Journal Homepage: -www.journalijar.com
INTERNATIONAL JOURNAL OF ADVANCED RESEARCH (IJAR)
ISSN NO. 2320-5407
Article DOI:10.21474/IJAR01/6523
DOI URL: http://dx.doi.org/10.21474/IJAR01/6523

RESEARCH ARTICLE

COMPARATION OF THEORETICAL PROPERTIES OF 3-METHYL-4-(3-BENZOXY-4-METHOXYBENZYLIDENAMINO)-4, 5-DIHYDRO-1*H*-1, 2, 4-TRIAZOL-5-ONE MOLECULE.

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Manuscript Info

Manuscript History

Received: 13 December 2017
Final Accepted: 15 January 2018
Published: February 2018

Key words:-
GIAO, 631G (d,p) and 6311G(d,p), mulliken charge, B3LYP, HF.

Abstract

3-Methyl-4-(3-benzoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule was optimized by using the B3LYP/HF 631G(d,p) and B3LYP/HF 6311G(d,p) basis sets. This optimized structures used to calculation of the different theoretical properties of the compound. ^{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. The veda4f program was used in defining IR data. IR absorption frequencies were compared with experimental data. Infrared spectrums were composed by using the data calculated. Additionally, bond lengths, dipole moments, HOMO-LUMO energys, mulliken charges by using the B3LYP/HF 631G(d,p) and B3LYP/HF 6311G(d,p) basis sets of this compound were theoretically calculated. Finally, theoretical properties of the compound according to two different basis sets were compared.

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Introduction:-

Schiff base compounds are used as starting materials in the synthesis of important drugs, such as antibiotics and antiallergic, antiphlogistic, and antitumor substances (Barton & Ollis, 1979; Ingold, 1969; Layer, 1963). On the industrial scale, they have a wide range of applications, such as dyes and pigments (Taggi et.al., 2002). Schiff bases have also been employed as ligands for the complexation of metal ions (Aydoganet.al., 2001). Schiff bases are also becoming increasingly important in the dye and plastic industries as well as for the liquidecrystal technology and mechanistic investigation of drugs used in pharmacology, biochemistry and physiology (Casaszar et.al., 1985, Sheikhshoaie & Sharif, 2006).

In the past years, by increasing development of computational chemistry, theoretically properties of Schiff bases were investigated. Quantum chemical calculation methods have widely been used to theoretically predict the structural, spectroscopic, thermodynamic and electronic properties of molecular systems. The quantum chemical calculation methods provide support for experimental structural and spectroscopic studies (Yüksek et.al., 2005a; Yüksek et.al., 2005b; Yüksek et.al., 2008a; Yüksek et.al., 2008b; Gökçe et.al., 2013; Gökçe et.al., 2014).

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Experimental data of 3-methyl-4-(3-benzoxy-4-methoxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule was described in the literature (Bahçeci et.al., 2016).

In the present paper, theoretical values of compound were calculated theoretically on the computer. Molecule was optimized by using the B3LYP/HF 631G(d,p) and B3LYP/HF 6311G(d,p) basis sets (Frisch et al., 2009; Wolinski, Hilton & Pulay, 1990). Starting from this optimized structure with ^{1}H-NMR and ^{13}C-NMR spectral data (Table **1**) and IR spectral values according to GIAO (Wolinski et al., 1990) method was calculated using the method of Gaussian G09W program package in gas phase. Theoretically and experimentally values (Bahçeci et.al., 2016) were plotted according to exp =a +b. δ calc Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program (Table **2**).The correlation graphs for chemical shifts drawn with ^{1}H-NMR, ^{13}C-NMR and ^{1}H-NMR(DMSO), ^{13}C-NMR(DMSO) spectral data of the molecule (Fig. **3**). Theoretically calculated IR data are multiplied with appropriate adjustment factors (Merrick et.al., 2007) and the data obtained according to HF and DFT method are formed using theoretical infrared spectrum (Fig. **4, 5**). The identification of calculated IR data was used in veda4f program (Jamróz, 2004) (Table **3**). Additionally, bond lengths (Table **4**), mulliken charges (Mulliken, 1955) (Table **5**), the HOMO(the highest occupied molecular orbitals)-LUMO(lowest unoccupied molecular orbitals) energy (Fig. **5, 6**) and dipole moments (Table **6**) of this compound was found by using two basis sets.

