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Spectroscopic Aspects (Experimental/Theoretical (FT-IR, NMR)) and Electronic Properties of 3-*p*-Chlorobenzyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one

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Abstract: 3-*p*-Chlorobenzyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one were optimized using DFT(B3LYP)/HF methods and 6-311G(d) and 3-21G levels. The ^{13}C-NMR and ^{1}H-NMR (in gas phase/DMSO solvent with GIAO method), FT-IR and UV-vis spectral values were performed using Gaussian09W program package. Theoretical spectral values of the molecule were calculated and compared with experimental data. The FT-IR spectrums were drawn the same methods and levels. Furthermore, the molecular potential surfaces such as the molecular electrostatic potential (MEP), electron density, electron spin potential (ESP), total density and contour maps of titled molecule have been drawn. The electron affinity (A), electronegativity (χ), global hardness (η)/softness (σ), ionization potential (I), E_{LUMO}-E_{HOMO} energies, energy gap (ΔE), thermal capacity (CV), mulliken atomic charges, entropy (S), total energy, thermal energies (E), bond angles, dipole moments and bond lengths of the molecule were performed with Gaussian09W program.

Keywords: 1,2,4-triazol-5-one, 6-311G(d), 3-21G, GIAO, HOMO-LUMO.

1. INTRODUCTION

1,2,4-Triazol-5-on derivatived Schiff bases are the most important organic compounds that obtained by condensation between a primary amine and an aldehyde or ketone to form an imine or azomethine group (-HC=N-) (Du et al., 2018; Jiao et al., 2018; Akın et al., 2019; Gao et al., 2019; Irak ve Beytur, 2019; Özil et al., 2019). It is known that many compounds have numerous biological activities. The derivatives of 1,2,4-triazole form a broad family of compounds that exhibit wide range of interesting properties; several of them show biological and pharmacological activities such as anti-depressants, antiparasitic, anticancer, antibacterial, anti-inflammatory and fungicides while these compounds find use in coordination chemistry and material field (non-linear optics properties magnetic and multidentate ligands) (Yüksek et al., 2013; Madeira et al., 2018; Mohameda et al., 2018; Beytur et al., 2019; Kukuljan and Kranjc, 2019) 1,2,4-Triazol-5-on derivatived Schiff bases

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are used as fungicides, insecticides, pesticides, bacteriocides as well. (Cui et al., 2002; Saadaoui et al., 2019). Recently, these compounds have also begun to draw attention with quantum chemical calculations. On the other hand, it is known that were intensively studied and numerous of their properties are highlighted by spectroscopic, optical, structural, thermal and theoretical calculations methods. In addition, it is reported in literature that the derivatives of 1,2,4-triazole are playing important role in biochemical processes ranging from anticancer to antioxidants and antiviral agents (Akyıldırım et al., 2016; Özdemir et al., 2018; Kotan and Yüksek, 2018; Boursas et al., 2019; Raouf et al., 2019).

We investigate in the present work, vibrational spectroscopy, $^{1}H/^{13}C$-NMR isotropic shift values, UV-vis. spectroscopy, structural, thermodynamic, electronic properties and theoretical calculations of 3-*p*-chlorobenzyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one were investigated by both experimental and DFT(B3LYP) and ab initio HF methods.

2. MATERIALS AND METHODS

2.1. Theoretical Details

The theoretical calculations have been performed with density functional theory (DFT) and Hartree-Fock (HF) methods and 6-311G(d)/3-21G levels on the Gaussian09W program package (Frisch et al., 2010). Firstly, the above cited compound was optimized and then calculated $^{13}C/^{1}H$-NMR isotropic shift values with method of GIAO (Wolinski et al., 1990), vibrational spectroscopy, UV-vis. spectroscopy, structural, thermodynamic, electronic properties. Furthermore, the HOMO-LUMO energy, molecular electrostatic potential (MEP), electron density, electron spin potential (ESP), total density and contour maps of titled molecule have been performed and drawn with the same methods and levels.

3. RESULT AND DISCUSSION

3.1. The Structural Results

The structural geometric values such as mulliken atomic charges, bond angles, bond lengths have been calculated by HF and B3LYP methods with 6-311G(d)/3-21G levels and The structural values are summarized in Table **1**-**3**. when the results are evaluated the average aromatic bond lengths (C-C) are 1.425 (B3LYP/6-311G(d)), 1.419 (HF/6-311G(d)), 1.424 ((B3LYP/3-21G) and 1.414 (HF/3-21G) Å. Also, the bond lengths of 1,2,4-triazole ring N25-N26, N25-C1, C2-O29, C2-N27, N27-C1 are calculated as 1,380/1.370/1.369; 1,297/1.295/1,268; 1.216/1,214/1.196; 1.420/1.415/1.387 Å, respectively for B3LYP/HF

methods and 6-311G(d) and 3-21G levels (Table **1**). In the literature, the N-N, N=C, C=O bond lengths are measured as 1.404 , 1.280, 1.212 Å (Ocak et al., 2003; Ustabaş et al., 2007). The calculated bond length values are consistent with literature values. All atomic charges (Mulliken, 1955) were calculated by the same methods and levels. All electronegative atoms (oxygen (O) nitrogen (N), and chlorine (Cl)) have negative atomic charge values. The carbon atoms that weren't surrounded electronegative atoms have negative atomic charge values. On the other hand, the C1 atom surrounded by two electronegative atoms (N25, N27) and C2 atom which is surrounded by three electronegative atoms (N26, N27, O29) have negative charges values. All hydrojen atoms of titled molecule (H25-H43) have positive atomic charge values (Table **3**).

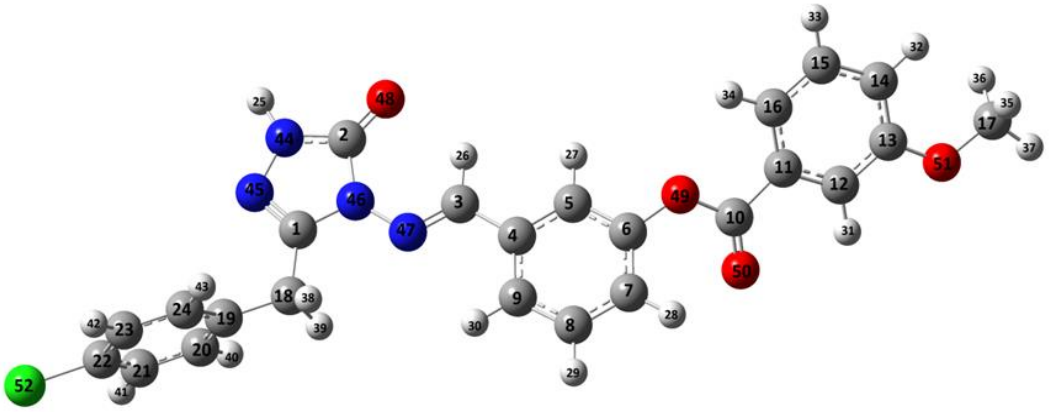


Figure 1. The Gaussview structure of the molecule.

Table 1. The calculated bond lenghts (A^0) of the molecule

	Bond Lenghts (A^0)	**HF 6-311G(d)**	**B3LYP 6-311G(d)**	**HF 3-21G**	**B3LYP 3-21G**
1	C1-N45	1.2651	1.2948	1.2776	1.3122
2	C1-N46	1.3802	1.3889	1.3817	1.3887
3	C1-C18	1.4987	1.4983	1.4937	1.4953
4	C18-C19	1.5116	1.5120	1.5130	1.5290
5	C18-H38	1.0838	1.0949	1.0835	1.0928
6	C18-H39	1.0837	1.0947	1.0835	1.0930
7	C19-C20	1.3865	1.3964	1.3854	1.3993
8	C19-C24	1.3865	1.3960	1.3854	1.4011
9	C20-H40	1.0757	1.0858	1.0721	1.0842
10	C20-C21	1.3835	1.3917	1.3834	1.3974
11	C21-H41	1.0732	1.0833	1.0695	1.0817
12	C21-C22	1.3804	1.3902	1.3728	1.3861
13	C22-Cl52	1.7456	1.7611	1.8183	1.8345
14	C22-C23	1.3804	1.3899	1.3728	1.3872
15	C23-H42	1.0732	1.0834	1.0695	1.0818
16	C23-C24	1.3835	1.3920	1.3834	1.3958
17	C24-H43	1.0756	1.0858	1.0721	1.0829
18	N44-N45	1.3679	1.3783	1.4263	1.4365
19	N44-H25	0.9886	1.0054	0.9919	1.0088
20	N44-C2	1.3470	1.3696	1.3539	1.3758
21	C2-O48	1.1950	1.2145	1.2196	1.2389
22	C2-N46	1.3885	1.4214	1.3950	1.4327
23	N46-N47	1.3637	1.3698	1.4030	1.4181

24	N47-C3	1.2583	1.2865	1.2678	1.2982
25	C3-H26	1.0713	1.0843	1.0630	1.0780
26	C3-C4	1.4770	1.4645	1.4637	1.4558
27	C4-C5	1.3854	1.4074	1.3915	1.4123
28	C4-C9	1.3959	1.4038	1.3874	1.4028
29	C5-O49	1.3773	1.3781	1.3970	1.4086
30	C5-C6	1.3835	1.3945	1.3833	1.3969
31	C6-H27	1.0733	1.0840	1.0630	1.0758
32	C6-C7	1.3779	1.3898	1.3828	1.3950
33	C7-H28	1.0748	1.0849	1.0716	1.0836
34	C7-C8	1.3898	1.3962	1.3839	1.3984
35	C8-H29	1.0746	1.0845	1.0710	1.0831
36	C8-C9	1.3761	1.3862	1.3786	1.3896
37	C9-H30	1.0726	1.0834	1.0700	1.0827
38	O49-C10	1.3437	1.3964	1.3625	1.3999
39	C10-O50	1.1780	1.1961	1.2053	1.2279
40	C10-C11	1.4900	1.4891	1.4795	1.4803
41	C11-C12	1.3794	1.3925	1.3779	1.3940
42	C11-C16	1.3940	1.4036	1.3928	1.4068
43	C12-H31	1.0710	1.0819	1.0678	1.0805
44	C12-C13	1.3923	1.3992	1.3917	1.4041
45	C13-O51	1.3456	1.3603	1.3681	1.3830
46	C13-C14	1.3833	1.3976	1.3804	1.3986
47	C14-H32	1.0726	1.0826	1.0694	1.0814
48	C14-C15	1.3918	1.3973	1.3879	1.3986
49	C15-H33	1.0749	1.0850	1.0714	1.0835
50	C15-C16	1.3746	1.3854	1.3727	1.3863
51	C16-H34	1.0722	1.0827	1.0691	1.0815
52	O51-C17	1.3975	1.4199	1.4349	1.4589
53	C17-H35	1.0785	1.0952	1.0834	1.0971
54	C17-H36	1.0848	1.0881	1.0722	1.0900
55	C17-H37	1.0851	1.0953	1.0834	1.0971

Table 2. The calculated bond angles (^{0}) of the molecule

	Bond Angles (^{0})	**HF**	**B3LYP**	**HF**	**B3LYP**
		6-311G(d)	**6-311G(d)**	**3-21G**	**3-21G**
1	C1-N45-N44	105.059	104.740	104.136	103.281
2	C1-N46-N47	121.157	121.325	120.435	120.701
3	C1-N46-C2	108.028	108.189	109.187	109.217
4	C1-C18-H38	108.025	108.316	108.085	108.272
5	C1-C18-H39	108.029	108.276	108.083	108.272
6	N45-N44-H25	120.716	120.194	119.993	119.350
7	N45-N44-C2	113.825	114.545	112.920	114.045
8	N45-C1-C18	126.725	126.192	127.152	126.275
9	N46-C1-C18	121.974	122.355	121.132	121.141
10	H25-N44-C2	125.459	125.261	127.087	126.605
11	N44-C2-N46	101.787	101.072	102.042	101.143
12	N44-C2-O48	129.599	130.145	130.279	130.933
13	O48-C2-N46	128.614	128.783	127.679	127.923
14	C2-N44-N45	113.825	114.545	112.920	114.045
15	C2-N46-N47	130.812	130.485	130.378	130.082
16	C1-C18-C19	113.582	113.546	112.307	112.379
17	H38-C18-C19	110.609	110.605	110.769	110.683
18	H39-C18-C19	110.610	110.613	110.768	110.682
19	H38-C18-H39	105.630	105.102	106.608	106.323
20	C18-C19-C20	120.748	120.821	120.487	120.508
21	C18-C19-C24	120.744	120.725	120.494	120.507

