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Research Article

Investigation of electronic, geometric and spectroscopic properties of 3-methyl-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule

Gül Kotan[1,*], Önder Albayrak[2], Haydar Yüksek[3]

[1]*Kafkas University, Kars Vocational School, Kars, Turkey*
[2]*Kafkas University, Atatürk Health Services Vocational School, Kars, Turkey*
[3]*Kafkas University, Department of Chemistry, Kars, Turkey*

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Gaussian G09W,
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GIAO,
1,2,4-triazol-5-one

ABSTRACT

3-Methyl-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule was optimized by using the DFT/6-311G (d,p) and HF/6-311G (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. Theoretical and experimental 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. Furthermore, the veda4f program was used in defining of IR data theoretically. The data obtained with using HF and DFT method are formed using theoretical infrared spectrum. In addition, geometric properties (bond lengths, bond angles and mulliken atomic charges), electronic properties (ELUMO-EHOMO (ΔEg), electronegativity (χ), electron affinity (A), softness (σ), global hardness (η), dipole moment, ionization potential (I), total energy of the molecule), thermodynamics properties, HOMO and LUMO, have been calculated by using Gaussian 09W program.

TR

3-Metil-4-(3-metil-2-tiyenilmetilenamino)-4,5-dihidro-1*H*-1,2,4-triazol-5-one molekülünün elektronik, geometrik ve spektroskopik özelliklerinin incelenmesi

Anahtar Kelimeler:
Gaussian G09W,
Veda4f,
HOMO-LUMO,
GIAO,
1,2,4-triazol-5-on

ÖZET

3-Metil-4-(3-metil-2-tiyenilmetilenamino)-4,5-dihidro-1*H*-1,2,4-triazol-5-on molekülü HF/ B3LYP6-311G(d,p) temel setleri kullanılarak optimize edilmiştir. Sonra, Gaussian 09W paket programı kullanılarak GIAO metoduna göre ^{1}H- ve ^{13}C-NMR isotropik kayma değerleri hesaplanmıştır. Teorik ve deneysel değerler δ exp=a+b. δ calc. eşitliğine göre grafiğe geçirilmiştir. Standart hata değerleri a, b sabitlerinin regresyon katsayısı ile Sigmaplot programı kullanılarak bulunmuştur. Ayrıca, Veda 4f programı teorik olarak IR verilerini belirlemede kullanılmıştır. DFT ve HF metodları ile elde edilen veriler teorik infrared spectrumu çizilmesinde kullanılmıştır. Ek olarak, geometrik özellikler (bağ uzunlukları ve açıları, mulliken atomik yükleri), elektronik özellikler (ELUMO-EHOMO kapasitesi (ΔEg), elektronegatiflik (χ), elektron yoğunluğu (A), global sertlik (η), yumuşaklık (σ), iyonizasyon potansiyeli (I), molekülün toplam enerjisi, dipol moment), termodinamik özellikleri, HOMO ve LUMO, Gaussian 09W paket programı kullanılarak hesaplanmıştır.

1. Introduction

Schiff bases are fundamental compounds for organic chemistry. These compounds are include -C=N- (azomethine group). Generally, synthesized by condensation of active -C=O- and -NH_2 containing compounds [1]. Schiff base compounds exhibit an order of biological properties [2, 3] and have been used as insecticides, bacteriocides, pesticides, and fungicides [4, 5]. If heteroatoms such as sulfur, oxygen, nitrogen are added to the structure of the Schiff base compounds, the biological activity is increased [6]. The most know biological activities: anti-viral activity [7], antifungal [8], anti-oxidant [9], antiinflammatory [10], antitumor [11, 12], anticancer [13, 14], antibacterial activities [15, 16] and anti-pyretic applications [17]. In the past years, by increasing development of computational chemistry, theoretically properties of Schiff bases were investigated. Quantum chemical calculation manners have commonly been used to theoretically estimate the structural, electronic properties, thermodynamic, spectroscopic of molecular systems. The quantum chemical calculation ensure support for spectroscopic studies and experimental structural [18-23]. Firstly, the target molecule optimized by using HF 6-311G (d,p) and DFT 6-311G (d,p) basis sets [24, 25]. Then, LUMO-HOMO, bond lengths, mulliken charges, ELUMO-EHOMO energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), Nucleophilic index (IP), ionization potential (I), chemical potential (Pi), total energy of the molecule, electrophilic index(ω), thermodynamics properties (thermal energies (E), thermal capacity (CV), entropy (S), dipole moments were calculated. Otherwise, IR data were theoretically calculated and for