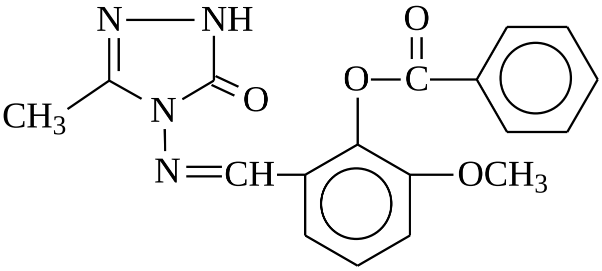

Figure 1:- Chemical formula of compound

Methods:-

The quantum chemical calculations were carried out with Density Functional Theory (DFT) and Hartree-Fock (HF) methods using 631G(d,p) and 6311G (d,p) basis set at the Gaussian 09W program package on a computing system (Frisch et al., 2009). Firstly, the compound was optimized by using the B3LYP/HF 631G(d,p) and B3LYP/HF 6311G(d,p) basis sets (Frisch et al., 2009; Wolinski, Hilton & Pulay, 1990). Thus, the most stable geometrical comformer of compoundwas obtained. Then, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with method of GIAO (Wolinski et al., 1990). The veda4f program was used in defining IR data (Jamróz, 2004). Otherwise, bond lengths, dipole moments, the HOMO-LUMO energy, and mulliken charges (Mulliken, 1955) of compound were calculated theoretically on the computer. Theoretical properties of the compound according to two different basis sets were compared.

Theoretical Calculations:-

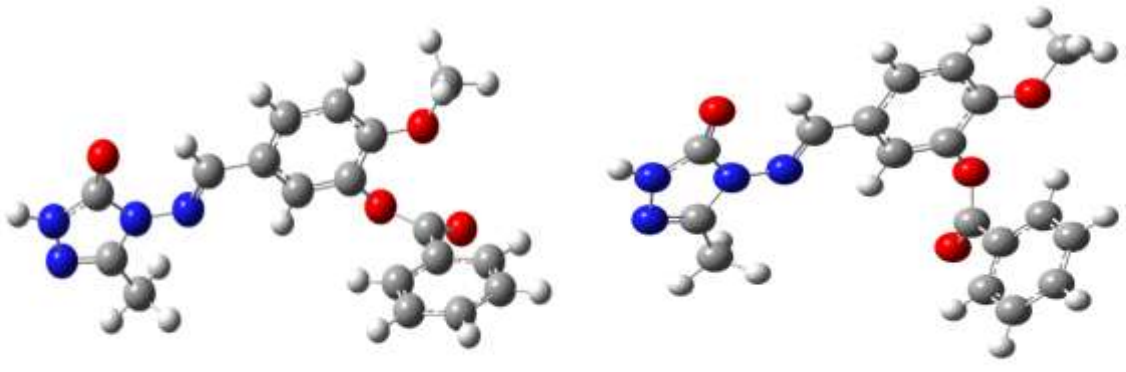

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Figure 2:- The optimized structure of the molecule with DFT/B3LYP/631G(d,p) (**1**) and DFT/B3LYP/6311G(d,p) (**2**) levels

Table 1:- The calculated and experimental ^{13}C and ^{1}H-NMR DMSO(B3LYP/HF 631G(d,p)/6311G(d,p))isotropic chemical shifts of the molecule (δ/ppm)

