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Spectroscopic and Thermodynamic Properties of Novel 1-(4-Methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzylideneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

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Abstract : In this study, 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one was optimized by using B3LYP/6-31G(d) HF/6-31G(d) basis sets. ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to 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. Also, calculated IR data of compound were calculated in gas phase by using of 631G(d) basis sets of B3LYP and HF methods and are multiplied with appropriate adjustment factors. Theoretical infrared spectrums are formed from the data obtained according to B3LYP and HF methods. In the identification of calculated IR data were used the veda4f program. Furthermore, molecule's theoretical angles, dipole moments, mulliken charges, HOMO-LUMO energies, total energy of the molecule, ionization potential, electron affinity, electronegativity and thermodynamic properties for both methods were calculated.

Key words : 4,5-Dihidro-1H-1,2,4-triazol-5-one, GIAO, B3LYP, HF, 6-31G(d).

Introduction

The optimized molecular structure, vibrational frequencies, UV–Vis spectroscopic parameters, atomic charges and frontier molecule orbitals (HOMO and LUMO) of the titled compound have been calculated by using DFT/B3LYP and HF method with 6-311G(d) basis set. All quantum chemical calculations were carried out by using Gaussian 09W [1, 2] program package and the GaussView molecular visualization program [3]. The molecular structure and vibrational calculations of the molecule was computed by using Becke-3-Lee Yang Parr (B3LYP) [4, 5] density functional method with 6-311G(d) basis set in ground state. IR absorption frequencies of analyzed molecule were calculated by two methods. Then, they were compared with experimental data, which are shown to be accurate. Infrared spectrum was composed by using the data obtained from both methods [6, 7]. The assignments of fundamental vibrational modes of the title molecule were

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performed on the basis of total energy distribution analysis by using VEDA 4f program [8]. In this study, 3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one [9] was treated with N-methylpiperazine in the presence of formaldehyde according to the Mannich reaction to synthesize novel 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one.

Experimental

The molecular structure of the title compound in the ground state (in vacuo) is computed by performing both Hartree-Fock (HF) and the density functional theory (DFT) by a hydrid functional B3LYP functional (Becke's three parameter hybrid functional using the LYP correlation functional) methods [1, 2] at 6-31G(d) level. In all these theoretical calculations, the basic or stimulated state of molecules or atoms can be used [1, 10]. The geometric optimizations of all structures can be generated by the MM2 method and then the semi-empirical PM3 method [11].

Results

Molecular Structure

The optimized molecular geometric parameters (bond angles) of the molecule by using B3LYP/6–311G(d) and HF/6–311G(d) levels are listed in Table **1**.

Table 1.The calculated bond angles of the molecule.

