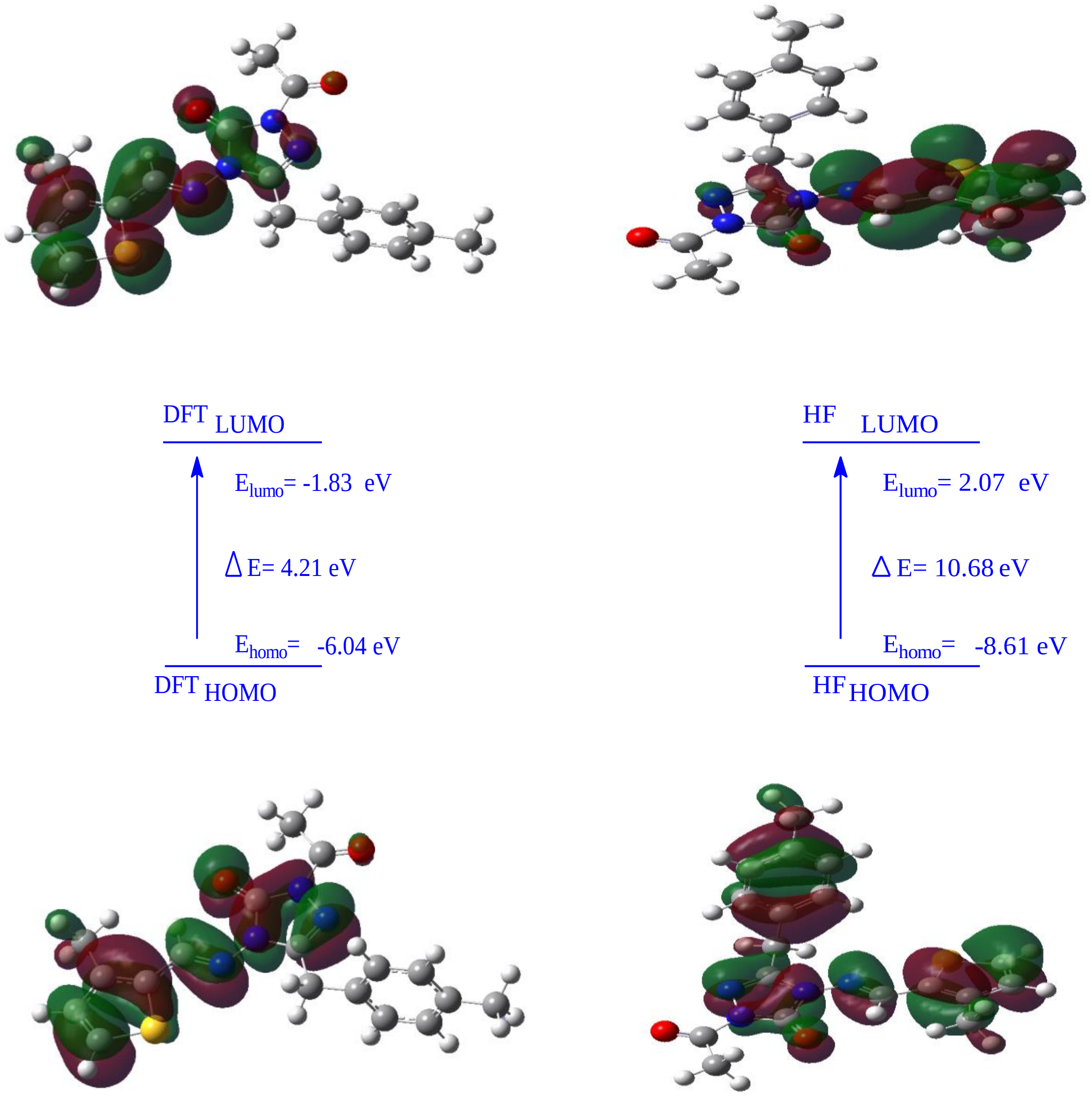

Figure 5. HOMO-LUMO energy gap.