No	**Exp.**	**B3LYP 631G**	**B3LYP 6311G**	**Differ. B3LYP 631G**	**Differ. B3LYP 6311G**	**HF631G**	**HF631G**	**Differ. HF631G**	**Differ. HF 6311G**
C1	144.73	150,21	167,65	-5,48	-22,92	145,35	159,01	-0,62	-14,28
C2	151.75	152,93	171,12	-1,18	-19,37	146,61	160,48	5,14	-8,73
C3	153.21	154,04	169,98	-0,83	-16,77	149,16	161,98	4,05	-8,77
C4	126.93	132,34	148,86	-5,41	-21,93	119,97	132,70	6,96	-5,77
C5	121.42	119,70	135,69	1,72	-14,27	119,35	132,74	2,07	-11,32
C6	140.25	149,20	168,43	-8,95	-28,18	132,22	146,77	8,03	-6,52
C7	154.01	154,78	177,10	-0,77	-23,09	149,66	164,23	4,35	-10,22
C8	113.20	116,34	132,34	-3,14	-19,14	105,68	117,28	7,52	-4,08
C9	128.72	134,40	151,54	-5,68	-22,82	131,71	145,16	-2,99	-16,44
C10	164.39	170,95	189,63	-6,56	-25,24	157,13	170,48	7,26	-6,09
C11	130.13	134,83	151,17	-4,70	-21,04	123,04	135,96	7,09	-5,83
C12	130.33	132,19	154,55	-1,86	-24,22	129,48	143,58	0,85	-13,25
C13	129.46	130,38	150,53	-0,92	-21,07	122,67	136,76	6,79	-7,30
C14	134.59	136,22	156,22	-1,63	-21,63	133,00	147,48	1,59	-12,89
C15	129.46	132,05	149,67	-2,59	-20,21	122,78	136,90	6,68	-7,44
C16	130.33	135,65	151,51	-5,32	-21,18	130,37	144,03	-0,04	-13,70
C17	56.93	61,07	73,18	-4,14	-16,25	46,25	54,59	10,68	2,34
C18	11.53	20,84	29,86	-9,31	-18,33	10,40	18,37	1,13	-6,84
H19	11.80	8,45	7,93	3,35	3,87	7,62	7,18	4,18	4,62
H20	9.65	11,02	10,61	-1,37	-0,96	10,27	10,06	-0,62	-0,41
H21	7.76	9,09	8,21	-1,33	-0,45	8,90	8,76	-1,14	-1,00
H22	7.28	7,69	7,72	-0,41	-0,44	7,60	7,33	-0,32	-0,05
H23	7.74	8,14	7,96	-0,40	-0,22	8,32	8,19	-0,58	-0,45
H24	8.13	8,50	8,96	-0,37	-0,83	9,15	9,01	-1,02	-0,88
H25	7.60	8,15	8,38	-0,55	-0,78	8,22	8,08	-0,62	-0,48
H26	7.61	8,51	8,40	-0,90	-0,79	8,54	8,40	-0,93	-0,79
H27	7.72	8,52	8,10	-0,80	-0,38	8,23	8,09	-0,51	-0,37
H28	8.13	9,05	8,39	-0,92	-0,26	9,10	8,91	-0,97	-0,78
H29	3.83	4,17	4,69	-0,34	-0,86	4,31	3,65	-0,48	0,18
H30	3.83	4,80	5,05	-0,97	-1,22	3,84	4,08	-0,01	-0,25
H31	3.83	4,49	4,50	-0,66	-0,67	4,02	3,86	-0,19	-0,03
H32	2.24	3,32	3,02	-1,08	-0,78	2,71	2,66	-0,47	-0,42
H33	2.24	3,33	2,96	-1,09	-0,72	2,75	2,62	-0,51	-0,38
H34	2.24	2,95	2,72	-0,71	-0,48	2,43	2,39	-0,19	-0,15

The relation between R^2 values of the compound:-

The optimized R^2 values of the compound with B3LYP/HF 631G(1) level:-
B3LYP/631G(d,p) (DMSO): ^{13}C: 0.9934, ^{1}H: 0.8617; HF/631G(d,p) (DMSO): ^{13}C: 0.9898, ^{1}H: 0.8220.

The optimized R^2 values of the compound with B3LYP/HF 6311G(2) level:-
B3LYP/6311G(d,p) (DMSO): ^{13}C: 0.9936, ^{1}H: 0.8437; HF/6311G(d,p) (DMSO): ^{13}C: 0.9885, ^{1}H: 0.8009.

There is such a relationship between R^2-values of the compound. Found standard error rate and a, b constants regression values were calculated according to formuleexp =a +b. δ calc Eq. These values for compound were shown in the table **2**. Theoretical and experimental carbon and proton chemical shifts ratios between acording to a, b ve R^2 values, lineer a correlation were observed.

Table 2:-The correlation data for chemical shifts of the molecule

^{13}C (DMSO)					^{1}H(DMSO)			
2	**R^{2}**	**S. error**	**a**	**b**	**R^{2}**	**S. error**	**a**	**b**
DFT/631G	0.9934	2.9357	1.0244	-6.8507	0.8617	1.1174	1.0485	0.8687
HF/631G	0.9898	3.7732	0.9869	5.8241	0.8220	1.2678	0.9617	0.0200
^{13}C (DMSO)					**^{1}H(DMSO)**			
2	**R^{2}**	**S. error**	**a**	**b**	**R^{2}**	**S. error**	**a**	**b**
DFT/6311G	0.9936	2.9800	0.9547	-14.369	0.8437	1.1880	1.0751	0.8786
HF/6311G	0.9885	4.0078	0.9416	0.9226	0.8009	1.3410	0.9589	0.1621