22	C19-C20-H40	119.886	119.755	119.881	119.725
23	C19-C24-H43	119.889	119.765	119.884	119.725
24	C19-C20-C21	121.131	121.202	120.771	120.864
25	H40-C20-C21	118.983	119.043	119.349	119.411
26	C20-C21-C22	119.166	119.053	118.727	118.484
27	C20-C21-H41	120.652	120.765	120.981	121.136
28	H41-C21-C22	120.182	120.183	120.291	120.380
29	C21-C22-C23	120.901	121.033	121.986	122.319
30	C21-C22-Cl52	119.547	119.488	119.006	118.841
31	Cl52-C22-C23	119.552	119.479	119.008	118.841
32	C22-C23-H42	120.185	120.186	120.293	120.380
33	C22-C23-C24	119.167	119.054	118.727	118.484
34	H42-C23-C24	120.648	120.760	120.980	121.136
35	C23-C24-H43	118.983	119.031	119.345	119.411
36	H43-C24-C19	119.889	119.765	119.884	119.725
37	C24-C19-C20	118.507	118.455	119.018	118.985
38	N46-N47-C3	119.992	119.158	119.012	117.196
39	N47-C3-H26	122.295	121.900	122.459	122.349
40	N47-C3-C4	120.468	120.363	120.137	119.776
41	H26-C3-C4	117.237	117.737	117.404	117.875
42	C3-C4-C5	117.988	118.133	117.774	117.947
43	C3-C4-C9	119.879	122.788	121.685	121.685
44	C5-C6-O49	118.002	115.727	124.889	125.421
45	C4-C5-C6	119.879	120.217	119.063	119.186
46	H27-C5-C6	119.127	118.951	119.990	119.753
47	C4-C5-H27	120.993	120.832	120.947	121.061
48	C5-C6-C7	121.105	120.950	120.796	120.612
49	O49-C6-C7	120.812	123.215	114.314	113.967
50	C6-C7-H28	120.025	120.548	118.710	118.552
51	C6-C7-C8	118.976	118.664	119.719	119.832
52	H28-C7-C8	120.998	120.783	121.571	121.616
53	C7-C8-H29	119.438	119.052	119.587	119.508
54	C7-C8-C9	120.690	121.139	120.319	120.347
55	H29-C8-C9	119.872	119.809	120.093	120.146
56	C8-C9-H30	120.474	120.793	121.084	121.518
57	C8-C9-C4	119.936	119.950	119.561	119.655
58	H30-C9-C4	119.590	119.258	119.355	118.827
59	C9-C4-C5	119.414	119.079	120.541	120.368
60	C6-O49-C10	119.934	121.342	128.220	125.475
61	O49-C10-O50	123.339	123.702	123.427	124.123
52	O49-C10-C11	111.914	111.141	111.459	110.215
63	O50-C10-C11	124.747	125.157	125.114	125.662
64	C10-C11-C16	122.175	122.693	122.038	122.595
65	C10-C11-C12	117.234	116.980	116.958	116.565
66	C11-C12-H31	120.470	120.165	120.627	120.143
67	C11-C12-C13	120.283	120.340	120.062	120.241
68	H31-C12-C13	119.247	119.495	119.312	119.616
69	C12-C13-O51	115.787	115.696	116.042	115.821
70	C12-C13-C14	119.424	119.513	119.354	119.182
71	C13-O51-C17	119.951	118.632	120.972	118.220

72	O51-C13-C14	124.789	124.791	124.604	124.997
73	O51-C17-H35	111.461	111.557	111.303	111.601
74	O51-C17-H36	111.456	111.528	111.303	111.600
75	O51-C17-H37	106.187	105.746	105.460	104.860
76	H35-C17-H36	109.435	109.427	109.452	109.316
77	H35-C17-H37	109.102	109.234	109.621	109.686
78	H36-C17-H37	109.107	109.251	109.621	109.686
79	C13-C14-C15	119.790	119.677	120.134	120.139
80	H32-C14-C15	119.097	119.304	119.173	119.231
81	C14-C15-H33	119.033	119.062	119.259	119.180
82	H33-C15-C16	119.836	119.795	119.945	119.916
83	C15-C16-H34	120.741	120.821	121.392	121.675
84	C15-C16-C11	118.780	119.000	118.651	118.694
85	C16-C11-C12	120.592	120.326	121.004	120.840
86	H34-C16-C11	120.480	120.179	119.957	119.631

Table 3. The Mulliken atomic charges of the molecule

	HF	**HF**	**B3LYP**	**B3LYP**
	6-311G(d)	**3-21G**	**6-311G(d)**	**3-21G**
C1	0.569	0.818	0.450	0.680
C2	0.782	1.250	0.584	0.942
C3	0.038	0.197	-0.055	0.111
C4	-0.044	-0.165	-0.016	-0.056
C5	-0.270	-0.24	-0.234	-0.211
C6	0.328	0.384	0.231	0.301
C7	-0.211	-0.253	-0.178	-0.191
C8	-0.208	-0.227	-0.205	-0.183
C9	-0.194	-0.204	-0.158	-0.173
C10	0.647	1.008	0.434	0.707
C11	-0.203	-0.246	-0.160	-0.107
C12	-0.241	-0.199	-0.203	-0.165
C13	0.369	0.417	0.272	0.322
C14	-0.300	-0.267	-0.259	-0.207
C15	-0.195	-0.227	-0.193	-0.182
C16	-0.211	-0.209	-0.160	-0.182
C17	-0.416	-0.273	-0.464	-0.336
C18	-0.586	-0.505	-0.589	-0.514
C19	0.064	-0.034	0.081	0.045
C20	-0.216	-0.203	-0.187	-0.166
C21	-0.128	-0.187	-0.115	-0.154
C22	-0.163	-0.318	-0.167	-0.261
C23	-0.128	-0.187	-0.115	-0.154
C24	-0.216	-0.203	-0.186	-0.166
H25	0.400	0.405	0.374	0.356
H26	0.307	0.332	0.260	0.264
H27	0.241	0.325	0.217	0.247
H28	0.238	0.268	0.228	0.207
H29	0.228	0.253	0.203	0.196
H30	0.242	0.270	0.210	0.205

H31	0.264	0.305	0.229	0.230
H32	0.242	0.255	0.229	0.197
H33	0.225	0.251	0.216	0.196
H34	0.244	0.274	0.200	0.205
H35	0.208	0.200	0.211	0.200
H36	0.208	0.200	0.212	0.200
H37	0.234	0.239	0.233	0.227
H38	0.268	0.274	0.251	0.243
H39	0.268	0.274	0.252	0.243
H40	0.222	0.253	0.197	0.197
H41	0.252	0.277	0.223	0.218
H42	0.252	0.277	0.223	0.218
H43	0.223	0.253	0.197	0.197
N44	-0.592	-0.759	-0.497	-0.592
N45	-0.247	-0.384	-0.185	-0.335
N46	-0.478	-0.856	-0.373	-0.629
N47	-0.275	-0.364	-0.206	-0.324
O48	-0.530	-0.668	-0.389	-0.518
O49	-0.510	-0.815	-0.369	-0.600
O50	-0.436	-0.616	-0.319	-0.480
O51	-0.461	-0.735	-0.337	-0.550
Cl52	-0.111	0.093	-0.081	0.082

3.2. FT-IR spectral analysis

3-*p*-Chlorobenzyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one have 52 atoms. The numbers of all vibrational frequencies of titled compound is 150. The vibrational frequencies have been performed with veda4f program and each vibrational frequencies were multiplied by appropriate scala factors (Merrich et al., 2007). The negative frequency values weren't observed. The unscaled IR spectrums were drawn according to DFT(B3LYP), HF methods and 6-311G(d)/3-21G levels. Between the two values were observed connected and consistent results (Table **4-5** and Figure **2**).

Table 4. The calculated IR frequencies of titled compound (cm^{-1}) (6-311G(d))

	Vibrational Frequencies	**HF**	**B3LYP**
1	τ NCCC(35), τ CCCN(23), τ COCC(18)	**5**	**4**
2	τ CNNC(25), τ COCC(61), τ CCCC(11), τ NCCC(14)	**6**	**8**
3	τ CCCC(12), τ COCC(32), τ CCOC(47)	**14**	**10**
4	δ CCN(10), τ CCOC(30), τ NCCC(24), τ CCCC(36)	**16**	**15**
5	τ CNNC(15), τ CCOC(16), τ CCCC(13), δ NCC(12)	**27**	**27**
6	τ CNNC(12), τ CCOC(11), τ CCCC(33), τ NCCC(27)	**29**	**28**
7	τ CCCC(18)	**43**	**48**
8	τ CCOC(11), τ CCNN(13)	**56**	**54**
9	δ COC(13), τ CCCN(12), τ CCNN(14)	**62**	**62**
10	δ CCO(13), δ COC(13)	**65**	**66**
11	τ HCOC(11), τ CCCC(13), τ COCC(64)	**70**	**83**
12	τ CNNC(29), τ NNCC(20), τ NCCC(14), τ CCCN(11)	**106**	**109**
13	δ NCC(19)	**124**	**118**
14	δ CCC(15), τ CCCC(24), τ ClCCC(20)	**147**	**139**
15	τ CNNC(20), τ NNCC(17), τ NCNC(10), τ NCCC(12)	**152**	**155**
16	τ CCCN(12)	**163**	**165**
17	τ CCCC(21)	**178**	**172**