Bond lenghts		**B3LYP**	**HF**	**Bond lenghts**		**B3LYP**	**HF**
1	C(1)-N(65)-N(64)	105.24	105.65	61	H(60)-C(29)-N(68)	108.83	109.08
2	C(1)-N(66)-N(67)	121.27	121.18	52	C(29)-N(68)-C(27)	111.40	111.68
3	C(1)-N(66)-C(2)	108.15	107.96	63	N(65)-C(1)-C(19)	126.42	126.88
4	C(1)-C(19)-C(20)	113.65	113.68	64	C(26)-N(64)-C(2)	124.53	125.19
5	C(1)-C(19)-H(44)	108.11	107.91	65	N(65)-C(2)-N(66)	101.93	102.60
6	C(1)-C(19)-H(45)	108.22	107.93	66	N(65)-C(2)-O(70)	129.37	129.10
7	H(44)-C(19)-C(20)	110.58	110.54	67	O(70)-C(2)-N(66)	128.69	128.29
8	H(45)-C(19)-C(20)	110.59	110.60	68	C(2)-N(66)-N(67)	130.55	130.82
9	C(19)-C(20)-C(21)	120.68	120.66	69	N(66)-C(1)-C(19)	122.27	122.01
10	C(19)-C(20)-C(25)	120.58	120.56	70	N(66)-N(67)-C(3)	118.76	119.89
11	C(20)-C(21)-H(46)	119.48	119.67	71	N(67)-C(3)-H(32)	122.06	122.38
12	C(20)-C(21)-C(22)	120.73	120.70	72	N(67)-C(3)-C(4)	120.06	120.24
13	H(46)-C(21)-C(22)	119.80	119.63	73	H(32)-C(3)-C(4)	117.88	117.37
14	C(21)-C(22)-H(47)	119.78	119.79	74	C(3)-C(4)-C(5)	117.91	117.99
15	C(21)-C(22)-C(23)	120.08	120.11	75	C(3)-C(4)-C(9)	122.42	122.42
16	H(47)-C(22)-C(23)	120.14	120.10	76	C(4)-C(5)-H(33)	120.25	120.74
17	C(22)-C(23)-H(47)	120.18	120.19	77	C(4)-C(5)-C(6)	119.51	119.70
18	C(22)-C(23)-C(24)	119.64	119.61	78	H(33)-C(5)-C(6)	120.24	119.56
19	H(48)-C(23)-C(24)	120.18	120.20	79	C(5)-C(6)-O(71)	122.56	120.46
20	C(23)-C(24)-H(49)	120.13	120.12	80	C(5)-C(6)-C(7)	120.01	121.10
21	C(23)-C(24)-C(25)	120.08	120.09	81	O(71)-C(6)-C(7)	116.31	118.33
22	H(49)-C(24)-C(25)	119.79	119.79	82	C(6)-C(7)-H(34)	119.18	119.56
23	C(24)-C(25)-H(50)	119.79	119.61	83	C(6)-C(7)-C(8)	119.31	119.14
24	C(24)-C(25)-C(20)	120.72	120.60	84	H(34)-C(7)-C(8)	121.52	121.29
25	H(50)-C(25)-C(20)	119.48	119.68	85	C(7)-C(8)-H(35)	119.48	119.51
26	C(25)-C(20)-C(21)	118.75	118.78	86	C(7)-C(8)-C(9)	120.52	120.53
27	N(65)-C(1)-N(66)	111.31	111.11	88	H(35)-C(8)-C(9)	120.00	119.96

28	N(65)-N(64)-C(26)	121.82	121.98	88	C(8)-C(9)-H(36)	120.95	120.58
29	N(64)-C(26)-N(68)	112.92	113.13	89	C(8)-C(9)-C(4)	119.98	119.95
30	N(64)-C(26)-H(51)	106.30	106.69	90	H(36)-C(9)-C(4)	119.07	119.48