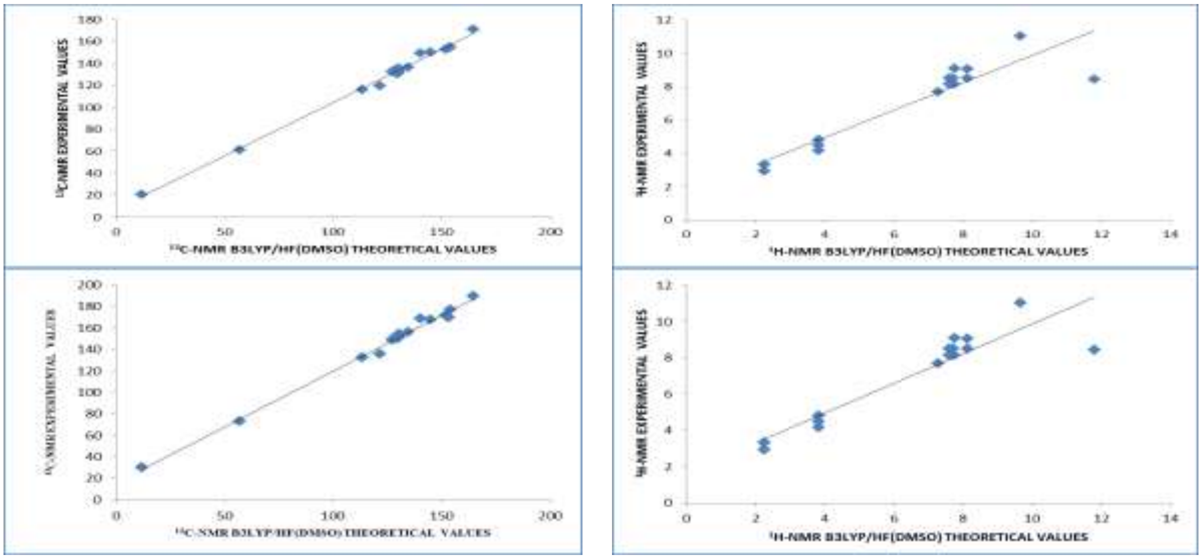


Figure 3:- The correlation graphs for B3LYP/HF 631G(d,p)/6311G(d,p) chemical shifts of the molecule

The vibration frequency of the compound:-

Theoretically IR values were calculation veda 4f programme and scala values were obtain. Theoretically calculated IR data are multiplied with appropriate adjustment factors respectively 0.9617, 0.8992, 0,9688, 0.9059 for DFT/631G(d,p), HF/631G(d,p) and DFT/6311G(d,p), HF/6311G(d,p) basis sets. The negative frequency in the data was not found. This result, structure of compound were shown stable. IR spectrums were drawn with obtained values according to HF and DFT method. Theoretically IR values were compare with experimentally IR values.The result of this compare were found corresponding with each other of values. Experimentally carbonyl peak (C=O) in 1704, 1730 cm^{-1} and theoretically (C=O) peak in 1768 cm^{-1} for 631G(d,p), 1762 cm^{-1} for 6311G(d,p) were observed.

Table 3:-The calculated frequencies values of the molecule optimized with **1** and **2** levels

Vibration Types (1)	**Experimental**	**Skalalı dft(1)**	**Skalalı hf(1)**	**Skalalı dft(2)**	**Skalalı hf(2)**
τ HCCC(16)	700	692	724	682	684
τ HCCC(11)	771	779	809	797	826
τ HCOC(27)	1262	1268	1277	1179	1197
ν NC(54)	1603	1591	1625	1613	1710
ν OC(90)	1730, 1704	1768	1809	1762	1809
ν NH(100)	3172	3557	3556	3566	3561