*Corresponding author: ozlemgursoy@gmail.com
+90 (474) 225 11 50 – 3057

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this was used the veda4f program [26]. Experimental data obtained from the literature [27]. The experimental and the calculated values were compared and found by regression analysis that are accurate. Theoretical IR data are multiplied with appropriate scale factors [28] and the theoretical infrared spectrums were plotted for obtained this results. Finally, $^{13}C/^{1}H$-NMR isotropic shift values were calculated with method of GIAO [25] Theoretical and experimental [27] parameters of investigated molecules were inserted into the grafic according to equatation of δ exp=a+b. δ calc. The standard error and regression coefficient (a, b) and were found with SigmaPlot program.

2. Computational details

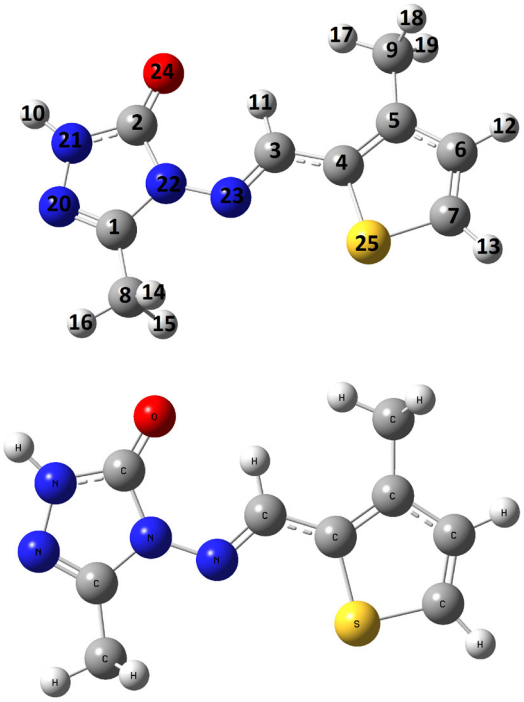


Fig. 1. The Gaussview structure [24, 25]

Table 1. The experimental and calculated ^{1}H /^{13}C-NMR isotropic chemical shifts (DMSO)

No	Exp.	DFT/DMSO	Differ/DMSO	HF/DMSO	Differ/DMSO
C1	148,59	167,51	-18,92	158,82	-10,23
C2	152,08	171,40	-19,32	160,43	-8,35
C3	144,55	164,22	-19,67	157,02	-12,47
C4	132,26	159,56	-27,30	138,57	-6,31
C5	143,63	168,25	-24,62	156,59	-12,96
C6	130,59	151,52	-20,93	137,60	-7,01
C7	131,95	155,87	-23,92	145,21	-13,26
C8	11,72	30,07	-18,35	18,27	-6,55
C9	14,47	31,36	-16,89	18,41	-3,94
H10	11,79	8,00	3,79	7,18	4,61
H11	9,84	11,16	-1,32	10,27	-0,43
H12	7,01	7,68	-0,67	7,17	-0,16
H13	7,68	8,18	-0,50	7,88	-0,20
H14	2,19	3,04	-0,85	2,61	-0,42
H15	2,19	3,04	-0,85	2,61	-0,42
H16	2,19	2,75	-0,56	2,39	-0,20
H17	2,32	3,05	-0,73	2,62	-0,30
H18	2,32	2,97	-0,65	2,62	-0,30
H19	2,32	2,97	-0,65	2,46	-0,14

3.The R^2 data analysis

B3LYP/6-311G(d,p) (DMSO): ^{13}C: 0,9987, ^{1}H: 0,9990; HF/6-311G(d,p) (DMSO): ^{13}C: 0,9255, ^{1}H: 0,9171. There is such a relationship between R^2 values. Found a, b constants regression data and standard error rate were calculated according to formule exp =a +b. δ calc Eq. Based values for molecule were given in the table 2. ^{13}C and ^{1}H chemical shifts ratios between acording to R^2, (a, b) data lineer a correlation were observed.