31	N(64)-C(26)-H(52)	106.39	106.38	91	C(9)-C(4)-C(5)	119.70	119.58
32	C(26)-N(68)-C(27)	112.89	112.68	92	C(6)-O(71)-C(10)	120.51	119.84
33	C(26)-N(68)-C(29)	113.24	113.48	93	O(71)-C(10)-O(72)	123.95	123.44
34	H(51)-C(26)-N(68)	113.44	112.94	94	O(71)-C(10)-C(11)	109.38	110.28
35	H(52)-C(26)-N(68)	108.47	108.61	95	O(72)-C(10)-C(11)	126.67	126.27
36	N(68)-C(27)-H(53)	112.02	111.79	96	C(10)-C(11)-H(37)	116.82	116.52
37	N(68)-C(27)-H(54)	108.62	108.71	97	C(10)-C(11)-C(12)	119.82	119.68
38	N(68)-C(27)-C(28)	109.32	109.62	98	H(37)-C(11)-C(12)	123.35	123.80
39	H(51)-C(27)-C(28)	110.08	110.31	99	C(11)-C(12)-H(38)	116.27	116.75
40	H(52)-C(27)-C(28)	109.38	109.06	100	C(11)-C(12)-C(13)	127.87	127.69
41	C(27)-C(28)-N(69)	113.94	113.75	101	H(38)-C(12)-C(13)	115.86	115.56
42	C(27)-C(28)-H(55)	110.08	110.04	102	C(12)-C(13)-C(14)	118.51	118.39
43	C(27)-C(28)-H(56)	107.91	108.02	103	C(12)-C(13)-C(18)	123.23	123.13
44	H(55)-C(28)-N(69)	108.98	109.18	104	C(13)-C(14)-H(39)	119.05	119.43
45	H(56)-C(28)-N(69)	107.89	108.05	105	C(13)-C(14)-C(15)	121.06	120.99
46	C(28)-N(69)-C(30)	109.78	110.13	106	H(39)-C(14)-C(15)	119.89	119.58
47	C(28)-N(69)-C(31)	114.25	114.62	107	C(14)-C(15)-H(40)	119.85	119.86
48	N(69)-C(31)-H(61)	109.01	109.20	108	C(14)-C(15)-C(16)	119.93	119.88
49	N(69)-C(31)-H(62)	109.01	109.20	109	H(40)-C(15)-C(16)	120.22	120.26
50	N(69)-C(31)-H(63)	115.68	115.09	110	C(15)-C(16)-H(41)	120.18	120.18
51	C(31)-N(69)-C(30)	114.27	114.60	111	C(15)-C(16)-C(17)	119.75	119.78
52	N(69)-C(30)-C(29)	113.90	113.67	112	H(41)-C(16)-C(17)	120.07	120.04
53	N(69)-C(30)-H(57)	107.81	107.99	113	C(16)-C(17)-H(42)	119.99	120.00
54	N(69)-C(30)-H(58)	108.93	109.13	114	C(16)-C(17)-C(18)	120.31	120.25
55	H(57)-C(30)-C(29)	108.18	108.27	115	H(42)-C(17)-C(18)	119.70	119.74
56	H(58)-C(30)-C(29)	110.06	110.03	116	C(17)-C(18)-H(43)	119.43	119.18
57	C(30)-C(29)-N(68)	109.52	109.71	117	C(17)-C(18) -C(13)	120.69	120.60
58	C(30)-C(29)-H(59)	110.45	110.52	118	H(43)-C(18)-C(13)	119.88	120.21
59	C(30)-C(29)-H(60)	110.02	109.54	119	C(18)-C(13) -C(14)	118.26	118.48
60	H(59)-C(29)-N(68)	111.08	111.02				