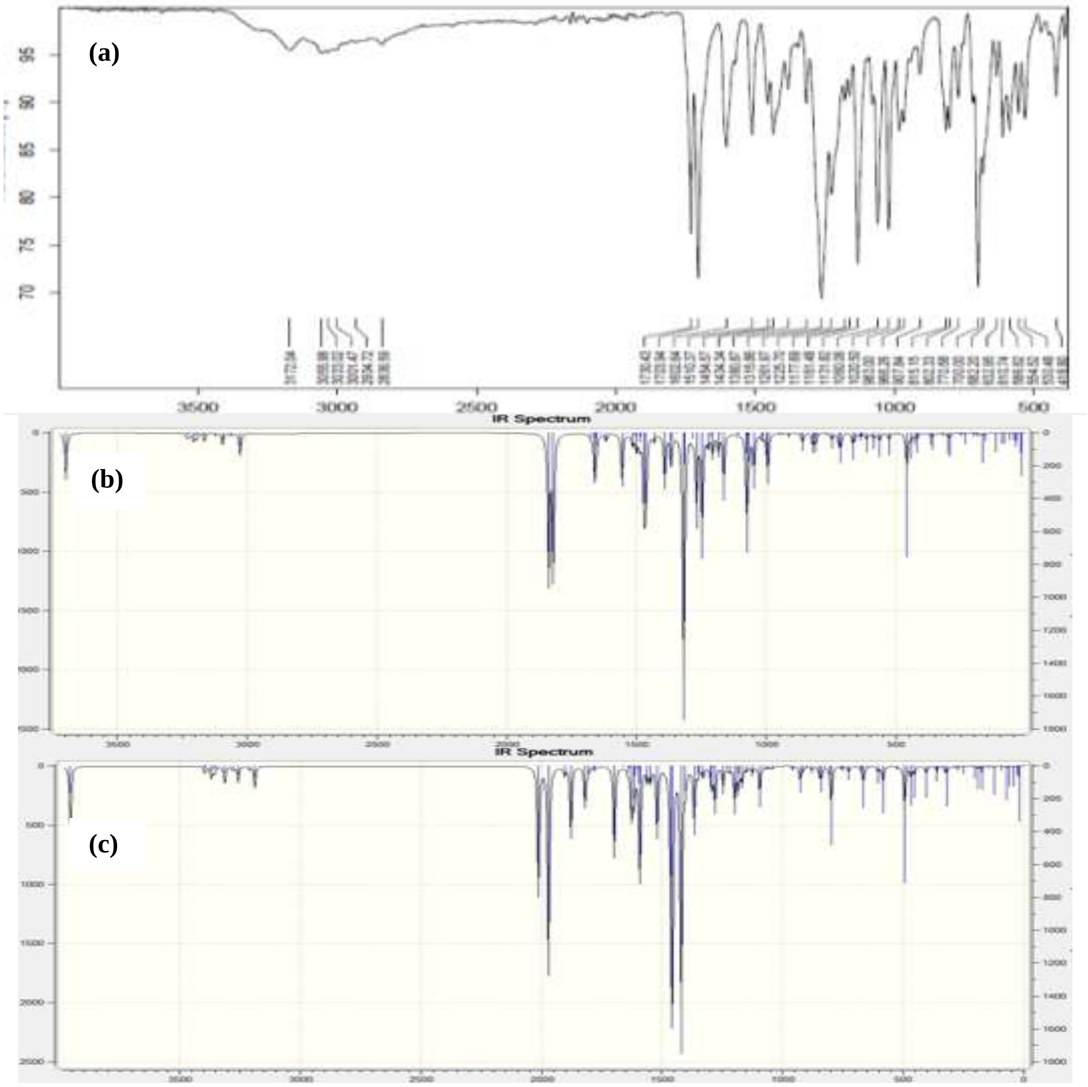
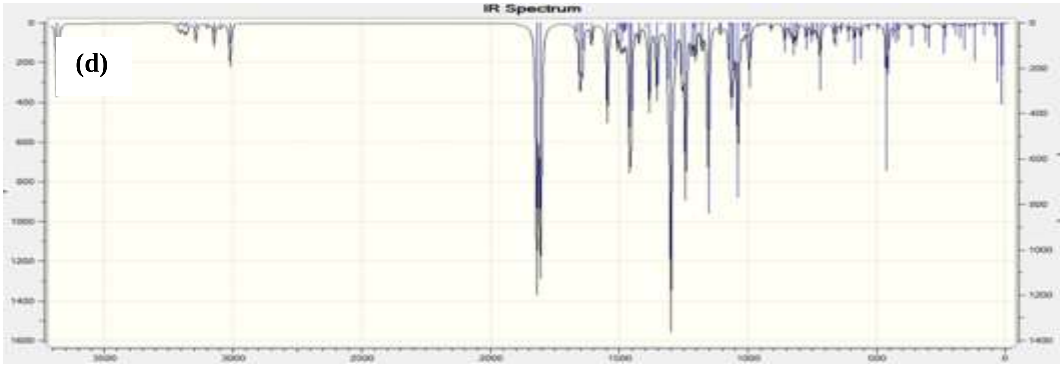


Figure 4:-Experimental **(a)** and theoretical IR spectrums and simulated with DFT/B3LYP/631G(d,p) **(b)** and HF/B3LYP/631G(d,p) **(c)** levels of the molecule.