18	τ CCCC(20)	**195**	**190**
19	τ HCOC(20), τ CCCC(27), τ COCC(12),τ OCCC(22), τ CCCN(20)	**223**	**213**
20	δ NCN(12), τ HCOC(20), τ CCCC(30),τ OCCC(11)	**225**	**222**
21	τ CCCN(40), τ NNCC(21), δ CNN(11), δ CCC(10), δ NNC(11)	**228**	**238**
22	δ ClCC(47), τ CNNC(12), δ CCC(10)	**255**	**248**
23	δ COC(27), τ CCCN(17)	**267**	**258**
24	τ HCOC(41), τ CCCC(26), δ ClCC(11), τ HNNC(20), τ NNCC(39)	**288**	**278**
25	τ HNNC(18), τ HCCC(11), τ CNNC(22), τ NNCC(19), τ CCCC(24), τ HCOC(40)	**292**	**286**
26	δ COC(20), τ CCCN(12), δ OCO(14)	**307**	**292**
27	δ OCO(13), δ COC(17)	**311**	**300**
28	τ CCCC(19), τ ClCCC(33)	**326**	**310**
29	τ CCCN(10), τ CCNN(35)	**361**	**346**
30	δ CCC(22), δ ClCC(29)	**379**	**366**
31	δ NCN(10), δ NNC(14), δ OCN(11), δ COC(12)	**401**	**378**
32	ν ClC(27), δ OCN(13), δ CCC(10)	**433**	**414**
33	τ HCCC(17), τ CCCC(81)	**435**	**415**
34	δ CCC(38), τ HNNC(26), δ COC(11)	**439**	**429**
35	τ CCCC(47)	**460**	**440**
36	τ HNNC(55), τ ONNC(10)	**462**	**454**
37	τ HNNC(26), δ CCC(38), δ COC(11), τ HCCC(11), τ CCCN(18)	**481**	**457**
38	τ HNNC(12), τ HCCC(11), δ COC(10)	**487**	**465**
39	δ CCO(10), δ CCC(20)	**504**	**491**
40	τ HCCC(23), τ CCCC(18), τ ClCCC(22)	**527**	**501**
41	δ COC(13), τ HCCC(11), τ CCCC(13),τ OCOC(10),τ OCCC(36), δ CCC(13)	**581**	**551**
42	δ CCC(18), δ COC(16),τ OCCC(15)	**582**	**566**
43	δ CCC(12)	**596**	**577**
44	δ OCN(10), δ CCO(10)	**609**	**590**
45	τ CCCN(18), τ COCC(11), τ CCOC(11)	**625**	**598**
46	δ CCC(27), δ OCN(14)	**639**	**618**
47	δ CCC(46)	**662**	**643**
48	τ HNNC(10), τ NNCC(11), τ NCNC(35), ν CC(12), ν ClC(21), δ CCC(15)	**687**	**656**
49	ν CC(11), ν ClC(22), δ CCC(19), τ HNNC(11), τ HCCC(12)	**689**	**664**
50	τ HCCC(12), δ CCC(20)	**706**	**683**
51	τ HCCC(28), τ CCCC(17)	**716**	**683**
52	τ HCCC(20), τ CCCC(40)	**719**	**691**
53	τ HCCC(29), τ CCCC(20), τ CCCN(19)	**725**	**693**
54	τ CCCC(14)	**767**	**738**
55	τ ONNC(76)	**802**	**738**
56	τ HCCC(24),τ OCOC(45)	**808**	**753**
57	τ HCCC(18), τ CNNC(10), τ ONNC(83)	**813**	**770**
58	τ HCCC(34), ν NC(12), ν CC(11), δ CNN(12)	**824**	**786**
59	ν NC(15), δ CNN(32), τ HCCC(32)	**832**	**792**
60	τ HCCC(51),τ OCOC(25), ν CC(15)	**851**	**802**
61	ν CC(14), τ HCCC(50),τ OCOC(28)	**861**	**819**
62	τ HCCC(99)	**864**	**821**
63	δ OCO(17), τ HCCC(99)	**886**	**822**
64	δ NCN(15), δ CCN(12)	**887**	**837**
65	τ HCCC(71), τ CCCC(15)	**909**	**859**
66	ν OC(19), τ HCCC(18)	**926**	**880**
67	τ HCCC(40), τ CCCC(10)	**966**	**891**
68	τ HCCC(38), τ CCOC(10)	**967**	**894**
69	τ HCCC(49), ν CC(11), δ HCC(31), τ CCCC(10)	**973**	**913**
70	τ HCCC(40)	**982**	**918**
71	δ HCC(32), τ HCCC(30), τ CCCC(11), ν OC(10), ν CC(11)	**985**	**931**
72	τ HCCC(84), τ CCCC(13)	**995**	**944**
73	τ HCCC(71), τ CCCC(18)	**1019**	**946**
74	ν CC(29), δ CCC(24)	**1027**	**960**
75	τ HCCC(84), τ CCCC(14)	**1033**	**962**
76	τ HCCC(56), ν CC(19), δ CCC(39)	**1035**	**969**
77	ν CC(28), δ CCC(29), τ HCCC(46)	**1044**	**1002**
78	τ HCNN(88), τ HCCC(57), τ CCCC(11)	**1049**	**1005**
79	ν CC(25), δ CCC(61), δ HCC(10)	**1055**	**1007**
80	δ CCC(43), δ NNC(15), τ HCNN(86)	**1083**	**1025**
81	δ CCC(13), δ NNC(38), δ CNN(14)	**1089**	**1026**
82	ν OC(62), ν CC(59), δ HCC(20)	**1117**	**1062**
83	ν OC(41), δ HCC(17), δ CCC(10)	**1126**	**1087**
84	ν NC(12), ν NN(35), ν CC(12), δ HCC(25)	**1129**	**1089**
85	ν CC(54), ν ClC(19), δ HCC(14), ν OC(11)	**1137**	**1092**
86	ν CC(48), δ HCC(22), ν OC(11), ν ClC(19)	**1138**	**1104**
87	ν CC(30), δ HCC(34)	**1142**	**1109**
88	ν CC(19), δ HCC(55)	**1151**	**1124**
89	δ HCC(25), ν NC(10), ν NN(30), δ HNN(10)	**1159**	**1158**
90	δ HCH(25), τ HCOC(26), ν CC(36)	**1168**	**1171**
91	ν CC(21), δ HCC(30), τ HCCC(12)	**1191**	**1185**
92	ν CC(13), δ HCC(48)	**1211**	**1187**
93	ν CC(22), δ HCC(70), δ HCH(25), τ HCOC(26)	**1232**	**1197**

94	δ HCH(13), τ HCOC(22), ν CC(25), δ HCC(64)	**1235**	**1199**
95	ν NC(19), ν NN(16), δ OCN(10), δ HCC(11)	**1251**	**1204**
96	ν CC(11), δ HCC(39), τ HCCC(26)	**1251**	**1207**
97	ν CC(20), δ HCC(14), τ HCCC(11)	**1261**	**1217**
98	ν OC(10), ν CC(11), δ HCC(12)	**1267**	**1223**
99	ν CC(14), ν NC(25), ν NN(13), δ CNN(14)	**1276**	**1254**
100	ν NN(11), τ HCCC(11), ν CC(12), δ HCC(48), τ HCCC(17)	**1288**	**1275**
101	ν CC(23), ν OC(16)	**1312**	**1285**
102	δ HCC(24), ν OC(16), ν CC(23)	**1326**	**1305**
103	δ HCC(24), ν NC(10), δ CNN(16), τ HCCC(23)	**1351**	**1310**
104	ν CC(51), δ HCC(31), ν OC(18)	**1368**	**1311**
105	δ HCC(26), τ HCCC(21)	**1373**	**1323**
106	ν CC(11), δ HCC(74)	**1377**	**1335**
107	ν CC(20), δ HCC(80)	**1383**	**1343**
108	ν CC(62), δ HCC(17), ν NC(11), ν NN(16), δ CNN(16), τ HCCC(14)	**1410**	**1349**
109	δ HNN(29), δ HCN(47), τ HCCC(15)	**1464**	**1391**
110	δ HNN(43), δ HCN(19), ν CC(30), δ HCC(37)	**1484**	**1401**
111	ν CC(30), δ HCC(38), ν OC(12), δ HNN(64)	**1485**	**1431**
112	ν CC(23), ν NC(13)	**1507**	**1441**
113	ν CC(28), δ HCC(14)	**1525**	**1462**
114	ν CC(18), δ HCN(11), δ HCH(74)	**1535**	**1467**
115	δ HCH(88), δ HCN(17), τ HCCC(15)	**1542**	**1477**
116	δ HCH(60)	**1546**	**1480**
117	δ HCH(74), τ HCOC(13)	**1562**	**1498**
118	δ HCH(71), τ HCOC(12)	**1570**	**1509**
119	δ HCC(41), δ HCH(16), δ CCC(13)	**1574**	**1511**
120	δ HCC(24), δ CCC(10)	**1577**	**1514**
121	ν CC(12), δ HCC(60), δ CCC(11)	**1587**	**1519**
122	ν CC(29), δ HCC(11), δ CCC(12)	**1679**	**1603**
123	ν CC(33), δ CCC(15)	**1691**	**1607**
124	δ HCH(60), ν CC(33), δ HCC(11), δ CCC(11)	**1696**	**1610**
125	ν NC(28), ν CC(46), δ HCC(21)	**1713**	**1628**
126	ν NC(17), ν CC(21)	**1717**	**1632**
127	ν NC(14), ν CC(35), δ HCC(10)	**1719**	**1635**
128	ν CC(63), ν NC(42)	**1772**	**1638**
129	ν NC(44), ν CC(11)	**1801**	**1653**
130	ν OC(88), ν NC(12)	**1865**	**1784**
131	ν OC(88), ν NC(12)	**1903**	**1792**
132	ν CH(91)	**3030**	**2982**
133	ν CH(99)	**3066**	**3016**
134	ν CH(50)	**3086**	**3040**
135	ν CH(99)	**3096**	**3041**
136	ν CH(46)	**3149**	**3116**
137	ν CH(46)	**3182**	**3137**
138	ν CH(46)	**3183**	**3139**
139	ν CH(70)	**3188**	**3140**
140	ν CH(46)	**3191**	**3146**
141	ν CH(41)	**3200**	**3149**
142	ν CH(66)	**3216**	**3158**
143	ν CH(73)	**3216**	**3172**
144	ν CH(76)	**3217**	**3173**
145	ν CH(41)	**3219**	**3176**
146	ν CH(67)	**3220**	**3178**
147	ν CH(41)	**3226**	**3185**
148	ν CH(56)	**3236**	**3195**
149	ν CH(97)	**3239**	**3203**
150	ν NH(100)	**3769**	**3654**

*ν, stretching; δ, bending; τ, torsion

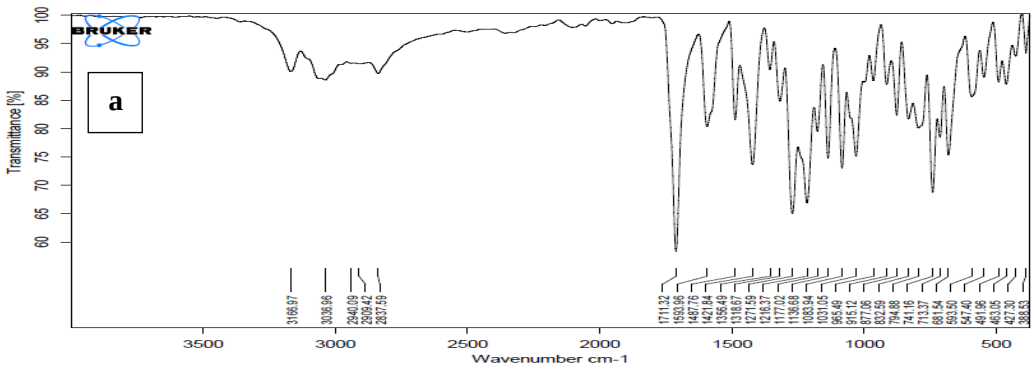
Table 5. The calculated IR frequencies of titled compound (cm^{-1}) (3-21G)

	Vibrational Frequencies	**HF**	**B3LYP**
1	τ CNNC(12), τ NCNC(24), τ CCCC(26)	**5**	**5**
2	τ CNNC(13), τ CCCC(37), τ CCCN(13)	**7**	**14**
3	δ CCC(10), δ CNN(16), δ CCN(16), τ CCCC(13), τ CCOC(18),τ COCC(51)	**17**	**17**
4	τ CCOC(28), τ COCC(51), τ CCCC(11)	**18**	**18**
5	τ NCNC(25), τ CCCC(26), τ CCOC(17)	**22**	**21**
6	τ CNNC(11), τ CCCC(11), τ CCOC(24), τ CCCN(16)	**31**	**34**
7	δ COC(21), τ CCCC(18)	**40**	**39**
8	τ NCNC(10), τ CCNN(41), τ COCC(24)	**63**	**63**
9	δ CNN(11), δ CCN(12), τ CCCC(13)	**64**	**64**
10	τ HCOC(11), τ COCC(56), τ CCNN(12)	**67**	**78**
11	τ CCCC(22), τ COCC(27), δ CCO(20), δ CCC(13)	**87**	**94**