Table 9. The electronic structure parameters of the molecule (HF 631G(d))

		Hatree	**eV**	**kcal/mol**	**kJ/mol**
	LUMO	0,07637	2,07808	47,9224	200,509
	HOMO	-0,31677	-8,61953	-198,774	-831,68
A	Electron affinity	-0,07637	-2,07808	-47,9224	-200,509
I	Ionization potential	0,31677	8,61953	198,774	831,68
ΔE	Energy gap	0,39314	10,6976	246,697	1032,19
χ	Electronegativity	0,1202	3,27073	75,4259	315,585
Pi	Chemical potential	-0,1202	-3,27073	-75,4259	-315,585
ω	Electrophilic index	0,001420026	0,03864	0,89107	3,72828
IP	Nucleophilic index	-0,02362771	-0,64293	-14,8265	-62,0346
S	Molecular softness	5,0872	138,428	3192,26	13356,6
η	Molecular hardness	0,19657	5,34881	123,348	516,095

2.6. Investigation of thermodynamics properties of compound

Thermodynamic parameters are shown in Table 10. Thermodynamic parameters of molecule were calculated 233.044 K and 1 atm of pressure. Also, the standard thermodynamic functions of enthalpy H^0, heat capacity CV^0 and entropy S^0 were obtained at the B3LYP/DFT/HF631G(d) level.

Table 10. The calculated thermodynamic parameters of the molecule

Rotational temperatures (Kelvin)	**DFT**	**HF**
A	0.01331	0.00948
B	0.00501	0.00772
C	0.00375	0.00477
Rotational constants (GHZ)		
A	0.27733	0.19759
B	0.10443	0.16088
C	0.07804	0.09934
Thermal Energies E (kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	223.632	239.054
Total	225.410	240.831
Thermal Capacity CV (cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	82.425	76.126
Total	88.386	82.088
Entropy S (cal/mol-K)		
Translational	43.487	43.487
Rotational	36.207	35.875
Vibrational	99.970	90.736
Total	179.664	170.098
Zero-point correction (Hartree/Particle)	0.334969	0.361125
Thermal correction to Energy	0.359213	0.383789
Thermal correction to Enthalpy	0.360157	0.384733
Thermal correction to Gibbs Free Energy	0.274793	0.303914
Sum of electronic and zero-point Energies	-1464.045482	-1456.760883
Sum of electronic and thermal Energies	-1464.021237	-1456.738219
Sum of electronic and thermal Enthalpies	-1464.020293	-1456.737275
Sum of electronic and thermal Free Energies	-1464.105658	- 1456.818094
Zero-point vibrational energy (Kcal/mol)	210.19598	226.60957

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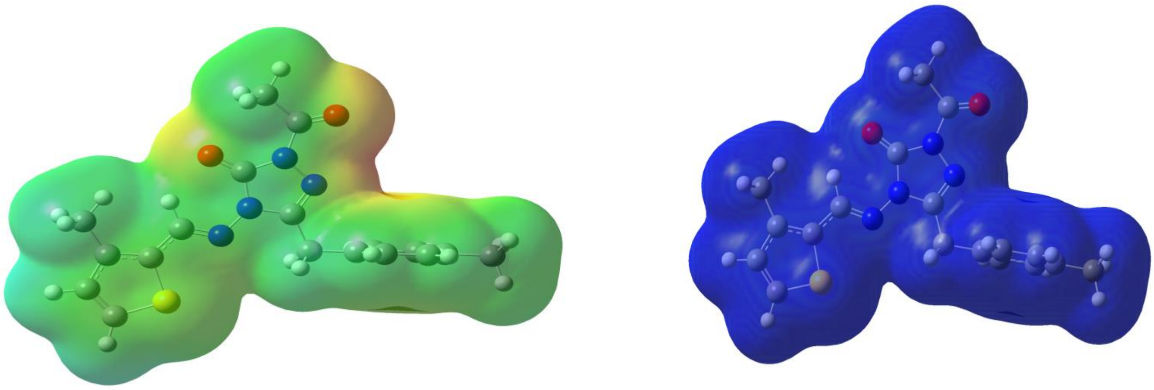
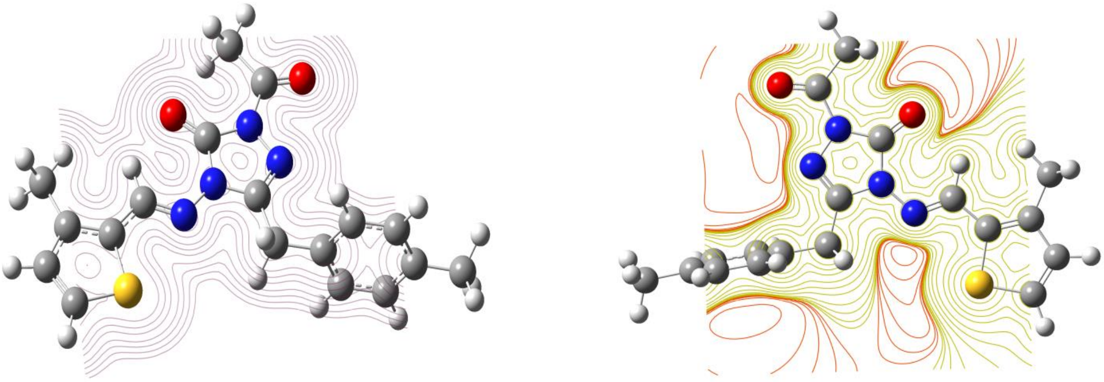