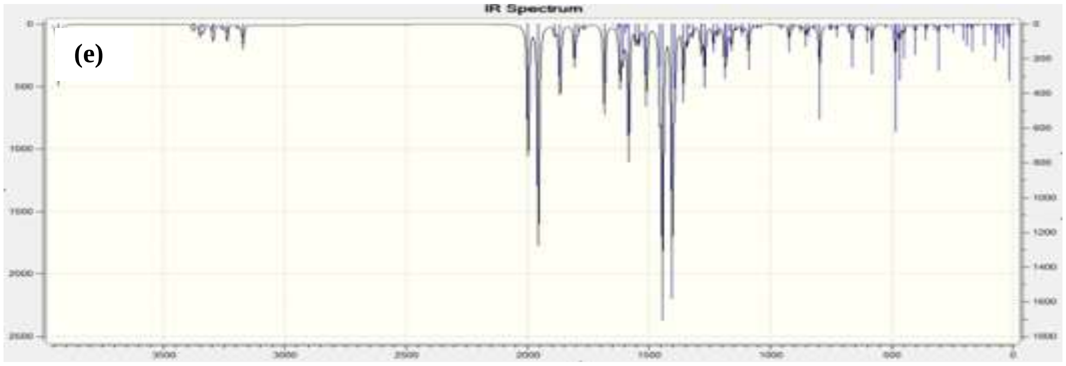
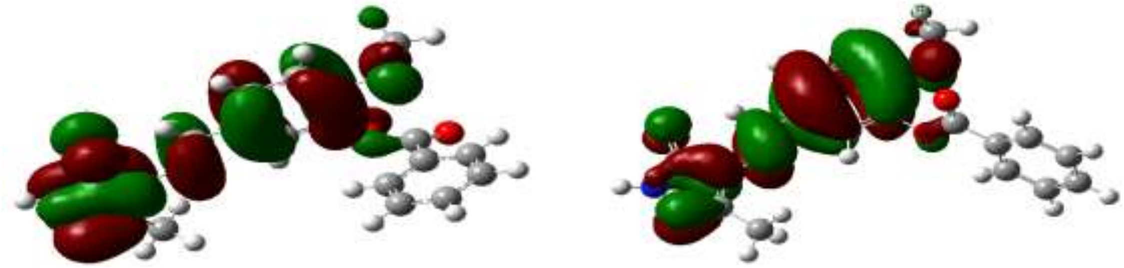


Figure 5:-Theoretical IR spectrums and simulated with DFT/B3LYP/6311G(d,p) **(d)** and HF/B3LYP/6311G(d,p) **(e)** levels of the molecule

Table 4:-The calculated bond lengths B3LYP/HF 631G(d,p) and B3LYP/HF 6311G(d,p) of the molecule.

	Bond Lengths	**DFT/631G**	**HF/631G**	**DFT/6311G**	**HF/6311G**
1	C(1)-N(35)	1.300	1.269	1.296	1.266
2	C(1)-N(37)	1.388	1.378	1.388	1.378
3	C(1)-C(18)	1.486	1.488	1.485	1.487
4	N(35)-N(36)	1.382	1.371	1.380	1.370
5	N(36)-H(19)	1.006	0.990	1.005	0.990
6	N(36)-C(2)	1.370	1.346	1.368	1.346
7	C(2)-O(39)	1.223	1.203	1.216	1.196
8	C(2)-N(37)	1.417	1.385	1.419	1.387
9	N(37)-N(38)	1.373	1.367	1.370	1.365
10	N(38)-C(3)	1.290	1.260	1.285	1.258
11	C(3)-H(20)	1.088	1.075	1.086	1.075
12	C(3)-C(4)	1.461	1.470	1.461	1.471
13	C(4)-C(5)	1.408	1.399	1.406	1.399
14	C(4)-C(9)	1.399	1.380	1.395	1.378
15	C(5)-H(21)	1.083	1.072	1.082	1.072
16	C(5)-C(6)	1.382	1.364	1.379	1.362
17	C(6)-O(40)	1.382	1.375	1.380	1.374
18	C(6)-C(7)	1.415	1.401	1.413	1.401
19	C(7)-O(41)	1.356	1.337	1.355	1.335
20	C(7)-C(8)	1.396	1.381	1.394	1.380
21	C(8)-H(22)	1.083	1.072	1.081	1.071
22	C(8)-C(9)	1.395	1.390	1.393	1.390
23	C(9)-H(23)	1.086	1.076	1.084	1.075
24	O(40)-C(10)	1.386	1.341	1.388	1.340
25	C(10)-O(42)	1.204	1.185	1.197	1.178
26	C(10)-C(11)	1.493	1.488	1.491	1.489
27	C(11)-C(12)	1.401	1.389	1.399	1.388
28	C(11)-C(16)	1.402	1.390	1.399	1.389
29	C(12)-H(24)	1.083	1.072	1.082	1.072
30	C(12)-C(13)	1.394	1.384	1.389	1.383
31	C(13)-H(25)	1.085	1.075	1.083	1.074
32	C(13)-C(14)	1.395	1.384	1.394	1.384
33	C(14)-H(26)	1.086	1.075	1.084	1.075
34	C(14)-C(15)	1.397	1.386	1.393	1.386
35	C(15)-H(27)	1.085	1.075	1.083	1.074
36	C(15)-C(16)	1.391	1.382	1.391	1.381
37	C(16)-H(28)	1.084	1.073	1.082	1.073