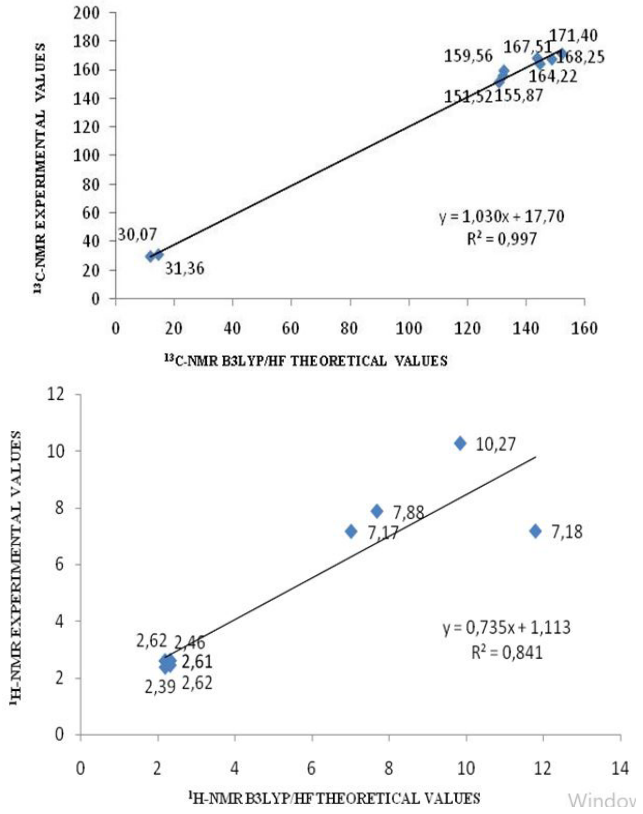


Fig. 2. The correlation graphs for B3LYP/HF 6-311G(d,p) chemical shifts of the molecule

4. FT-IR study of molecule

Theoretically IR data were calculation veda 4f programme and scala vibration values were obtain. Theoretical IR data are multiplied with appropriate adjustment factors respectively 0.9688, 0.9059 for DFT/HF 6-311G(d,p) basis sets and showed in the Table 3. The data was positive found. Structure were stable according to this result. IR spectrums were drawn with obtained data according to HF and DFT method. Theoretically IR details were compare with experimentally IR values, summarized in table 3.

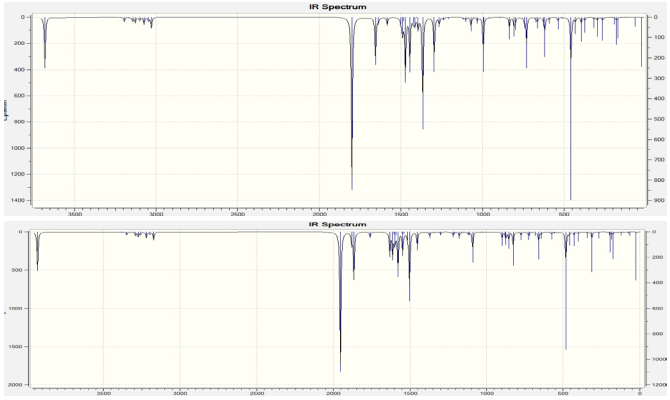


Fig. 3. Theoretical IR spectrums simulated with DFT/6-311G(d,p)(a) ,HF/6-311G(d,p)(b)