12	δ CCC(13), δ CCO(20), τ CCCC(18), τ COCC(13)	**95**	**95**
13	τ CNNC(22), τ NCNC(17), τ CCCN(12), τ NNCC(23)	**120**	**120**
14	δ CCC(14), τ CCCC(30), τ ClCCC(20)	**142**	**136**
15	τ CNNC(20),τ CCCC(10), τ CCNN(13),τ CCCN(17)	**165**	**160**
16	τ CCCN(31), τ CCCC(23)	**176**	**174**
17	ν CC(10), δ CNN(11), δ COC(11)	**183**	**184**
18	δ NCC(12), δ CCN(10), δ COC(30)	**196**	**197**
19	τ HCOC(44), τ COCC(10), τ CCCC(13), τ OCCC(18)	**210**	**208**
20	δ CNN(11), δ CCO(10)	**215**	**214**
21	δ ClCC(60)	**236**	**230**
22	τ CCCN(36), τ CCCC(13), τ CCNN(15)	**263**	**257**
23	δ COC(39)	**265**	**266**
24	τ HCOC(18), τ CCCC(31), τ OCCC(10)	**273**	**268**
25	τ CNNC(14), τ CCCN(27), τ CCNN(25), τ OCCC(10)	**280**	**286**
26	τ CCCC(16), τ ClCCC(32), δ COC(17)	**310**	**304**
27	δ COC(17), τ ClCCC(30), τ CCCC(18)	**319**	**311**
28	τ NCNC(31), τ NNCC(19)	**338**	**323**
29	δ CCC(23), δ ClCC(22), τ HCCC(11), δ COC(18), δ OCO(16)	**356**	**349**
30	δ OCO(19), δ CCC(22), δ ClCC(19), τ HCCC(12)	**360**	**350**
31	τ CCCN(10), τ CCNN(29), τ NNCC(15)	**370**	**354**
32	ν ClC(37), δ OCN(14)	**405**	**396**
33	τ HCCC(17), τ CCCC(80), δ CCC(17)	**422**	**416**
34	τ HCCC(19), τ CCCC(80)	**433**	**416**
35	δ CCC(23), δ COC(10)	**438**	**434**
36	τ CCCC(48)	**464**	**446**
37	τ HCCC(20), τ CCCN(19), τ CCOC(16), τ CCCC(18)	**485**	**467**
38	δ CCC(20)	**491**	**485**
39	τ HCCC(24), τ CCCC(24), τ ClCCC(21)	**520**	**492**
40	τ HNNC(89), δ CCC(17), δ COC(19)	**557**	**542**
41	τ HCCC(10), τ CCCC(16), τ OCOC(11), τ OCCC(32), δ OCN(18), δ CNN(13), δ NNC(20)	**572**	**551**
42	δ CCC(13), δ COC(21), τ OCOC(13), τ OCCC(21), τ HCCC(12)	**573**	**553**
43	δ OCN(17), δ NNC(21), τ HNNC(95)	**584**	**559**
44	δ CCO(16), δ COC(12), δ CCC(22)	**591**	**582**
45	ν NN(13), δ CCC(25), δ CNN(10)	**610**	**597**
46	τ CCCN(19), τ COCC(19), τ CCOC(17),τ OCCC(19)	**637**	**608**
47	ν CC(13), ν ClC(15), δ CCC(20), τ NNCC(15), τ NCNC(42), τ CCNN(12)	**653**	**638**
48	ν CC(13), ν ClC(15), δ CCC(20), τ NNCC(15), τ NCNC(42), τ CCNN(12)	**661**	**644**
49	δ CCC(41), τ NNCC(12), τ CCNN(12), τ NCNC(34)	**670**	**650**
50	ν CC(12), δ CCC(31)	**694**	**682**
51	τ CCCC(31)	**705**	**685**
52	τ HCCC(31), τ CCCC(18)	**727**	**702**
53	τ HCCC(44), τ COCC(10), τ CCOC(15), τ CCCN(15)	**737**	**710**
54	τ CCCC(14), ν NN(11)	**739**	**722**
55	τ ONNC(78), ν NC(13), δ CNN(28)	**770**	**733**
56	τ HCCC(13), τ OCOC(54)	**784**	**744**
57	ν NC(10), δ CNN(10), ν CC(12), τ HCCC(16), τ CCCC(16)	**786**	**754**
58	δ NCN(13), δ NCC(12), τ HCCC(12), τ CCCC(10), δ OCO(26), τ ONNC(74)	**792**	**760**
59	ν CC(10), ν OC(12), δ OCO(27), τ ONNC(74)	**793**	**771**
60	ν NC(10), δ CCN(16)	**820**	**800**
61	ν CC(11), δ CCC(11), τ HCCC(12), CCN(15)	**822**	**805**
62	τ HCCC(33), τ CCOC(15)	**861**	**809**
63	τ HCCC(63), τ CCCC(10), τ OCOC(10)	**865**	**811**
64	τ HCCC(100), ν OC(20), ν CC(13)	**876**	**826**
65	τ HCCC(99), τ CCCC(11)	**895**	**849**
66	ν CC(10), ν OC(18), τ HCCC(55), τ CCCC(12)	**912**	**858**
67	HCC(33), τ HCCC(30), ν CC(13)	**933**	**913**
68	τ HCCC(30), HCC(33), ν CC(13)	**939**	**920**
69	τ HCCC(49), δ NCC(41)	**979**	**924**
70	ν CC(11), δ CCC(11), τ HCCC(31)	**995**	**925**
71	τ HCCC(27), τ CCCC(13)	**997**	**944**
72	δ NCN(15), δ NCC(39), δ CCC(13), ν CC(41)	**1002**	**948**
73	τ HCCC(60), τ CCCC(10), νCC(17), δ CCC(26)	**1011**	**968**
74	τ HCCC(84), τ CCCC(14)	**1017**	**970**
75	τ HCCC(26), τ CCOC(12), NC(31), δ CNN(12)	**1035**	**978**
76	ν CC(21), ν OC(21), δ CCC(53)	**1041**	**985**
77	ν NC(35), δ CNN(10), τ HCCC(17), τ HCNN(13)	**1042**	**990**
78	τ HCCC(57), ν NC(26), ν NN(15), ν OC(56)	**1050**	**994**
79	τ HCCC(82), τ CCCC(17)	**1059**	**995**
80	ν CC(29), δ CCC(18), τ HCCC(82), τ CCCC(17)	**1060**	**998**
81	ν OC(35), δ CCC(15), τ HCCC(62)	**1074**	**1012**
82	δ CCC(63), τ HCCC(47)	**1078**	**1024**
83	τ HCNN(84), τ HCOC(28), δ HCH(16), δ HCC(12), ν CC(61), ν ClC(15)	**1082**	**1046**
84	ν CC(60), ν ClC(14), δ HCC(18)	**1090**	**1067**
85	ν OC(12), δ HCC(17), δ CCC(12)	**1099**	**1069**
86	ν CC(36), δ HCC(20)	**1100**	**1086**
87	ν CC(32), δ HCC(20), τ HCNN(74)	**1107**	**1092**

88	ν CC(45), δ HCC(47)	**1107**	**1112**
89	ν NC(26), ν NN(15), ν OC(56), ν CC(13)	**1142**	**1115**
90	δ HCH(24), τ HCOC(26), ν CC(19)	**1155**	**1118**
91	ν OC(13), δ HCC(13), ν CC(19), τ HCOC(26)	**1156**	**1136**
92	ν CC(61), δ HCH(16), τ HCOC(28), δ HCC(16), τ HCCC(13)	**1158**	**1149**
93	ν CC(27), ν OC(12), δ HCC(16), τ HCCC(13)	**1158**	**1172**
94	ν NC(10), ν NN(12), δ NNC(11), δ HCC(21)	**1171**	**1180**
95	ν CC(10), δ HCC(36), δ HCH(13), τ HCOC(24)	**1184**	**1188**
96	ν CC(21), δ HCC(14), δ CCC(12)	**1198**	**1191**
97	ν CC(16), δ HCC(69), τ HCCC(25)	**1214**	**1199**
98	ν CC(16), δ HCC(60), τ HCCC(25)	**1218**	**1199**
99	ν CC(14), ν OC(11), δ HCC(41)	**1219**	**1202**
100	ν CC(14), ν OC(12), δ HCC(14)	**1245**	**1238**
101	ν CC(13), ν OC(10), ν NN(13), ν NC(12), δ NNC(18), δ HCC(79)	**1257**	**1255**
102	ν CC(17), ν NC(11), δ HCN(10), τ HCCC(18), HCC(45)	**1260**	**1270**
103	ν CC(60), δ HCC(14), ν OC(42)	**1276**	**1283**
104	ν CC(30), τ HCCC(11), ν OC(23), δ HCC(10)	**1294**	**1287**
105	ν CC(32), δ HCC(13), ν NC(12), τ HCCC(28), δ HCN(11)	**1312**	**1294**
106	ν CC(26), δ HCC(40)	**1334**	**1309**
107	δ HNN(79), δ HCC(74)	**1352**	**1318**
108	δ HCC(74), δ HNN(78)	**1355**	**1324**
109	δ HCC(79), ν NN(13), δ NNC(18)	**1360**	**1335**
110	ν CC(10), δ HCN(33), τ HCCN(36)	**1387**	**1353**
111	ν NC(12), δ HCN(26)	**1420**	**1392**
112	ν CC(26), δ HCC(42)	**1427**	**1404**
113	ν CC(17), δ HCC(10), δ HCN(18)	**1453**	**1418**
114	ν CC(30), δ HCC(15)	**1458**	**1432**
115	δ HCC(10), δ HCH(91)	**1477**	**1452**
116	δ HCH(86)	**1483**	**1460**
117	δ HCC(46)	**1508**	**1482**
118	δ HCC(25), ν CC(21)	**1513**	**1483**
119	ν CC(11), δ HCC(65)	**1524**	**1492**
120	δ HCH(76), τ HCOC(11)	**1525**	**1502**
121	δ HCH(74), τ HCOC(10)	**1534**	**1514**
122	ν NC(54), ν CC(27), δ HCC(12), δ CCC(12)	**1593**	**1531**
123	ν NC(49), ν CC(21), δ HCC(10), δ CCC(10)	**1598**	**1543**
124	ν CC(35), δ HCC(16), δ CCC(12)	**1600**	**1557**
125	ν CC(43), δ HCC(26), δ CCC(13)	**1610**	**1561**
126	ν CC(42), δ HCC(22), δ CCC(10)	**1613**	**1567**
127	δ HCC(22), ν CC(28)	**1623**	**1567**
128	ν NC(39), ν CC(28), δ CCC(10)	**1636**	**1572**
129	ν CC(61), δ HCC(11), ν NC(45)	**1671**	**1585**
130	ν OC(85), δ CNN(12)	**1734**	**1676**
131	ν OC(85)	**1745**	**1711**
132	ν CH(91)	**2907**	**2923**
133	ν CH(100)	**2939**	**2959**
134	ν CH(50)	**2957**	**2976**
135	ν CH(100)	**2971**	**2988**
136	ν CH(46)	**3016**	**3051**
137	ν CH(69)	**3056**	**3076**
138	ν CH(64)	**3057**	**3088**
139	ν CH(73)	**3062**	**3089**
140	ν CH(52)	**3063**	**3093**
141	ν CH(36)	**3079**	**3095**
142	ν CH(67)	**3091**	**3120**
143	ν CH(67)	**3091**	**3122**
144	ν CH(69)	**3092**	**3124**
145	ν CH(74)	**3093**	**3125**
146	ν CH(72)	**3097**	**3126**
147	ν CH(56)	**3108**	**3134**
148	ν CH(48)	**3119**	**3150**
149	ν CH(28)	**3138**	**3169**
150	ν NH(100)	**3538**	**3514**