38	C(7)-O(41)	1.356	1.337	1.355	1.335
39	O(41)-C(17)	1.422	1.402	1.423	1.402
40	C(17)-H(29)	1.096	1.085	1.095	1.079
41	C(17)-H(30)	1.089	1.084	1.088	1.085
42	C(17)-H(31)	1.096	1.079	1.094	1.085
43	C(18)-H(32)	1.094	1.083	1.092	1.083
44	C(18)-H(33)	1.094	1.083	1.092	1.083
45	C(18)-H(34)	1.090	1.080	1.089	1.080



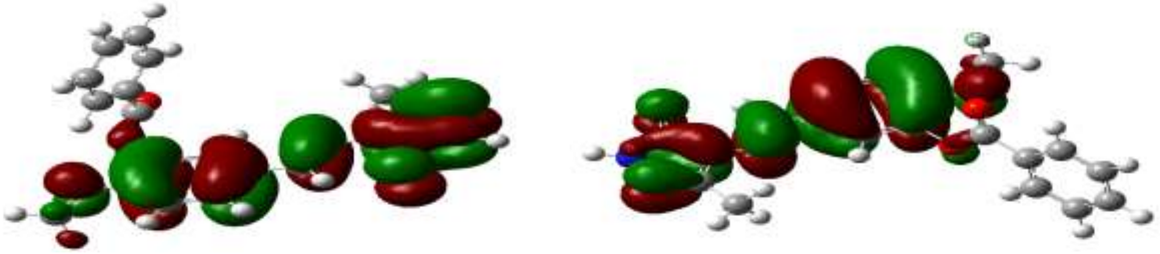
E_{HOMO} (B3LYP) : -0.21409 Hatree

E_{HOMO} (HF) : -0.30218 Hatree

E_{LUMO} (B3LYP) : -0.05666 Hatree

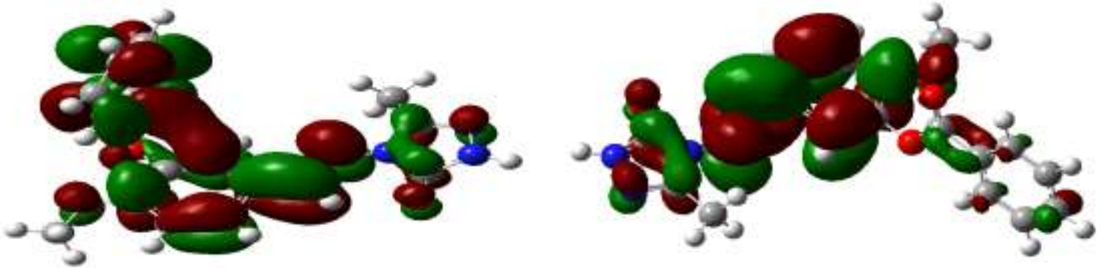
E_{LUMO} (HF) : 0.09319 Hatree

Figure 6:-HOMO-LUMO energy calculated with DFT/B3LYP/631G(d,p) and HF/B3LYP/631G(d,p) levels of the molecule.



E_{HOMO} (B3LYP) : -0.22090 Hatree

E_{HOMO} (HF) : -0.30611 Hatree



E_{LUMO} (B3LYP) : -0.06669 Hatree

E_{LUMO} (HF) : 0.08729 Hatree

Figure 7:-HOMO-LUMO energy calculated with DFT/B3LYP/6311G(d,p) and HF/B3LYP/6311G(d,p)levels of the molecule

Table 5:-The calculated mulliken charges datas B3LYP/HF 631G(d,p)/ 6311G(d,p) of the molecule