Table 2. The correlation values for chemical shifts of the molecule [25]

	^{13}C (DMSO)				^{1}H(DMSO)			
	R^2	S. error	a	b	R^2	S. error	a	b
DFT	0,9987	3,0761	2,6820	0,0185	0,9990	2,6352	2,1076	0,0158
HF	0,9255	1,5023	0,9695	0,1599	0,9171	1,5816	0,9775	0,1756

Table 3. Significant vibrational frequencies (cm^{-1}) [26, 27]

Vibration	Experimental	Theoretical
ν (NH)	3173	3556
ν (C=N)	1608, 1603	1604
ν (C=O)	1714	1744

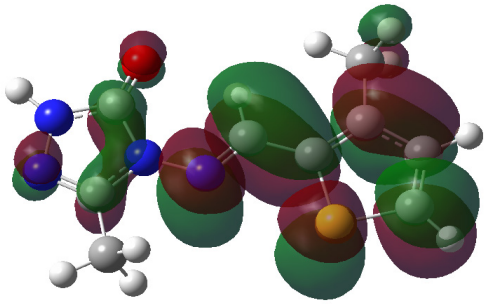
Table 4. The calculated IR frequencies of title compound (cm^{-1}) [28]

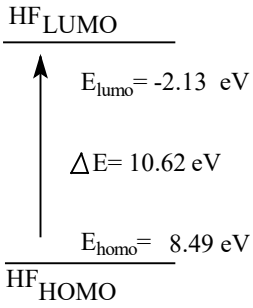
Vibration Types	Scaled DFT	Scaled HF
τ CNCC (19), τ CNNC(39), τ NCCN(15)	24	22
τ HCCC(70)	38	60
τ CNNC(10), τ CCCC(17), τ CCNN(31), τ NCCN(29)	63	66
δ CCN(41), δ CNN(30), δ CCC(12)	64	69
τ HCCN(68), τ CNNC(17)	117	111
τ CCCC(14), **τ CNCN(20),**	146	159
τ CNNC(11), τ CCCN(17), τ CNNC(24)	166	167
δ CNN(12), δ CCC(17), δ NNC(22)	174	176
δ CCN(16), δ CCC(19)	187	178
δ CCC(11), τ CCCC(15), τ NNCN(11)	200	200
τ CCCN(12), τ CCCC(19), τ NCCN(30)	257	243
τ HNNC(20), τ CNNC(17), τ NCNN(16)	288	283
δ CCN(38), δ CCC(34)	308	310
τ CCCC(10), τ CCNN(29), τ SCCC(21), τ CCCC(12)	361	363
δ OCN(18), δ CNN(10), δ NNC(13), δ CCC(15)	383	389
δ CCC(24)	417	417
τ HNNC(59), τ ONNC(10)	444	437
τ CCCC(17), τ CCNN(12), τ SCCC(49)	497	505
ν CC(21), δ SCC(29)	521	521
ν NC(12), δ OCN(37), δ NNC(10), δ CCN(13)	574	583
ν NN(10), ν CC(21), δ CNN(29)	599	598
τ HCCS(15), τ HCCC(11), τ CCCN(30), τ SCCC(10)	606	618
τ HNNC(12), τ NCNN(54), τ CNNC(11)	642	653
ν SC(22), δ CCC(17)	651	659
ν CC(10), ν SC(14), δ CCC(24), δSCC(16)	707	702
τ HCCS(80)	708	749
τ ONNC(81)	721	775
ν NN(18), δ NNC(10)	775	792
ν OC(10), ν NC(21), ν CC(10), δ CNN(27)	782	795
ν SC(44), δ SCC(26)	810	814
τ HCCS(82), τ SCCC(10)	865	931
ν CC(12), δ HCS(10),δ CCC(17), τ HCCC(17)	932	931
τ HCNN(93)	962	988
δ HCH(12), δ NNC(15), τ HCCN(36)	965	1008
ν CC(10), τ HCCC(35)	1000	1014
δ HCH(11), τ HCCC(51), τ CCCC(10)	1020	1043
δ HCH(21), τ HCCN(59)	1035	1056
ν NN(12), ν NC(15), δ NNC(19)	1037	1067
ν NN(27), δ HNN(10), τ HCCN(28)	1070	1098
δ HCC(31), ν CC(16), δ HCS(34),	1083	1103
ν CC(11), ν NC(20), ν NN(16), δ CNN(15)	1171	1178
δ HCS(13), δ HCC(14), δ CCC(13)	1200	1218
ν NC(39)	1226	1242
ν NN(22), δ CNN(24)	1256	1315
δ HNN(65)	1324	1361
τ HCCC(62)	1351	1371
ν CC(12), δ HCS(14),δ HCC(10), δ HCH(23)	1361	1392
δ HCH(56), **ν CC(14),**	1371	1402
δ HCH(56)	1379	1404
ν CC(16), ν NC(12), δ HCH(12)	1400	1429
δ HCH(77), τ HCCN(22)	1425	1441
δ HCH(19), ν CC(25)	1427	1448
δ HCH(38)	1440	1452
ν CC(65), τ HCCN(16)	1444	1461
ν CC(11), δ HCH(17), τ HCCC(13)	1453	1478
ν CC(52)	1534	1595
ν NC(53), τ HCN(10)	1587	1690
ν CC(10), ν NC(55)	1604	1703
ν NC(10), ν OC(72)	1744	1770
ν CH(83)	2934	2874
ν CH(92)	2951	2895
ν CH(100)	2978	2917
ν CH(100)	3003	2952
ν CH(82)	3029	2966
ν CH(92)	3044	2981
ν CH(54)	3066	3034
ν CH(50)	3095	3061
ν CH(50)	3140	3074
ν NH(100)	3556	3560