*ν, stretching; δ, bending; τ, torsion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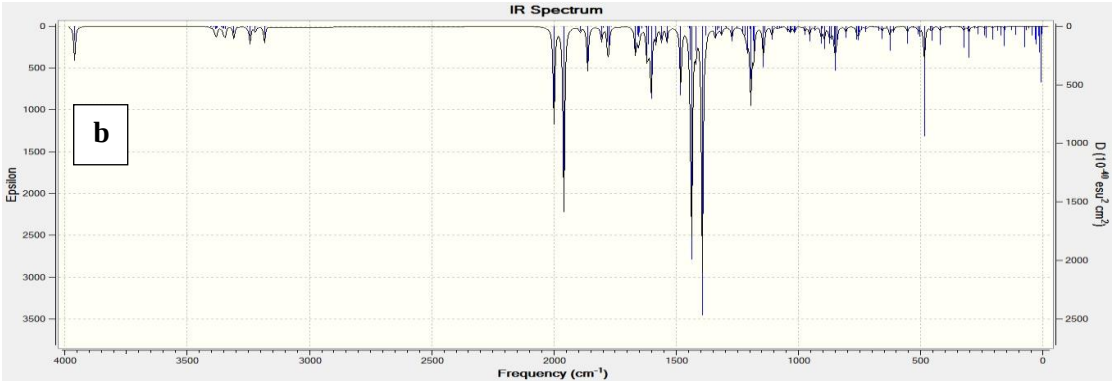
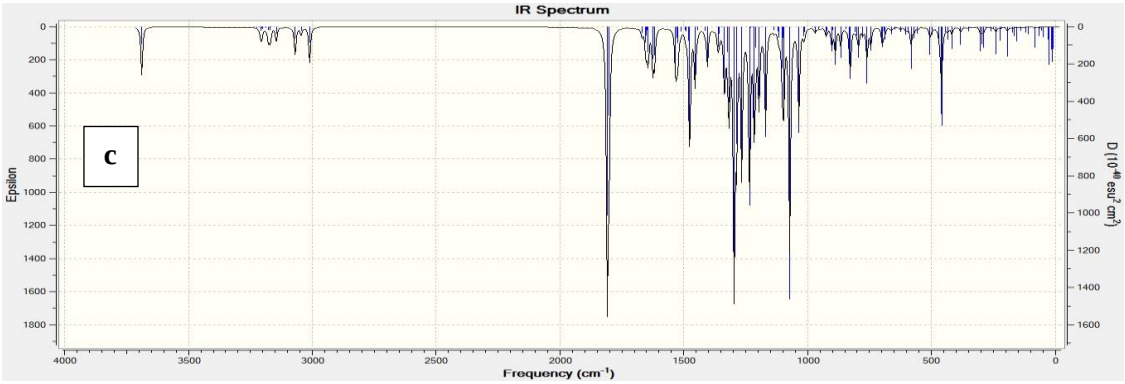
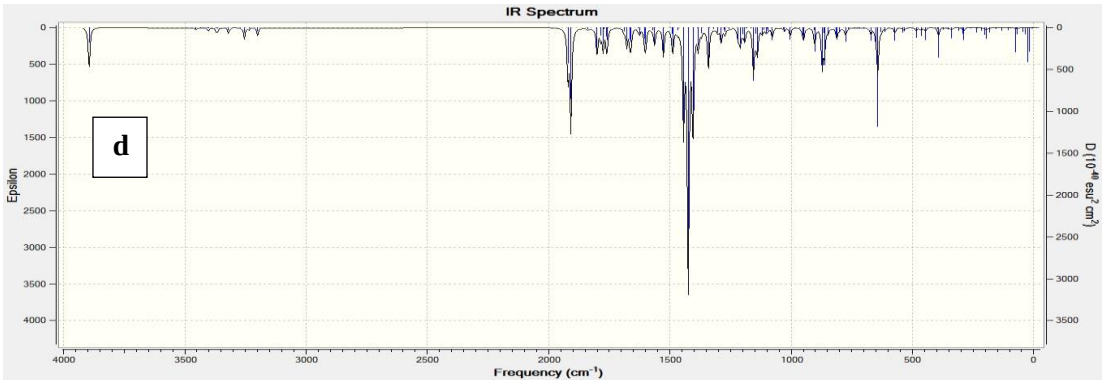
Transmittance [%]
Wavenumber cm-1
3166.97
3038.96
2940.09
2909.42
2837.59
1711.32
1593.96
1487.76
1421.84
1356.49
1318.67
1271.59
1216.37
1177.02
1136.68
1083.94
1031.05
965.49
915.12
877.06
832.59
794.88
741.16
713.37
681.54
593.50
547.40
491.96
463.05
427.20
388.83


IR Spectrum
b
Epsilon
D (10⁻⁴⁰ esu² cm²)
Frequency (cm⁻¹)


IR Spectrum
c
Epsilon
D (10⁻⁴⁰ esu² cm²)
Frequency (cm⁻¹)


IR Spectrum
d
Epsilon
D (10⁻⁴⁰ esu² cm²)
Frequency (cm⁻¹)

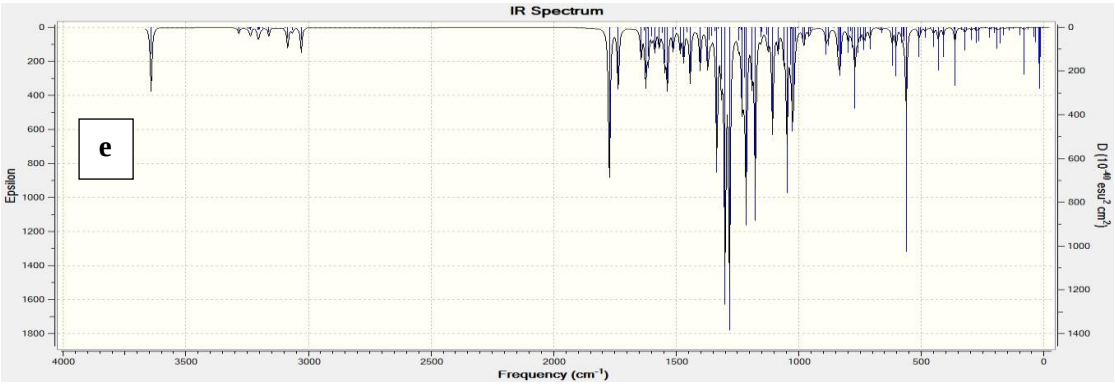


Figure 2. The calculated FT-IR spectrums of titled compound (Experimental (a) calculated (6-311G(d) HF (b) ve B3LYP (c), 3-21G HF (d) and B3LYP (e))

3.3. ^{13}C and ^{1}H NMR Chemical Shift and Regression Analyses

The ^{1}H and ^{13}C NMR chemical shifts values in gase phase and DMSO solvent of the above cited molecule have been carried out by DFT (B3LYP) and Hartree Fock (HF) methods with 6-311G(d) and 3-21G levels (Table **6**, **7** and Figure **3**). The results were indicated lineer correlation. The calculated R^2 (6-311G(d)/3-21G) have been 0.9932/0.99825 (gas phase), 0.9942/0.9831 (DMSO) for ^{13}C-NMR chemical shifts values and 0.6591/0.6130 (gas phase), 0.7011/0.6690 (DMSO) for ^{1}H-NMR chemical shifts values. All isotropic chemical shift values for titled compound were listed in Table **6** and **7**.

Theoretical and experimental carbon-proton chemical shifts ratios of titled compound were observed a lineer correlation according to R^2 values.

Table 6. The ^{1}H and ^{13}C NMR isotropic chemical shifts of titled compound (with respect to TMS, all values in ppm) (6-311G(d)).

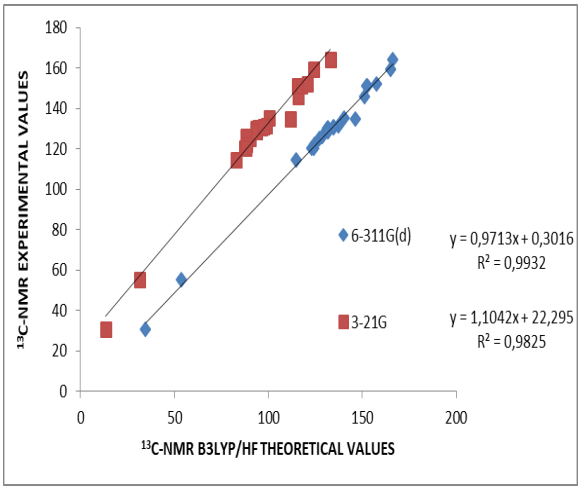
	$\delta_{Exp.}$	$\delta_{cal.}$ HF (Vacum)	$\delta_{cal.}$ HF (DMSO)	Different	Different (DMSO)	$\delta_{cal.}$ B3LYP (Vacum)	$\delta_{cal.}$ B3LYP (DMSO)	Different	Different (DMSO)
C1	145,91	151,30	153,18	-5,39	-7,27	140,80	143,26	5,11	2,65
C2	151,15	152,48	153,42	-1,33	-2,27	141,62	142,58	9,53	8,57
C3	151,02	152,25	152,73	-1,23	-1,71	142,60	143,07	8,42	7,95
C4	135,18	140,14	140,24	-4,96	-5,06	126,38	126,30	8,80	8,88
C5	124,88	127,17	127,58	-2,29	-2,70	118,08	118,44	6,80	6,44
C6	152,19	157,67	157,35	-5,48	-5,16	142,14	141,30	10,05	10,89
C7	125,92	128,52	128,25	-2,60	-2,33	118,94	119,02	6,98	6,90
C8	130,09	131,33	132,14	-1,24	-2,05	120,43	121,15	9,66	8,94
C9	120,22	123,13	123,63	-2,91	-3,41	114,13	114,92	6,09	5,30
C10	164,32	166,33	167,75	-2,01	-3,43	151,11	152,91	13,21	11,41
C11	130,27	134,79	133,90	-4,52	-3,63	122,76	121,78	7,51	8,49
C12	122,15	124,68	122,87	-2,53	-0,72	115,22	113,25	6,93	8,90

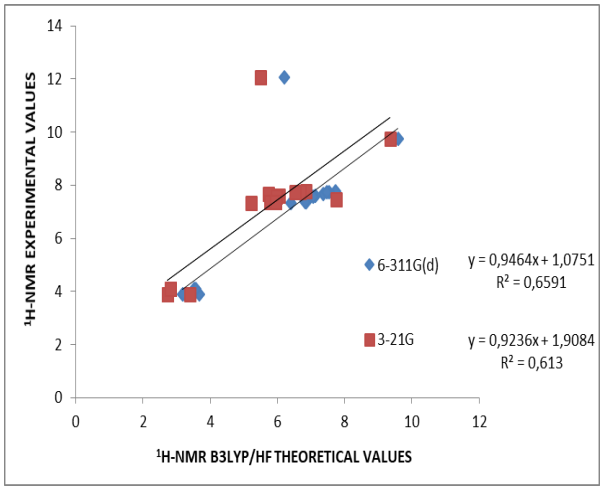
C13	159,45	165,21	165,45	-5,76	-6,00	149,53	149,41	9,92	10,04
C14	114,40	114,95	117,64	-0,55	-3,24	104,06	106,57	10,34	7,83
C15	130,19	131,73	133,24	-1,54	-3,05	120,83	122,37	9,36	7,82
C16	120,31	124,21	124,26	-3,90	-3,95	113,40	113,71	6,91	6,60
C17	55,47	53,56	54,11	1,91	1,36	35,29	35,76	20,18	19,71
C18	30,43	34,62	34,07	-4,19	-3,64	17,41	16,99	13,02	13,44
C19	131,40	137,32	138,91	-5,92	-7,51	125,47	127,11	5,93	4,29
C20	130,77	134,74	135,52	-3,97	-4,75	123,29	123,86	7,48	6,91
C21	128,30	131,61	131,85	-3,31	-3,55	120,92	121,15	7,38	7,15
C22	134,72	146,20	144,73	-11,48	-10,01	128,97	127,23	5,75	7,49
C23	128,30	131,74	131,98	-3,44	-3,68	120,97	121,16	7,33	7,14
C24	130,77	134,66	135,44	-3,89	-4,67	123,32	123,86	7,45	6,91
H25	12,05	6,20	6,67	5,85	5,38	5,39	5,8	6,66	6,25
H26	9,75	9,59	9,56	0,16	0,19	9,01	8,98	0,74	0,77
H27	7,46	6,80	6,98	0,66	0,48	6,66	6,87	0,80	0,59
H28	7,66	7,37	7,43	0,29	0,23	6,66	6,85	1,00	0,81
H29	7,61	7,13	7,35	0,48	0,26	6,85	7,11	0,76	0,50
H30	7,78	7,73	7,85	0,05	-0,07	7,57	7,74	0,21	0,04
H31	7,74	7,53	7,36	0,21	0,38	7,44	7,24	0,30	0,50
H32	7,34	6,41	6,79	0,93	0,55	6,06	6,47	1,28	0,87
H33	7,56	7,07	7,32	0,49	0,24	6,79	7,09	0,77	0,47
H34	7,73	7,48	7,58	0,25	0,15	7,19	7,32	0,54	0,41
H35	3,88	3,18	3,35	0,70	0,53	2,51	2,71	1,37	1,17
H36	3,88	3,18	3,36	0,70	0,52	2,51	2,72	1,37	1,16
H37	3,88	3,68	3,76	0,20	0,12	3,08	3,15	0,80	0,73
H38	4,09	3,53	3,70	0,56	0,39	2,93	3,14	1,16	0,95
H39	4,09	3,57	3,72	0,52	0,37	2,92	3,12	1,17	0,97
H40	7,37	6,84	7,08	0,53	0,29	6,59	6,86	0,78	0,51
H41	7,35	6,86	7,01	0,49	0,34	6,63	6,79	0,72	0,56
H42	7,35	6,85	6,99	0,50	0,36	6,63	6,79	0,72	0,56
H43	7,37	6,83	7,07	0,54	0,30	6,59	6,86	0,78	0,51

Table 7. The ^{1}H and ^{13}C NMR isotropic chemical shifts of titled compund (with respect to TMS, all values in ppm 3-21G)).