Table 2. The calculated frequencies values of the molecule.

	Vibration Types	**scaled DFT**	**scaled Hf**
1	τ NCCC (25), τ NCNN (22)	8	5
2	δ COC (20), τ NCCC (10)	12	6
3	τ NCCC (23), τ NCNN (17), τ CCOC (13)	14	8
4	τ COCC (26)	16	13
5	τ CCOC (16), τ COCC (18)	19	12
6	τ NCCC (28)	21	15
7	τ CCCC (16), τ COCC (18)	23	16
8	τ CNCN (45)	29	19
9	NCNN (11)	28	23
10	τ CCNN (19)	35	25
11	δ COC (13), τ CCNN (12)	37	38
12	τ CCOC (12), τ COCC (23)	40	41
13	τ CCCC (14), τ CCOC (10), τ COCC (18)	47	44
14	τ NCNN (18), τ CCNN (17)	56	57

15	δ NCC (10), δ CCC (10)	67	64
16	δ CCC (10), τ CCNC (13)	90	90
17	τ CCCO (19), τ CCOC (34)	93	97
18	τ COCC (18)	101	98
19	τ CNNC (19)	119	116
20	τ CCCO (26), τ CCOC (10)	148	133
21	τ CNNC (14), τ HCCN (54)	153	168
22	τ CCCN (18)	162	176
23	τ NCNN (13)	171	180
24	τ CNNC (24), τ NNCN (11)	178	183
25	τ CCCN (15)	189	191
26	δ CNC (19), τ CNCN (21)	198	199
27	δ CCC (11), CCO (12)	202	200
28	δ CCN (10), δ CNC (15), τ CNCN (10)	209	213
29	τ HCNC (24)	218	219
30	CC (15), δ CCC (12)	224	228
31	τ CCCC (25)	232	230
32	τ CCCC (21), τ NCNN (13)	238	233
33	τ CNNC (16)	250	252
34	τ COCC (18)	257	264
35	δ OCN (13)	276	283
36	τ CCCO (10), τ CCCC (20)	282	292
37	τ CCOC (13)	290	297
38	δ CNN (10), δ CCN (13), τ CCCN (13)	312	323
39	δ NNC (15), δ OCN (11)	322	346
40	δ COC (11), δ CCN (13), τ CNNC (16)	334	352
41	δ CNN (17), δ NNC (14)	348	357
42	δ HCN (11)	355	367
43	τ NCNN (10), τ CNNC (10), τ NNCN (11)	359	371
44	δ COC (11)	370	386
45	δ CNN (12), δ NNC (13), δ OCN (13)	387	409
46	τ HCCC (11), τ CCCO (35), τ CCCC (33)	409	430
47	δ CNC (11), τ HCCC (17)	413	437
48	δ CNC (43)	431	444
49	δ CNC (10)	440	450
50	δ HCH (44)	441	461
51	τ HCCC (16), τ CCCC (28), τ OCCC (14)	461	486
52	δ CCC (11)	470	490
53	δ CCN (16)	490	504
54	τ HCCN (139, δ CNC (30), δ HCH (44)	495	510
55	τ HCCC (15), τ CCCO (19), τ CCCC (20)	496	517
56	δ CCC (18), δ CCO (16), δ OCO (10)	558	573
57	δ CCC (11), δ NCN (12)	582	602
58	τ CCCC (16), τ OCCC (21)	594	614
59	δ CCC (28)	617	641
60	δ CNC (12)	627	647
61	δ CCC (40), ν CC (40)	628	649
62	δ CNN (14), δ CCN (11), δ OCN (14)	629	654
63	τ NNCN (14)	635	687
64	τ NNCN (14), ν NC (23), ν CC (13)	653	687
65	τ CCCO (18), τ OCOC (24)	686	721
66	τ HCCC (26), CCCC (43), ν CC (21), δ HCC (10)	691	724
67	τ HCCC (24)	700	732
68	τ ONNC (27)	701	734
69	τ HCCC (18), τ OCOC (40)	710	760
70	τ ONNC (46)	**716**	**781**

71	δ COC (10), δ OCO (28)	**751**	**799**
72	τ HCCC (12), τ OCOC (34)	769	801
73	τ HCCC (18)	773	806
74	τ HCCC (10)	776	812
75	ν NC (26)	779	822
76	δ NCC (13)	789	834
77	ν NC (24)	801	840
78	τ HCCC (31), τ CCCC (10)	808	855
79	ν NN (10), δ NCC (13)	833	874
80	τ HCNC (15), ν NC (10)	845	880
81	τ HCCC (40)	846	885
82	τ HCCC (48)	847	888
83	ν CC (10), δ CCC (11)	857	906
84	τ HCCC (32)	876	937
85	τ HCCC (25)	886	943
86	δ CNC (11), δ CCN (14)	902	960
87	τ HCCC (52)	915	981
88	δ CCC (18), ν CC (21)	921	989
89	τ HCCC (48)	926	995
90	δ CCC (11), ν CC (10), ν OC (17)	951	997
92	τ HCCC (55), ν CH (53)	961	1010
93	ν NN (13), ν NC (17), ν CC (20)	970	1029
94	τ HCCC (58), τ CCCC (10)	973	1037
95	δ CNC (10), ν CC (19)	984	1037
96	τ HCCC (35), δ CCC (18)	986	1038
97	τ HCCC (41), τ CCCC (13)	990	1039
98	ν OC (15)	993	1042
99	τ HCCN (12), ν CC (10)	995	1048
100	τ HCCN (12)	1000	1055
101	ν CC (25), δ CCC (24)	1007	1062
102	τ HCNN (39), δ CCC (13)	1009	1066
103	τ HCNN (47), δ CCC (11)	1009	1073
104	ν NC (26)	1026	1076
105	τ HCCC (49)	1030	1091
106	τ HCCN (24)	1037	1092
107	ν CC (28), δ HCC (19)	1048	1093
108	ν CC (17), δ HCN (22)	1049	1096
109	τ HCNC (12)	1061	1109
110	ν CC (14), δ HCN (10), τ HCNC (16)	1064	1112
110	δ HCC (17)	1070	1121
111	ν NC (11), δ HCC (11)	1080	1127
112	δ NNC (10), ν NC (22), δ CNN (11)	1089	1132
113	δ HCC (22)	1104	1135
114	ν CC (12), δ HCC (14)	1104	1153
115	ν NC (17)	1133	1162
116	δ NCN (13)	1151	1172
117	ν NC (12)	1154	1198
118	ν NC (12)	1163	1206
119	ν OC (15), δ HCC (50)	1175	1212
120	ν NC (16)	1178	1230
121	ν OC (18), δ HCC (27)	1182	1233
122	ν CC (10), δ HCC (41)	1184	1235
123	ν CC (14), ν OC (11), δ HCC (22)	1189	1242
124	δ HCC (21)	1204	1249
125	δ HCC (21)	1205	1251
126	τ HCNC (26)	1220	1264