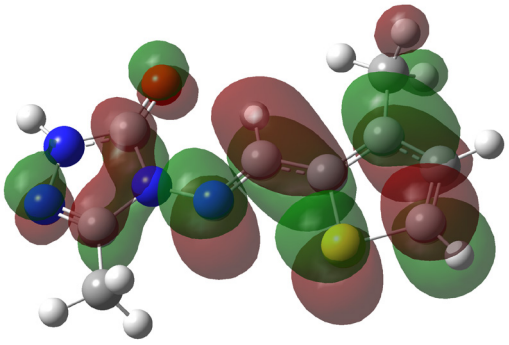
Table 5. Bond legths (A^0) and bond angles (^{0}) theoretical data

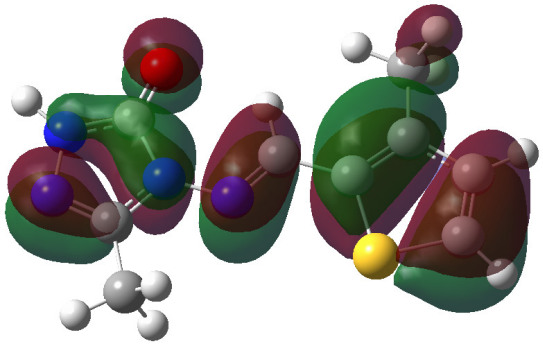
Bond legths	DFT	HF	Bond legths	DFT	HF
C(1)-C(8)	1.485	1.487	C(3)-H(11)	1.085	1.072
C(1)-N(20)	1.296	1.266	C(3)-C(4)	1.442	1.459
C(1)-N(22)	1.388	1.379	C(4)-C(5)	1.383	1.356
N(20)-N(21)	1.380	1.370	C(5)-C(9)	1.504	1.505
N(21)-C(2)	1.368	1.345	C(5)-C(6)	1.427	1.438
C(2)-N(22)	1.417	1.386	C(6)-H(12)	1.082	1.074
C(2)-O(24)	1.217	1.197	C(6)-C(7)	1.364	1.342
N(22)-N(23)	1.370	1.363	C(7)-H(13)	1.079	1.071
N(21)-H(10)	1.005	0.090	C(7)-S(25)	1.728	1.719
C(8)-H(14)	1.092	1.083	C(4)-S(25)	1.753	1.739
C(8)-H(15)	1.092	1.083	C(9)-H(17)	1.089	1.080
C(8)-H(16)	1.089	1.080	C(9)-H(18)	1.094	1.086
N(23)-C(3)	1.289	1.259	C(9)-H(19)	1.094	1.086