	$\delta_{Exp.}$	**$\delta_{cal.}$ HF (Vacum)**	**$\delta_{cal.}$ HF (DMSO)**	**Different**	**Different (DMSO)**	**$\delta_{cal.}$ B3LYP (Vacum)**	**$\delta_{cal.}$ B3LYP (DMSO)**	**Different**	**Different (DMSO)**
C1	145,91	115,91	117,21	30,00	28,70	113,16	115,13	32,75	30,78
C2	151,15	115,45	115,90	35,70	35,25	114,74	115,23	36,41	35,92
C3	151,02	117,71	117,78	33,31	33,24	115,66	115,83	35,36	35,19
C4	135,18	100,43	99,89	34,75	35,29	93,10	92,49	42,08	42,69
C5	124,88	90,47	89,72	34,41	35,16	84,30	83,53	40,58	41,35
C6	152,19	120,83	120,79	31,36	31,40	111,09	110,91	41,10	41,28
C7	125,92	88,09	88,99	37,83	36,93	83,78	84,63	42,14	41,29
C8	130,09	93,56	94,79	36,53	35,30	88,77	90,01	41,32	40,08
C9	120,22	87,23	87,58	32,99	32,64	82,91	83,42	37,31	36,80
C10	164,32	133,12	133,78	31,20	30,54	128,41	129,24	35,91	35,08
C11	130,27	96,54	95,74	33,73	34,53	90,18	89,31	40,09	40,96
C12	122,15	88,39	86,86	33,76	35,29	85,50	83,69	36,65	38,46

C13	159,45	124,08	124,18	35,37	35,27	115,71	115,4	43,74	44,05
C14	114,40	83,08	85,11	31,32	29,29	78,19	80,34	36,21	34,06
C15	130,19	94,38	95,67	35,81	34,52	88,93	90,44	41,26	39,75
C16	120,31	88,19	88,23	32,12	32,08	83,95	84,43	36,36	35,88
C17	55,47	31,41	32,05	24,06	23,42	15,57	16,18	39,90	39,29
C18	30,43	13,50	13,06	16,93	17,37	-0,91	-1,22	31,34	31,65
C19	131,40	99,20	100,62	32,20	30,78	93,57	95,17	37,83	36,23
C20	130,77	97,53	98,26	33,24	32,51	91,72	92,32	39,05	38,45
C21	128,30	93,60	93,69	34,70	34,61	89,17	89,29	39,13	39,01
C22	134,72	111,87	110,92	22,85	23,80	99,50	98,33	35,22	36,39
C23	128,30	93,60	93,69	34,70	34,61	89,17	89,29	39,13	39,01
C24	130,77	97,54	98,26	33,23	32,51	91,70	92,3	39,07	38,47
H25	12,05	5,51	6,01	6,54	6,04	4,55	4,96	7,50	7,09
H26	9,75	9,35	9,28	0,40	0,47	8,81	8,72	0,94	1,03
H27	7,46	7,76	7,66	-0,30	-0,20	7,38	7,26	0,08	0,20
H28	7,66	5,74	6,03	1,92	1,63	5,72	6,04	1,94	1,62
H29	7,61	6,06	6,38	1,55	1,23	5,88	6,25	1,73	1,36
H30	7,78	6,84	6,99	0,94	0,79	6,76	6,95	1,02	0,83
H31	7,74	6,68	6,50	1,06	1,24	6,81	6,56	0,93	1,18
H32	7,34	5,23	5,67	2,11	1,67	4,94	5,44	2,40	1,90
H33	7,56	5,98	6,30	1,58	1,26	5,74	6,13	1,82	1,43
H34	7,73	6,52	6,76	1,21	0,97	6,49	6,7	1,24	1,03
H35	3,88	2,73	2,97	1,15	0,91	1,74	2,03	2,14	1,85
H36	3,88	2,73	2,97	1,15	0,91	1,74	2,03	2,14	1,85
H37	3,88	3,39	3,52	0,49	0,36	2,73	2,82	1,15	1,06
H38	4,09	2,82	3,02	1,27	1,07	2,06	2,33	2,03	1,76
H39	4,09	2,82	3,02	1,27	1,07	2,05	2,32	2,04	1,77
H40	7,37	5,95	6,26	1,42	1,11	5,73	6,09	1,64	1,28
H41	7,35	5,77	5,96	1,58	1,39	5,56	5,77	1,79	1,58
H42	7,35	5,77	5,96	1,58	1,39	5,56	5,77	1,79	1,58
H43	7,37	5,95	6,26	1,42	1,11	5,73	6,09	1,64	1,28





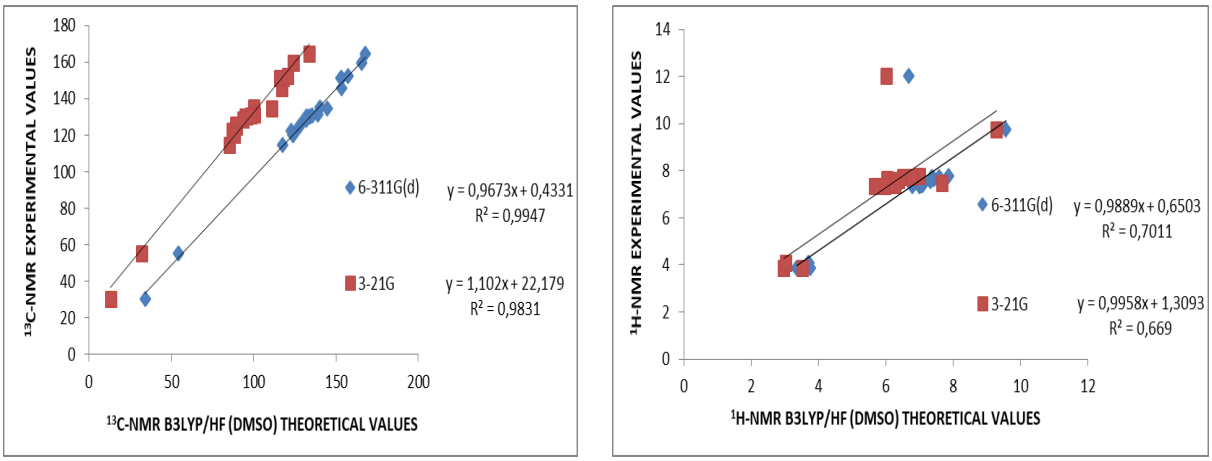
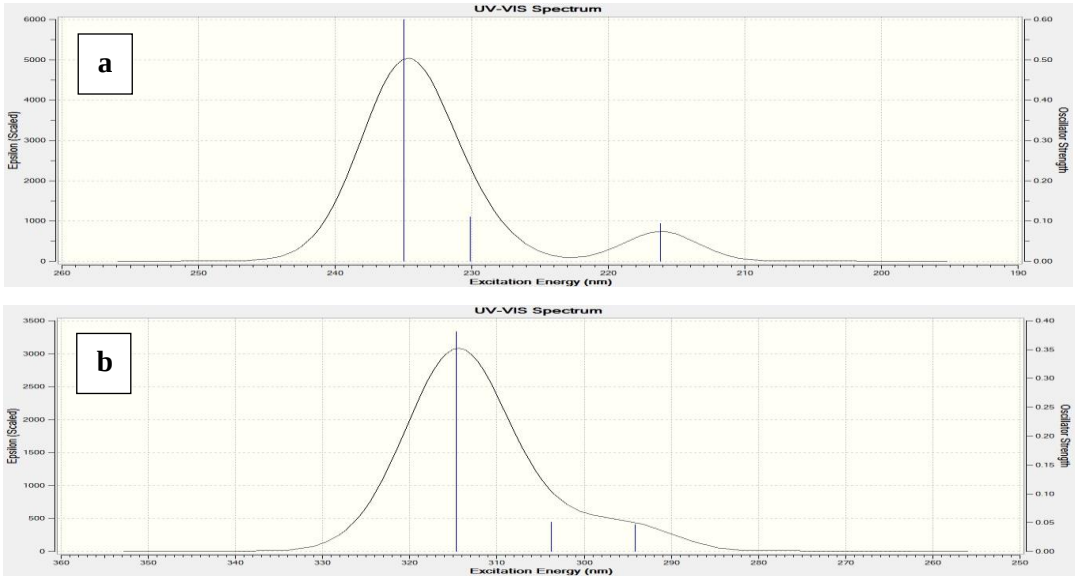
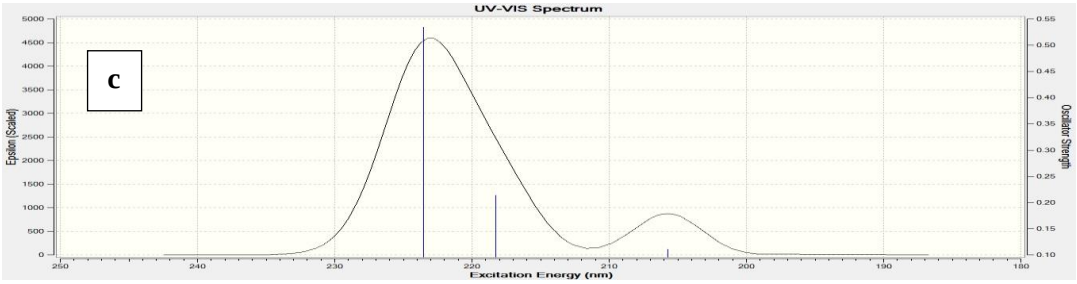


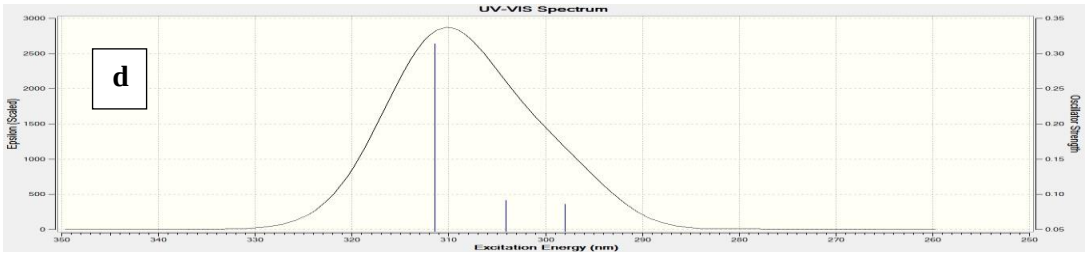
Figure 3. ^{13}C- and ^{1}H-NMR chemical shifts values of titled compound with 6-311G(d) ve 3-21G/B3LYP and HF (gas/DMSO)**.**