127	δ HCC (37), τ HCNC (11)	1224	1268
128	ν CC (11), δ HCC (29)	1228	1271
129	δ HCC (31)	1242	1276
130	ν OC (13), δ NCN (13)	1255	1279
131	δ HCC (14)	1277	1289
132	δ HCC (25), δ CCC (18)	1283	1298
133	ν CC (11), ν NN (10), δ NCN (14)	1291	1327
134	ν CC (19), δ HCC (17), δ CCC (10)	1313	1347
135	δ HCC (47)	1315	1351
136	δ HCC (45)	1318	1367
137	δ HCN (27)	1320	1375
138	δ HCC (54)	1328	1378
139	δ HCC (32)	1339	1381
140	δ HCN (11)	1345	1383
141	ν CC (34), δ HCC (18)	1348	1387
142	ν CC (40), δ HCC (23)	1356	1404
143	ν CC (43), δ HCC (21)	1359	1421
144	δ HCC (47)	1364	1431
145	δ HCC (47)	1364	1435
146	ν NC(10), δ HCN (39)	1383	1443
147	δ HCN (41)	1384	1443
148	δ HCC (17), τ HCNC (23)	1389	1461
149	τ HCNC (12)	1398	1472
150	τ HCNC (19)	1403	1478
151	δ HCN (16)	1417	1494
152	δ HCN (14), δ HCH (44)	1427	1496
153	δ HCH (10), τ HCNC (14)	1438	1512
154	ν CC (11), ν NC (14), δ HCH (12)	1450	1515
155	δ HCH (70)	1467	1530
156	ν CC (14), δ HCN (12), δ HCC (10)	1469	1535
157	δ HCH (45)	1482	1539
158	ν CC (14), δ HCC (24)	1484	1540
159	δ HCH (17)	1485	1550
160	δ HCH (44), τ HCCN (13)	1486	1557
161	δ HCH (32)	1489	1561
162	δ HCH (36), τ HCNC (13)	1497	1558
163	δ HCH (35), τ HCCN (11)	1499	1563
164	δ HCH (53)	1504	1567
165	δ HCH (47)	1508	1570
166	δ HCC (26)	1525	1587
167	δ HCH (42)	1528	1587
168	ν CC (12), δ HCC (32), δ CCC (12)	1532	1589
169	δ HCH (60)	1534	1591
170	ν CC (40)	1618	1693
171	ν CC (14), δ CCC (11)	1621	1708
172	ν NC (14), ν CC(19), δ HCC (12)	1638	1721
173	ν CC (13)	1644	1727
174	ν NC (23)	1644	1770
175	ν NC (50)	1664	1782
176	ν CC (21), δ HCC (10)	1681	1814
177	ν OC (72), ν NC (10)	1789	1863
178	ν OC (81)	1793	1906
179	ν CH (48)	2895	2960
180	ν CH (59)	2900	2965
181	ν CH (51)	2939	3004
182	ν CH (53)	2941	3006

183	ν CH (24)	2964	3047
184	ν CH (62)	2970	3054
185	ν CH (58)	3010	3059
186	ν CH (58)	3015	3065
187	ν CH (68)	3023	1072
188	ν CH (73)	3037	3076
189	ν CH (21)	3039	3083
190	ν CH (25)	3047	3092
191	ν CH (43)	3063	3102
192	ν CH (50)	3066	3108
193	ν CH (28)	3080	3119
194	ν CH (16)	3082	3126
195	ν CH (51)	3093	3136
196	ν CH (25)	3096	3156
197	ν CH (48)	3112	3163
198	ν CH (57)	3135	3168
199	ν CH (37)	3145	3196
200	ν CH (44)	3155	3202
201	ν CH (26)	3159	3209
202	ν CH (54)	3160	3210
203	ν CH (33)	3167	3214
204	ν CH (47)	3169	3223
205	ν CH (38)	3177	3226
206	ν CH (55)	3184	3230
207	ν CH (47)	3189	3232
208	ν CH (49)	3192	3240
209	ν CH (38)	3199	3246
210	ν CH (27)	3214	3248

Vibrational frequencies

The 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one has 72 atoms and the number of the normal vibrations are 210. The observed and calculated vibrational frequencies, the calculated IR intensities and assignments of vibrational frequencies for title compound are summarized in Table **2**.