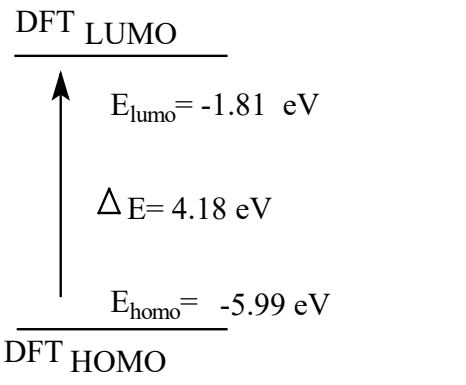
Bond angles	B3LYP	HF	Bond angles	B3LYP	HF
N(20)-C(1)-N(22)	111.37	111.24	N(22)-N(23)-C(3)	118.69	119.80
N(20)-N(21)-C(2)	114.36	113.68	N(23)-C(3)-H(11)	121.79	122.36
N(20)-N(21)-H(10)	120.46	120.98	H(11)-C(3)-C(4)	118.10	117.92
C(10)-N(21)-C(2)	125.16	125.33	C(3)-C(4)-C(5)	127.28	126.82
N(21)-C(2)-O(24)	130.06	129.59	C(3)-C(4)-S(25)	121.14	121.19
O(24)-C(2)-N(22)	128.69	128.49	C(4)-C(5)-C(6)	111.79	111.65
N(20)-C(1)-C(8)	125.19	125.50	C(4)-C(5)-C(9)	125.91	127.09
N(22)-C(1)-C(8)	123.43	123.24	H(17)-C(9)-H(18)	107.72	107.93
C(1)-C(8)-H(14)	110.93	110.43	H(17)-C(9)-H(19)	107.72	107.93
C(1)-C(8)-H(15)	110.93	110.43	H(18)-C(9)-H(19)	107.21	107.60
C(1)-C(8)-H(16)	108.55	108.44	C(9)-C(5)-C(6)	122.29	121.25
H(14)-C(8)-H(15)	107.29	107.84	C(5)-C(6)-C(7)	113.37	113.06
H(14)-C(8)-H(16)	109.54	109.83	H(12)-C(6)-C(7)	123.35	123,79
H(15)-C(8)-H(16)	109.54	109.83	C(6)-C(7)-S(25)	112.31	112.41
N(21)-C(2)-N(22)	101.23	101.91	C(6)-C(7)-H(13)	127.98	127.42
N(21)-N(20)-C(1)	104.71	105.02	H(13)-C(7)-S(25)	119.69	120.16
C(2)-N(22)-N(23)	130.31	130.74	C(4)-S(25)-C(7)	90.94	90.90