	DFT 631G	**HF 631G**		**DFT 631G**	**HF 631G**		**DFT 6311G**	**HF 6311G**		**DFT 6311G**	**HF 6311G**
C1	0.522	0.592	**H22**	0.098	0.167	**C1**	0.294	0.396	**H22**	0.111	0.115
C2	0.816	1.051	**H23**	0.100	0.171	**C2**	0.535	0.729	**H23**	0.098	0.101
C3	0.111	0.187	**H24**	0.106	0.190	**C3**	0.135	0.245	**H24**	0.111	0.119
C4	0.081	-0.106	**H25**	0.096	0.157	**C4**	-0.169	-0.199	**H25**	0.103	0.104
C5	-0.144	-0.111	**H26**	0.094	0.158	**C5**	0.016	-0.015	**H26**	0.103	0.105
C6	0.284	0.341	**H27**	0.095	0.158	**C6**	0.098	0.250	**H27**	0.099	0.105
C7	0.370	0.430	**H28**	0.116	0.196	**C7**	0.198	0.291	**H28**	0.124	0.124
C8	-0.142	-0.217	**H29**	0.121	0.117	**C8**	-0.120	-0.130	**H29**	0.114	0.119
C9	-0.136	-0.137	**H30**	0.137	0.126	**C9**	-0.050	-0.063	**H30**	0.138	0.100
C10	0.556	0.862	**H31**	0.121	0.148	**C10**	0.387	0.697	**H31**	0.120	0.091
C11	0.034	-0.191	**H32**	0.144	0.160	**C11**	-0.213	-0.293	**H32**	0.132	0.122
C12	-0.096	-0.102	**H33**	0.141	0.154	**C12**	-0.023	-0.034	**H33**	0.133	0.124
C13	-0.095	-0.165	**H34**	0.141	0.156	**C13**	-0.098	-0.092	**H34**	0.136	0.127
C14	-0.075	-0.128	**N35**	-0.335	-0.567	**C14**	-0.071	-0.077	**N35**	-0.220	-0.286
C15	-0.096	-0.164	**N36**	-0.435	-0.352	**C15**	-0.105	-0.091	**N36**	-0.312	-0.380
C16	-0.088	-0.105	**N37**	-0.411	-0.618	**C16**	-0.021	-0.035	**N37**	-0.365	-0.469
C17	-0.084	-0.034	**N38**	-0.327	-0.334	**C17**	-0.138	-0.031	**N38**	-0.215	-0.277
C18	-0.360	-0.359	**O39**	-0.542	-0.659	**C18**	-0.244	-0.182	**O39**	-0.392	-0.532
C19	0.288	0.339	**O40**	-0.528	-0.710	**C19**	0.250	0.259	**O40**	-0.322	-0.503
C20	0.157	0.227	**O41**	-0.524	-0.662	**C20**	0.140	0.164	**O41**	-0.277	-0.446
H21	0.121	0.197	**O42**	-0.432	-0.562	**H21**	0.117	0.116	**O42**	-0.338	-0.466

Table 6:-The calculated dipole moments datas B3LYP/HF 631G(d,p)/ 6311G(d,p) of the molecule

	DFT/631G	**DFT/6311G**	**HF/631G**	**HF/6311G**
μ_x	-0.9451	-0.9097	-1.6273	-1.6055
μ_y	4.1544	4.1733	5.9378	5.8610
μ_z	-0.1641	-0.1783	0.3787	0.2856
μ_{Toplam}	4.2637	4.2750	6.1684	6.0836

Results and Discussion:-

In this work, geometrical parameters and spectroscopic parameters such as IR, ^{1}H-NMR and ^{13}C-NMR spectra of molecule are calculated by Density Functional Theory (DFT) and Hartree-Fock (HF) methods with the 631G(d,p) and 6311G(d,p) two different basis sets. Obtained spectroscopic parameters are compared with experimental data. Furthermore, calculated theoretical data with the 631G(d,p) and 6311G(d,p) basis sets are compared with each other. The chemical shifts in the calculations ^{1}H-NMR and ^{13}C-NMR and IR vibrational frequencies are found to be compatible with the experimental data. Theoretical and experimental carbon and proton chemical shifts ratios between acording to a, b ve R^{2} values, lineer a correlation were observed.

Furthermore, IR vibrational frequencies experimentally carbonyl peak (C=O) in 1706 cm^{-1} and theoretically (C=O) peak in 1768 cm^{-1} for 631G(d,p), 1762 cm^{-1} for 6311G(d,p) were observed. The negative frequency in the IR data was not found. This result, structure of compound were shown stable. In addition, bond lengths, dipole moments, the HOMO-LUMO energy and mulliken charges are calculated theoretically by using the B3LYP/HF 631G(d,p) and 6311G(d,p) basis sets.

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