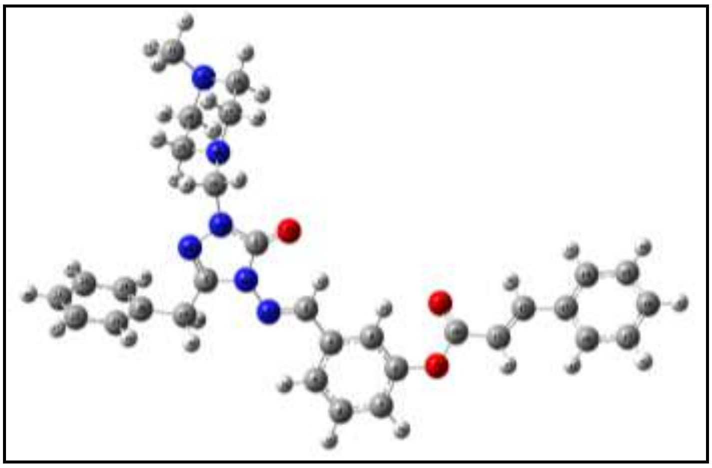


Figure 1. The optimized molecular structure of 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one (1) with DFT/HF 6–31G(d) level.

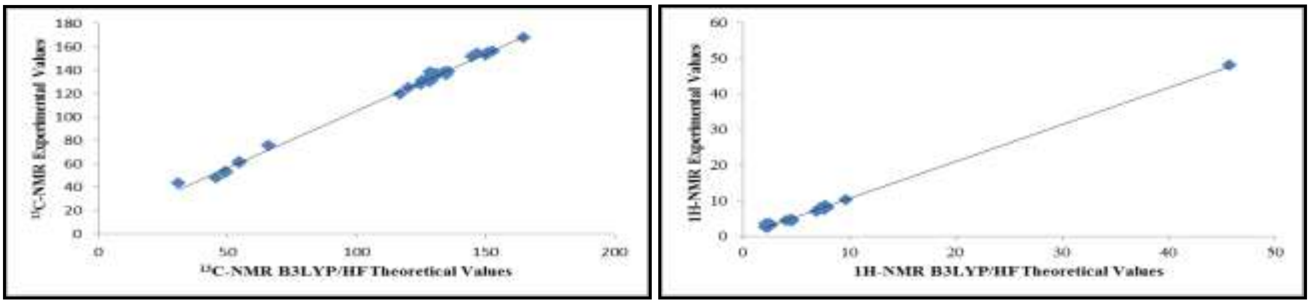
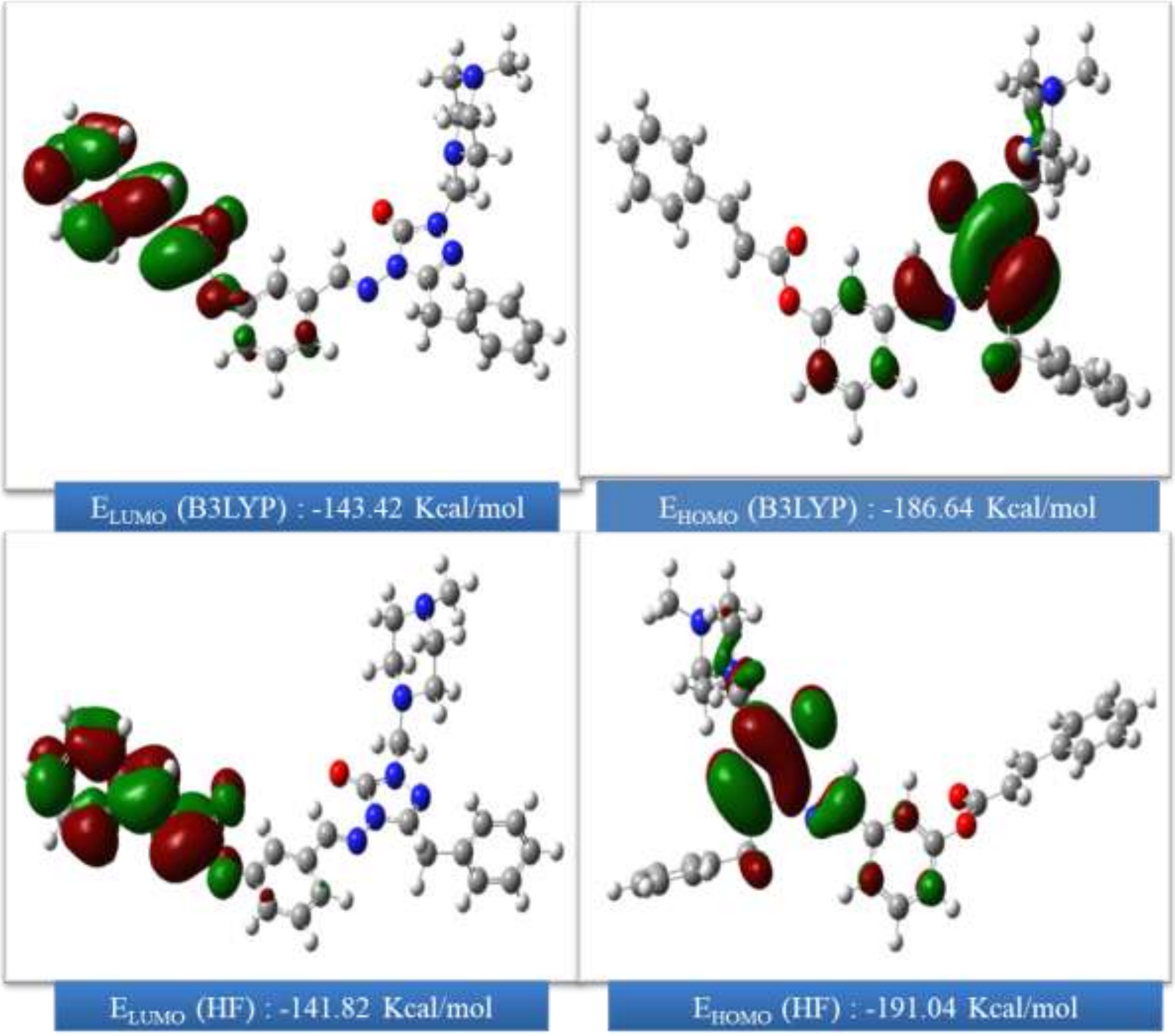


Figure 2. The correlation graphics for ^{13}C-NMR (DMSO) and ^{1}H-NMR (DMSO) chemical shifts of the molecule



E$_{LUMO}$ (B3LYP) : -143.42 Kcal/mol

E$_{HOMO}$ (B3LYP) : -186.64 Kcal/mol

E$_{LUMO}$ (HF) : -141.82 Kcal/mol

E$_{HOMO}$ (HF) : -191.04 Kcal/mol

Figure 3. The calculated HOMO-LUMO energies of the molecule according to DFT/B3LYP/6–31G(d) and HF/B3LYP/6–31G(d) levels

NMR spectral analysis

In nuclear magnetic resonance (NMR) spectroscopy, the isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties which provide the accurate predictions of molecular geometries [12-14]. In this framework, the optimized molecular geometry of the molecule was obtained by using B3LYP and HF methods with 6–31G(d) basis level in DMSO solvent. By considering the optimized molecular geometry of the title compound the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital (GIAO) method. Theoretical and experimental [9] values were plotted according to δ exp=a. δ calc.+ b, Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program.

Table 3. The calculated and experimental ^{13}C and ^{1}H NMR isotropic chemical shifts of the molecule.