The MEP of the molecule The total density of the molecule



The Electron Density of the molecule The Electrostatic Potential of the molecule

Figure 6. The calculated molecular surfaces of the molecule.

3. CONCLUSIONS

Spectroscopic parameters such as ^{13}C and ^{1}H-NMR, IR and geometrical parameters were calculated by HF and DFT methods with the 6-31G(d) basis sets of the program package Gaussian G09W. These calculations were compared with the experimental findings. The chemical shifts in the calculations $^{13}C/^{1}H$-NMR and IR values were found that this data approximately fitted to the experimental data. Experimental and theoretical ^{13}C and ^{1}H chemical shifts ratios between according to R^2 and a, b values linear a correlation were observed. In addition, Theoretical infrared vibration values were determined with Veda4f program and important results. Furthermore, total energy of the molecule, global hardness (η), bond lengths, softness (σ), LUMO-HOMO, E_{LUMO}-E_{HOMO} energy gap (ΔEg), mulliken charges, thermodynamics properties, dipole moments, ionization potential (I), electron affinity (A), electronegativity (χ) were calculated with B3LYP/ HF/DFT631G (d) basis sets.

Conflict of interest

Authors declare that there is no a conflict of interest with any person, institute, company, etc.

REFERENCES

1. Das, K.; Datta, A.; Nandi, S.; Mane, S.B.; Mondal, S.; Massera, C.; Sinha, C.; Hung, C.H.; Askun, T.; Çelikboyun, P.; Cantürk, Z.; Garribba, E.; Akitsu, T.; *Inorg.Chem. Front.* **2015**, 749-762.

2. Zahid, H.C.; Sajjad, H.S.; Moulay, H.Y.; Taibi, B.H. *Eur. J. Med. Chem*. **2010**, 45, 2739-274.

3. Balram, S.; Mahendra, S.R.; Rambabu, S.; Anil B.; Sanjay, S. *Eur. J. Med. Chem.* **2010**, 45, pp. 2938-2942.

4. Wang, B. L.; Shi, Y. X.; Ma, Y.; Liu, X. H.; Li, Y. H.; Song, H.B.; Li, B.J.; Li. Z. M. *J. Agric. Food Chem.* **2010,** 58, 5515-5522.

5. Hu, G. Q.; Wang, G. Q.; Duan, N. N.; Wen, X. Y.; Cao, T. Y.; Xie, S. Q.; Huang, W.L. *Acta Pharm. Sin. B.*, **2012**, 3, 312-317.

6. Young, D. W. *Heterocyclic Chemistry*, Frst ed., Longman group Ltd., London, 1975.

7. Kumar, K. S.; Ganguly, S.; Veerasamy, R.; De Clercq, E. *Eur. J. Med. Chem.* **2010**, 45 (11), 5474-5479.

8. Patel, R. V.; Park, S. W. *Eur.* J. Med. Chem. **2014**, 71, 24-30.

9. Shanty, A. A.; Philip, J. E.; Sneha, E. J.; Kurup, M. R. P.; Balachandran, S.; Mohanan, P. V. *Bioorg. Chem.* **2017**, 70, 67-73.