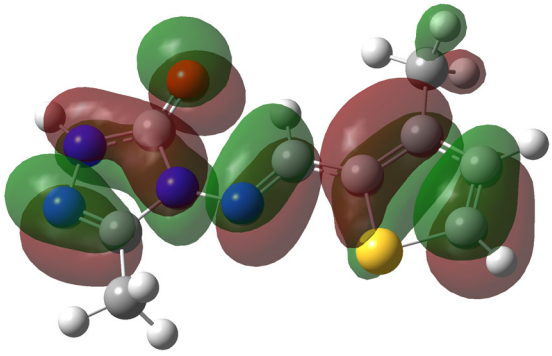


Fig. 4. HOMO-LUMO energy gap

Table 6. The electronic structure parameters of the molecule

		Hatree	ev	kcal/mol	KJ/mol
	LUMO	-0,22053	6,00078	138,383	579,002
	HOMO	-0,06676	1,81659	41,8921	175,278
A	electron affinity	-0,22053	-6,00078	-138,383	-579,002
I	ionization potential	-0,06676	-1,81659	-41,8921	-175,278
ΔE	energy gap	0,15377	4,18419	96,4911	403,723
χ	electronegativity	-0,143645	-3,90868	-90,1377	-377,14
Pi	chemical potential	0,143645	3,90868	90,1377	377,14
ω	electrophilic index	0,000793	0,02158	0,49775	2,08259
IP	Nucleophilic index	0,011044	0,30052	6,93023	28,9964
S	molecular softness	13,0064	353,914	8161,58	34148,4
η	molecular hardness	0,076885	2,09209	48,2456	201,862

5.Investigation of thermodynamics properties of compound

Thermodynamic parameters shown in the table 7. Thermodynamic parameters of molecule were calculated 233.044 K and 1 atm of pressure. In addition to, the standard thermodynamic functions of heat capacity (CV^0), enthalpy (H^0), entropy (S^0) were calculated at the DFT/HF 6-311G(d,p) level.

Table 7. The calculated thermodynamic parameters of the molecule

Rotational temperatures (Kelvin)	DFT	HF
A	0.05404	0.05462
B	0.01435	0.01451
C	0.01137	0.01152
Rotational constants (GHZ)		
A	1.12596	1.14543
B	0.29893	0.30242
C	0.23691	0.23996
Thermal Energies E(kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	124.895	133.510
Total	126.673	135.287
Thermal Capacity CV(cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	46.747	43.263
Total	52.708	49.224
Entropy S(cal/mol-K)		
Translational	42.096	42.096
Rotational	32.666	32.625
Vibrational	48.685	44.541
Thermal correction to Energy	0.201865	0.215594
Thermal correction to Enthalpy	0.202810	0.216538
Thermal correction to Gibbs Free Energy	0.144156	0.159873
Zero-point correction (Hartree/Particle)	0.187422	0.201979
Sum of electronic and zero-point Energies	-1041.367425	-1036.729687
Sum of electronic and thermal Energies	-1041.352982	-1036.716072
Sum of electronic and thermal Enthalpies	-1041.352038	-1036.715128
Sum of electronic and thermal Free Energies	-1041.410691	-1036.771794
Zero-point vibrational energy (Kcal/mol)	117.60907	126.74390

Table 8. The calculated mulliken charges datas of the molecule

	DFT	HF		DFT	HF
C1	0.293	0.395	H14	0.135	0.126
C2	0.533	0.729	H15	0.135	0.126
C3	0.132	0.210	H16	0.131	0.126
C4	-0.294	-0.315	H17	0.120	0.106
C5	-0.037	-0.067	H18	0.128	0.115
C6	-0.056	-0.081	H19	0.128	0.115
C7	-0.277	-0.257	N20	-0.220	-0.285
C8	-0.244	-0.173	N21	-0.312	-0.379
C9	-0.246	-0.181	N22	-0.364	-0.469
H10	0.250	0.259	N23	-0.219	-0.266
H11	0.165	0.189	O24	-0.395	-0.534
H12	0.095	0.101	S25	-0.284	0.274
H13	0.135	0.135			

Table 9. The calculated dipole moments data

	μ_x	μ_y	μ_z	μ_{Toplam}
Dft	-0.7541	1.1416	-0.2600	1.3927
Hf	-0.6731	0.6095	0.2736	0.9483

Table 10. The calculated total energy data

Enerji (a.u.)	DFT	HF
	-1041.5548	-1036.9316

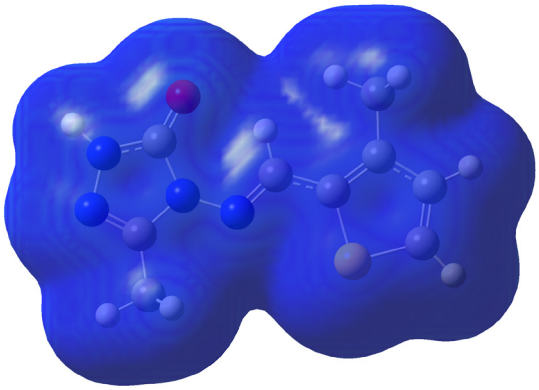


Fig. 5. The total density of the molecule.