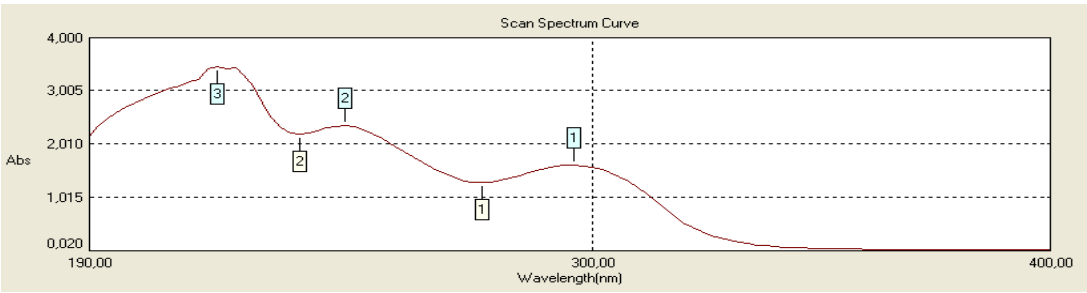
3.4.UV-vis. Spectral Values

The oscillator strengths (*f*), absorption wavelengths (λ) and excitation energies of UV–Vis electron absorption spectroscopy (in ethanol solvent) of the titled compound have been performed by B3LYP/HF strategies with 6-311G(d) and 3-21G levels. The experimental absorption wavelengths of titled compound have been exhibited as 296, 246 and 222, 218 nm (Medetalibeyoğlu 2015). The UV-vis. spectral values of titled compound have been calculated by TD-DFT/HF methods (in the ethanol). The wavelength, excitation energy, oscillator strength in ethanol of titled compound have been shown in Figure **4.**







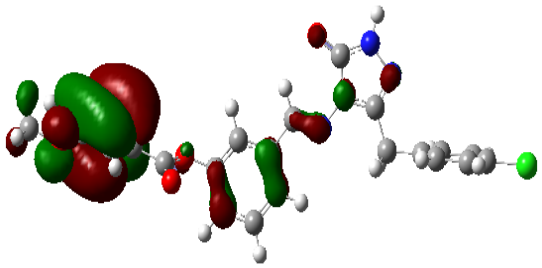


Experimental (nm)	λ (nm) HF/B3LYP 6-311G(d)	λ (nm) HF/B3LYP 3-21G	Excitation Energy (eV) HF/B3LYP 6-311G(d)	Excitation Energy (eV) HF/B3LYP 3-21G	*f* (osillatör strengths) HF/B3LYP 6-311G(d)	*f* (osillatör strengths) HF/B3LYP 3-21G
296.00	234.95/314.66	223.50/311.142	5.2771/3.9402	5.5475/3.9813	0.5996/0.3808	0.5346/0.3140
246.00	230.09/303.75	218.28/304.07	5.3885/4.0818	5.6799/4.0775	1.1098/0.0506	0.2134/0.0912
222.00	216.16/294.10	205.74/297.98	5.7356/4.2157	6.0262/4.1608	0.0933/0.0463	0.1106/0.0861

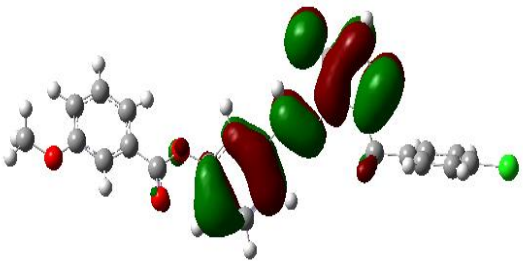
Figure 4. The wavelength (λ), excitation energy and oscillator strengths (*f*) and UV-vis Spectrums.

3.5. Frontier Molecular Orbital Analysis, Dipole Moment, Total Energy, Electronic Thermodynamics Properties

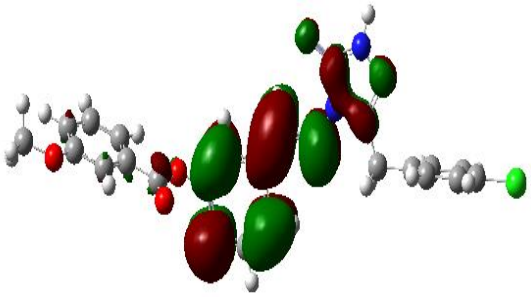
Frontier molecular orbitals (FMO) give information about the electronic transitions, kinetic stability, optical and electric properties (Fukui, 1982). The HOMO-LUMO energy values of titled compound were calculated with two computational levels and these values were found as 10.826/4.243 e.V (HF/B3LYP (6-311G(d)) and 10.881/6.062 (HF/B3LYP (3-21G)) e.V (Figure **5**). The electron affinity (A), global hardness (η)/softness (S), electronegativity (χ), chemical potential (μ), ionization potential (I), chemical potential (Pi) calculated by using HOMO-LUMO energies for the compound were given in Table **8.**



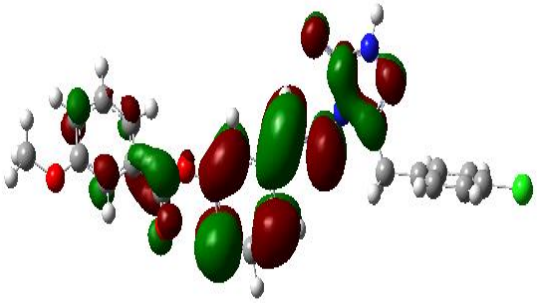
E_{HOMO}(HF (a)) : 8.748 eV



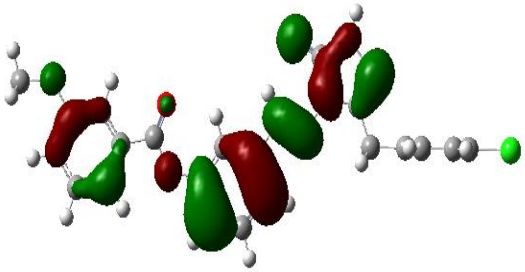
E_{HOMO}(B3LYP (a)) : -6.031 eV



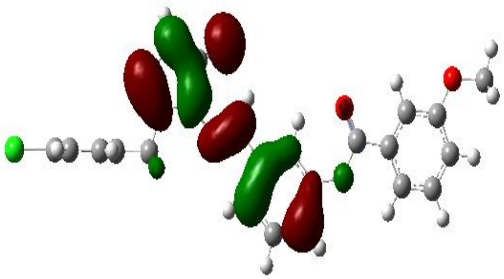
E_{LUMO}(HF (a)) : 2.078 eV



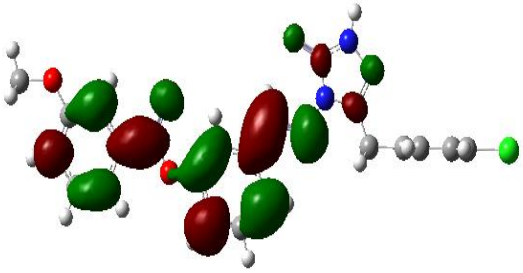
E_{LUMO}(B3LYP (a)) : -1.788 eV



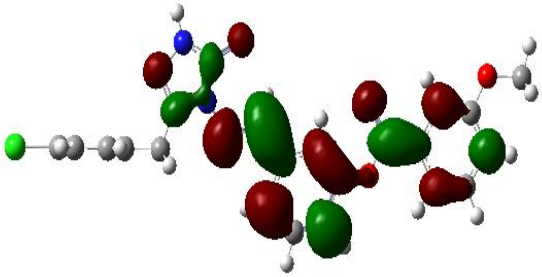
E_{HOMO}(HF (b)) : 2.078 eV



E_{HOMO}(B3LYP (b)) : -6.062 eV



E_{LUMO}(HF (b)) : -8.803 eV



E_{LUMO}(B3LYP (b)) : 1.674 eV

Figure 5. 3D plots of HOMO and LUMO energies of the compound

Table 8. Electronic properties of the compound

	HF/B3LYP 6-311G(d)	**HF/B3LYP 3-21G**
E_{HOMO} (eV)	-8.748/-6.031	-8.803/-6.062
E_{LUMO} (eV)	2.078/-1.788	2.078/1.674
$\Delta E = E_{LUMO}-E_{HOMO}$ (eV)	10.826/4.243	10.881/6.062
I (eV)	8.748/6.031	8.803/6.062
A(eV)	-2.078/1.788	-2.078/-1.674
χ (eV)	3.335/3.909	3.363/2.194
η (eV)	5.413/2.121	5.441/3.868
S (eV^{-1})	136.792/349.012	136.094/191.422

The dipole moments, total energy values, thermodynamic structure properties (Thermal energy, Zero-Point Vibrational energy (ZPVE), Rotational constants, etc.) of titled compound were carried out by using B3LYP/HF with 6-311G(d) and 3-21G methods and listed in Table **8, 9** and **10.** Thermodynamic structure properties (Thermal energy, Zero-Point Vibrational energy (ZPVE), Rotational constants, etc.) were calculated with DFT/HF method and 6-311G(d) and 3-21G basis set at 298.150 ^{o}K and under 1 atm. All thermodynamic structure parameters such as entropy, Zero-point vibrational energy, enthalpy, thermal capacity were examined and given in Table **9**. The calculated zero-point vibrational energy (ZPVE) values of titled compound were found as 246.31501/265.13393 (B3LYP/HF and 6-311G(d)) and 248.32801/267.75516 (B3LYP/HF and 3-21G) Kcal/mol, respectively. The total thermal energy(E)-entropy(S)-thermal capacity (CV) values of the compound are found as E; 263.831/282.187 Kcal/mol (DFT/HF, 6-311G(d)), 266.073/284.362 (DFT/HF, 3-21G) Kcal/mol, S; 196.064/198.870 (DFT/HF, 6-311G(d)), 192.667/194.721 Cal/mol-K (DFT/HF, 3-21G)), CV; 106.826/101.014 Cal/mol-K (DFT/HF, 6-311G(d)), 107.240/98.758 Cal/mol-K (DFT/HF 3-21G).

The total dipole moment values were calculated as 5.9887/5.8098 (HF/B3LYP (6-311G(d)), 5.6547/5.2542 (HF/B3LYP (3-21G)) and all dipole moment values were listed in Table **10**.

The calculated total energy values of titled compound were obtained as -874.645 a.u./-879.917 a.u. (HF/B3LYP (6-311G(d)) and -869.598 a.u./-874.874 a.u. (HF/B3LYP (3-21G)) (Table **11**).

Table 9. The thermodynamics parameters of the compound

Parameters	B3LYP 6-311G(d)	HF 6-311G(d)	B3LYP 3-21G	HF 3-21G
Rotational temperatures (Kelvin)				
A	0.02082	0.01998	0.02045	0.02073
B	0.00127	0.00131	0.00131	0.00133
C	0.00122	0.00127	0.00124	0.00126
Rotational constants (GHZ)				
A	0.43376	0.41632	0.42621	0.43186
B	0.02651	0.02725	0.02733	0.02768
C	0.02550	0.02644	0.02593	0.02626
Thermal Energies E(Kcal/mol)				
Translational	0.889	0.889	0.889	0.889
Rotational	0.889	0.889	0.889	0.889
Vibrational	262.053	280.410	264.295	282.584
Total	263.831	282.187	266.073	284.362
Thermal Capacity CV(cal/mol-K)				
Translational	2.981	2.891	2.981	2.981
Rotational	2.981	2.891	2.981	2981
Vibrational	100.864	95.052	101.278	92.796
Total	106.826	101.014	107.240	98.758
Entropy S(cal/mol-K)				
Translational	44.281	44.281	44.281	44.281
Rotational	38.236	38.214	38.207	38.168
Vibrational	113.547	116.376	117.671	112.272
Total	196.064	198.870	192.667	194.721
Zero-point correction (Hartree/Particle)	0.392528	0.422518	0.395736	0.426689
Thermal correction to Energy	0.420441	0.449694	0.424014	0.453160
Thermal correction to Enthalpy	0.421385	0.450638	0.424958	0.454104
Thermal correction to Gibbs Free Energy	0.328229	0.356148	0.329856	0.361586
Sum of electronic and zero-point Energies	-1906.034383	-1896.501120	-1895.50482	-1885.97203
Sum of electronic and thermal Energies	-1906.006470	-1896.473944	-1895.47655	-1885.94556
Sum of electronic and thermal Enthalpies	-1906.098682	-1896.47300	-1895.47556	-1885.94462
Sum of electronic and thermal Free Energies			-1895.57070	
Zero-point vibrational energy (Kcal/mol)	246.31501	265.13393	248.32801	267.75516

Table 10. The dipole moment of the compound

Dipole Moment	HF 6-311G(d)	HF 3-21G	B3LYP 6-311G(d)	B3LYP 3-21G
µx	-4.3029	-3.8842	-4.4915	-4.0223
µy	4.1064	4.0148	3.6630	3.3488
µz	-0.6977	-0.8776	-0.4041	-0.4621
µToplam	5.9887	5.6547	5.8098	5.2542

Table 11. The total energy values of the compound

Energy	HF 6-311G(d)	HF 3-21G	B3LYP 6-311G(d)	B3LYP 3-21G
(a.u.)	-874.645	-869.598	-879.917	-874.874

Having studied molecular surfaces of the compound the most high positive area is located on N44-H25 (on hydrogen atom) while the most high negative area is positioned on electronegative oxygen atoms (O48, O50, O51) of the molecule which can be regarded as possible site electrophilic attack (Figure **6**).