10. Pontiki, E.; Hadjipavlou-Litina, D.; Chaviara, A. *J. Enzym. Inhib. Med. Chem.* **2008**, 23 (6), 1011-1017.

11. Mari, S. K.; Bantwal, S. H.; Nalilu, S. K. *Eur. J. Med. Chem.*, **2008**, 43, 309-314.

12. Boraei, A. T. A.; Gomaa, M. S.; Ashry, S. H.; Duerkop, A. *Eur. J. Med. Chem*., **2017,** 125, 360-371.

13. Bensaber, S. M.; Allafe, H.; Ermeli, N. B.; Mohamed, S. B.; Zetrini, A. A.; Alsabri, S. G.; Erhuma, M.; Hermann, A.; Jaeda, M. I.; Gbaj, A. M. *Med. Chem. Res.* **2014**, 23 (12), 5120-5134.

14. Sinha, A., Banerjee, K., Banerjee, A., Das, S., Choudhuri, S. K. *J. Organomet. Chem.* **2014**, 772, 34-41.

15. Papadopoulou, M. V.; Bloomer, W. D.; Rosenzweig, H.S.; Chatelain, E.; Kaiser, M.; Wilkinson, S. R.; MaKenzie, C.; Ioset, J. R. *J. Med. Chem*. **2012**, 55, 5554-5565.

16. Li, Y. H.; Zhang, B.; Yang, H. K.; Li, Q.; Diao, P. C.; You, W. W.; Zhao, P. L. *Eur. J. Med. Chem.* **2017**, 125, 1098-1106.

17. Xia, Z. P.; Wang, X. D.; Wang, P. F.; Zhou, Y.; Zhang, J. W.; Zhang, L.; Zhou, J.; Zhou, S. S.; Ouyang, H.; Lin, X.Y.; Mustapa, M.; Reyinbaike, A. ; Zhu, H. L. *Eur. J. Med. Chem*., **2014**, 80, 92-100.

18. Yüksek, H.; Gürsoy, Ö.; Çakmak, İ.; Alkan, M. *Magn. Reson. Chem.* **2005**, 43, 585-587.

19. Yüksek, H.; Çakmak, İ.; Sadi, S.; Alkan, M. Baykara, H. *Int. J. Mol. Sci.* **2005**, 6, 219-229.

20. Yüksek, H.; Alkan, M.; Bahçeci, Ş.; Çakmak, İ.; Ocak, Z.; Baykara, H.; Aktaş, Ö.; Ağyel, E. *J. Mol. Struc*. **2008**, 873, 142-148.

21. Yüksek, H.; Alkan, M.; Çakmak, İ.; Ocak, Z.; Bahçeci, Ş.; Calapoğlu, M.; Elmastaş, M.; Kolomuç, A.; Aksu, H. *Int. J. Mol. Sci.* **2008**, 9, 12-32.

22. Gökçe, H.; Bahçeli, S.; Akyıldırım, O.; Yüksek, H.; Gürsoy-Kol, Ö. *Lett. Org. Chem.* **2013**, 10 (6), 395-441.

23. Gökçe, H.; Akyıldırım, O.; Bahçeli, S.; Yüksek, H.; Gürsoy-Kol, Ö. *J. Mol. Struc.* **2013**, 1056-1057, 273-284.

24. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X. et al. Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT. **2009**. 200.

25. Wolinski, K.; Hilton, J. F. Pulay, P. *J. Am. Chem. Soc.* **1990**, 112, 512.

26. Jamróz, M. H. Vibrational Energy Distribution Analysis: VEDA 4 program, Warsaw, 2004.

27. Gürsoy-Kol, Ö.; Yüksek, H.; İslamoğlu, F. *J. Chem. Soc. Pakistan* **2013**, 35(4), 1179-1190.

28. Merrick, J. P.; Moran, D.; Radom, L. *J. Phys. Chem*. **2007**, 111 (45), 11683-11700.

29. Ocak, N.; Çoruh, U.; Kahveci, B.; Şaşmaz, S.; Vazquez-Lopez, E. M.; Erdönmez, A. *Acta Cryst. Sec. E.* **2003**, 59(6), 750-752.

30. Ustabas, R.; Çoruh, U.; Sancak, K.; Ünver, Y.; Vazquez-Lopez, E.M. *Acta Cryst. Sec. E.* **2007**, 63, 2982-3051.

31. Fessenden, R. J.; Fessenden, J. S. Organic Chemistry, Third Edition, Brooks, Cole Publishing Company, California, 1986.

32. İkizler, A. A. Organik Kimyaya Giriş, Dördüncü Baskı, KTÜ Basımevi, Trabzon, Türkiye, 1996, 398 (in Turkish).

33. Mulliken, R S. *J. Chem Phys.* **1955**, 23, 1833-1840.

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