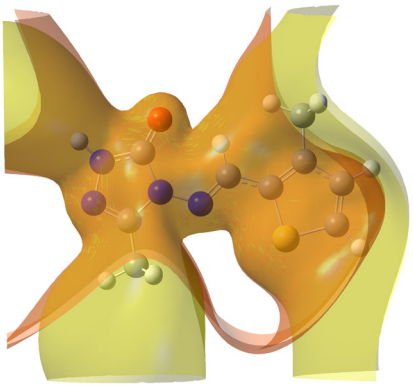


Fig. 6. The ESP of the molecule.

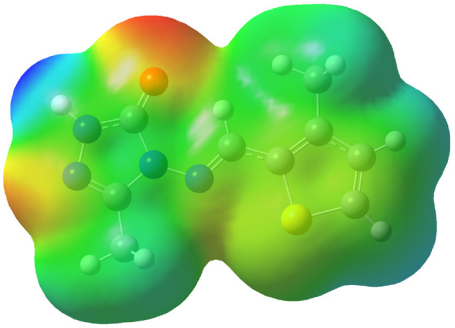


Fig. 7. The MEP of the molecule.

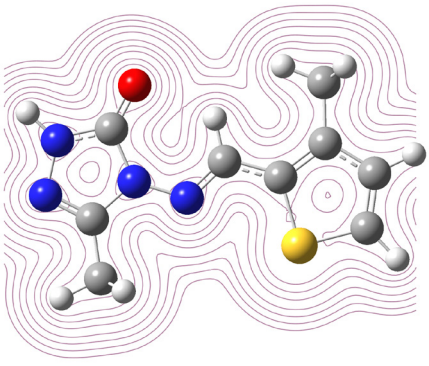


Fig. 8. The Electron Density

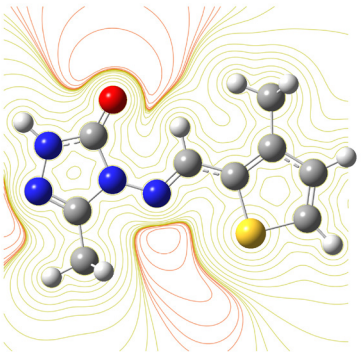


Fig. 9. The Electrostatic Potential

6. Conclusion

Spectroscopic parameters such as ^{13}C and ^{1}H-NMR, IR and geometrical parameters are calculated by Hartree-Fock (HF) and Density Functional Theory (DFT) methods with the 6-311G(d,p) basis sets of the program package Gaussian G09W. Spectroscopic parameters are compared with experimental data. The chemical shifts in the calculations $^{13}C/^{1}H$-NMR and IR values are found that this data to be compatible with the experimental data. Experimental and theoretical ^{13}C and ^{1}H chemical shifts ratios between acording to R^2 and a, b values lineer a correlation were observed. In addition, Thereotical IR vibration values determined with Veda4f program and important resuts given in Tablo 3. Furthermore, HOMO-LUMO, the bond lengths, bond angles, mulliken charges, ELUMO-EHOMO energy gap (ΔEg), electronegativity (χ), global hardness (η), softness (σ), electron affinity (A), total energy of the molecule, thermodynamics properties, ionization potential (I), dipole moments were calculated. All results showed that the calculated geometric (the bond lengths, bond angles, mulliken charges), spectroscopic (Proton Nuclear Magnetic Resonance (^{1}H-NMR), Carbon-13 Nuclear Magnetic Resonance (^{13}C-NMR)), electronic and thermodynamics parameters obtained by DFT/6-311G(d,p) method had a better agreement with the experimental values than HF/6-311G(d,p) method.

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