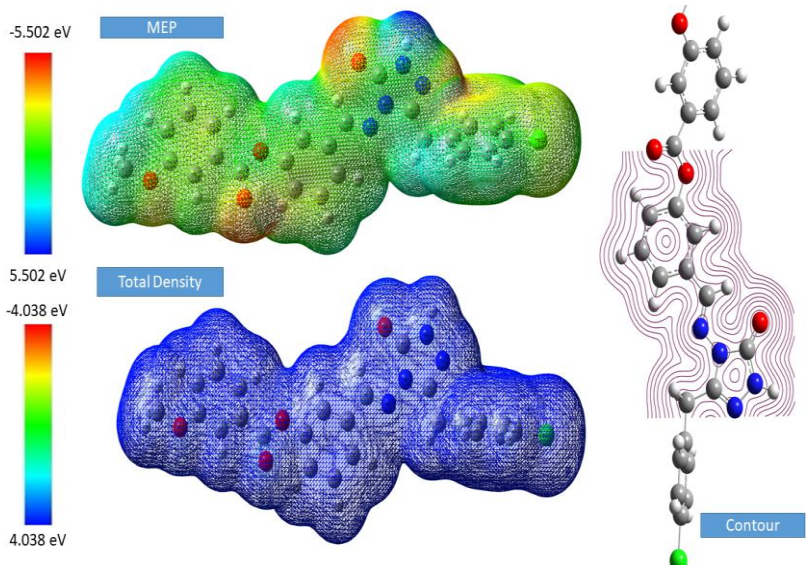


Figure 5. The molecular surfaces of titled compound

4. CONCLUSION

In this work, spectroscopic, electronic and geometric parameters of 3-*p*-chlorobenzyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule are calculated by HF/B3LYP with the 6-311G(d) and 3-21G levels. The vibrational frequencies and spectrums were obtained with the same methods and levels. All vibrational frequencies was found as possitive. It are shown that titled compound was stable. The FT-IR, UV-vis and $^{1}H/^{13}C$-NMR spectral values are found to be very compatible with the experimental spektral values. Evaluated ^{1}H- and ^{13}C-NMR isotropic shift ratios between theoretical and experimental values (Medetalibeyoğlu, 2015) were observed a lineer correlation and the best R^2 value is 0.9932 for ^{13}C-NMR isotropic shift ratio that obtained with DFT/6-311G(d) method in DMSO solvent. The experimental spectroscopic values are compared with obtained spectroscopic parameters. Also, the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO), E_{LUMO}-E_{HOMO} energy gap (ΔE), bond angles, mulliken charges, bond lengths, electronic parameters, thermodynamics properties, dipole moments, total energy were calculated with different methods and levels. Obtained and experimental spectral values were compared with each other and all spectral values appeared a reasonably great agreement.

REFERENCES

Akın Ş., Demir E.A., Colak A., Kolcuoglu Y., Yildirim N., Bekircan O. (2019). Synthesis, biological activities and molecular docking studies of some novel 2,4,5-trisubstituted-1,2,4-triazole-3-one derivatives as potent tyrosinase inhibitors. *Journal of Molecular Structure*, 1175, 280-286.

Akyıldırım O., Gökce H., Bahçeli S., Yüksek H. (2016). Theoretical and spectroscopic (FT-IR, NMR and UV–Vis.) characterizations of 3-*p* chlorobenzyl-4-(4-carboxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule. *Journal of Molecular Structure*, 1127, 114-123.

Beytur M., Manap S., Özdemir, G., Gürsoy Kol, Ö., Aytemiz, F., Alkan, M., Yüksek, H., Preparation of Some New Bis-[4-(3-alkyl/aryl-4,5-dihydro-1H-1,2,4-triazol-5-on-4-yl)-azomethinphenyl] Phtalate Derivatives with Their Antioxidant and Antimicrobial Activities. *Research Journal of Pharmaceutical Biological and Chemical Sciences*, 10 (1), 426-436.

Boursas, F., Berrah, F., Kanagathara, N., Anbalagan, G. & Bouacida, S. (2019). XRD, FT-IR, FT-Raman spectra and ab initio HF vibrational analysis of bis (5-amino-3-carboxy-1H-1,2,4-triazol-4-ium) selenate dihydrate. *Journal of Molecular Structure*, 1180, 532-541.

Cui D., Li Z., Song G., Qian X. (2002). Synthesis and biological activities of *N*-(1,2,4-triazole-4-yl)-*N*′-(fluorine-containing-phenyl)carbamimidothioates. *Journal of Fluorine Chemistry*, 115(1), 79-82.

Du H., Fan Z., Yang L., Bao X. (2018). Synthesis and Antimicrobial Activities of Novel 1, 2, 4-Triazole-acyl-hydrazone Derivatives Containing the Quinazolin-4-one Moiety. *Chinese Journal of Organic Chemistry*, 8(2), 531-538.

Fukui K., Yonezawa T., Shingu H.J. (1952). A molecular orbital theory of reactivity in aromatic hydrocarbons, *The Journal of Chemical Physics.* 20, 722-725.

Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Mennucci B., Petersson G.A., Nakatsuji H., Caricato M., Li X., Hratchian H.P., Izmaylov A.F., Bloino J., Zheng G., Sonnenberg J.L., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Montgomery J.A., Peralta J.E., Ogliaro F., Bearpark M., Heyd J.J., Brothers E., Kudin K.N., Staroverov V.N., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J.C., Iyengar S.S., Tomasi J., Cossi M., Rega N., Millam J.M., Klene M., Knox J.E., Cross J.B., Bakken V., Adamo C., Jaramillo J., Gomperts R., Stratmann R.E., Yazyev O., Austin A.J., Cammi R., Pomelli C., Ochterski J.W., Martin R.L., Morokuma K., Zakrzewski V.G., Voth G.A., Salvador P., Dannenberg J.J., Dapprich S., Daniels A.D., Foresman Farkas J.B., Ortiz J.V., Cioslowski J. Fox D.J. (2010). Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT,

Gao F., Wang T., Xiao J., Huang G. (2019). Antibacterial activity study of 1,2,4-triazole derivatives. *European Journal of Medicinal Chemistry*, 173, 274-281.

Irak Z.T., Beytur M. (2019). 4-Benzilidenamino-4,5-dihidro-1H-1,2,4-triazol-5-on Türevlerinin Antioksidan Aktivitelerinin Teorik Olarak İncelenmesi. *Iğdır Üniversitesi Fen Bilimleri Enstitüsü Dergisi*, 9(1), 512-521.

Jiao S., Wang, Z., Zhao Q., n Yu, W., Chang J. (2018). Synthesis of fused 3-amino-1,2,4-triazoles via sequential addition of aryl hydrazines to isothiocyanates and I_2-mediated cyclodesulfurization. *Tetrahedron*, 74(24), 3069-3073.

Ocak N., Çoruh U., Kahveci B., Şaşmaz S., Vazquez-Lopez E.M., Erdönmez A. (2003). 1- Acetyl-3-(p-chlorobenzyl)-4-(p-chlorobenzylidenamino)-4,5-dihydro-1*H*-1,2,4- triazol-5-one. *Acta Crystallographica Section E*. 59(6), 750-752.

Özdemir G., Kotan G., Yüksek H., (2018). Theoretical Investigation of Spectroscopic, Electronic and Thermodynamic Properties of [2-Methoxy-4-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl)-azomethinphenyl] Acetate Molecule. *Asian Journal of Chemical Sciences*, 4, 1-12.

Özil M., Balaydın H.T. Şentürk M. (2019). Synthesis of 5-methyl-2,4-dihydro-3H-1,2,4-triazole-3-one's aryl Schiff base derivatives and investigation of carbonic anhydrase and cholinesterase (AChE, BuChE) inhibitory properties. *Bioorganic Chemistry*, 86, 705–713.

Kotan G., Yüksek H., (2018). Investigation of Theoretical Properties of Novel 1-(Morpholine-4-yl-Methyl)-3-Methyl-4-(4-Ethoxybenzylidenamino)-4, 5-Dihydro-1*H*-1, 2, 4-Triazol-5-One Molecule. *International Journal of Pharmaceutical, Chemical & Biological Sciences*, 8(1). 147-156.

Kukuljan L. and Kranjc K. (2019). 3-(5-Amino-1,2,4-triazole)-1,2,4-oxadiazole: A new biheterocyclic scaffold for the synthesis of energetic materials. *Tetrahedron Letters*, 60, 207–209.

Madeira C.L., Field A. J., Simonich T.M., Tanguay R. L., Chorover J., Sierra-Alvarez R. (2018). Ecotoxicity of the insensitive munitions compound 3-nitro-1,2,4-triazol-5-one (NTO) and its reduced metabolite 3-amino-1,2,4-triazol-5-one (ATO). *Journal of Hazardous Materials*, 343, 340-346.

Mohameda N.G., Shehaa M.M., Hassana H.Y., Abdel-Hafezb L.J.M., Omarc F.A. (2018). Synthesis, antimicrobial activity and molecular modeling study of 3-(5-amino-(2H)-1,2,4-triazol-3-yl]-naphthyridinones as potential DNA-gyrase inhibitors. *Bioorganic Chemistry*, 81, 599–611.

Medetalibeyoğlu H., (2015). Bazı yeni 4-[3-(3-metoksibenzoksi)-benzilidenamino]-4,5dihidro-1H-1,2,4-triazol-5-on türevlerinin sentezi, deneysel ve teorik özelliklerinin incelenmesi. Doktora Tezi, Kafkas Üniversitesi Fen Bilimleri Enstitüsü, Kimya Anabilim Dalı, Kars.

Merrick J.P., Moran D., Radom L. (2007). An Evaluation of Harmonic Vibrational Frequency Scale Factors. *Journal of Physical Chemistry*, 111(45), 11683-11700.

Raouf H., Beyramabadi, S.A., Allameh, S., Morsali, A. (2019). Synthesis, experimental and theoretical characterizations of a 1,2,4-triazole Schiff base and its nickel(II) complex. *Journal of Molecular Structure*, 1179, 779-786.

Saadaoui I., Krichen F., Salah B.B., Mansour R.B., Miled N., Bougatef A., Kossentini M. (2019). Design, synthesis and biological evaluation of Schiff bases of 4-amino-1,2,4-triazole derivatives as potent angiotensin converting enzyme inhibitors and antioxidant activities. *Journal of Molecular Structure*, 1180, 2019, 344-354.

Ustabas R., Çoruh U., Sancak K., Ünver Y., Vazquez-Lopez EM. (2007). 1-(benzoylmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)4,5-dihydro-1*H*-1,2,4-triazol-5-one. *Acta Crystallographica Section E*. 63, 2982- 3051.

Wolinski K., Hinton J.F., Pulay P. (1990). Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. Journal of the American Chemical Society, 112, 8251-8260.

Yüksek H., Akyıldırım, O., Yola M.L., Gürsoy-Kol Ö., Çelebier M., Kart, D. (2013). Synthesis, *In Vitro* Antimicrobial and Antioxidant Activities of Some New 4,5-Dihydro-1*H*-1,2,4-triazol-5-one Derivatives. *Archiv der Pharmazie*, 346 (6), 470-480