No	Experim.	DFT/631d/DMSO	Diff./DMSO	HF/631d/DMSO	Diff/DMSO
C1	144,82	151,60	-6,78	125,92	18,90
C2	150,16	152,80	-2,64	128,98	21,18
C3	152,81	155,73	-2,92	128,88	23,93
C4	135,62	138,88	-3,26	111,41	24,21
C5	127,76	131,31	-3,55	107,59	20,17
C6	150,97	154,93	-3,96	125,31	25,66
C7	124,94	127,81	-2,87	105,69	19,25
C8	130,23	133,83	-3,60	108,33	21,90
C9	120,35	125,14	-4,79	102,34	18,01
C10	164,78	167,61	-2,83	142,75	22,03
C11	117,00	119,28	-2,28	94,23	22,77
C12	146,74	154,07	-7,33	128,16	18,58
C13	130,96	136,85	-5,89	108,55	22,41
C14	128,69	129,95	-1,26	105,65	23,04
C15	128,47	132,72	-4,25	106,47	22,00
C16	134,98	136,04	-1,06	111,10	23,88
C17	128,47	132,88	-4,41	106,65	21,82
C18	128,69	138,41	-9,72	112,16	16,53
C19	30,95	43,73	-12,78	16,33	14,62
C20	133,83	138,05	-4,22	111,11	22,72
C21	129,01	134,20	-5,19	109,38	19,63
C22	128,72	131,97	-3,25	107,09	21,63
C23	125,73	130,80	-5,07	106,41	19,32
C24	128,72	132,00	-3,28	107,16	21,56
C25	129,01	133,98	-4,97	109,19	19,82
C26	65,91	75,88	-9,97	41,85	24,06
C27	49,44	53,46	-4,02	20,65	28,79
C28	54,51	61,82	-7,31	26,71	27,80
C29	54,51	60,87	-6,36	26,04	28,47
C30	49,44	52,48	-3,04	19,65	29,79
C31	45,73	48,03	-2,30	18,49	27,24
H32	9,69	10,15	-0,46	9,28	0,41
H33	7,23	7,78	-0,55	6,63	0,60
H34	7,64	7,51	0,13	6,63	1,01
H35	7,58	7,94	-0,36	6,96	0,62
H36	7,7	8,44	-0,74	7,68	0,02
H37	6,94	6,87	0,07	5,89	1,05
H38	7,92	8,12	-0,20	7,57	0,35
H39	7,84	8,37	-0,53	7,46	0,38
H40	7,47	7,93	-0,46	6,87	0,60
H41	7,37	7,92	-0,55	6,91	0,46
H42	7,47	7,89	-0,42	9,82	-2,35
H43	7,84	7,75	0,09	6,88	0,96
H44	4,1	4,38	-0,28	2,89	1,21
H45	4,1	4,39	-0,29	2,92	1,18
H46	7,34	7,74	-0,40	6,72	0,62
H47	7,31	7,82	-0,51	6,69	0,62
H48	7,29	7,77	-0,48	0,65	6,64

H49	7,31	7,81	-0,50	6,69	0,62
H50	7,34	7,73	-0,39	6,71	0,63
H51	4,57	4,08	0,49	2,37	2,20
H52	4,57	4,63	-0,06	3,12	1,45
H53	2,29	2,54	-0,25	0,79	1,50
H54	2,29	3,27	-0,98	0,94	1,35
H55	2,6	3,01	-0,41	1,18	1,42
H56	2,6	3,48	-0,88	1,83	0,77
H57	2,6	2,94	-0,34	1,02	1,58
H58	2,6	3,28	-0,68	1,59	1,01
H59	2,29	2,63	-0,34	0,53	1,76
H60	2,29	2,87	-0,58	0,65	1,64
H61	2,13	2,45	-0,32	1,02	1,11
H62	2,13	2,47	-0,34	1	1,13
H63	2,13	3,39	-1,26	1,35	0,78

Table 4. Mulliken atomic charges of the molecule

	DFT	**HF**		**DFT**	**HF**		**DFT**	**HF**
C1	0.554	0.629	**C25**	-0.169	-0.208	**H49**	0.130	0.202
C2	0.847	1.110	**C26**	0.010	0.107	**H50**	0.127	0.204
C3	0.038	0.090	**C27**	-0.136	-0.135	**H51**	0.147	0.180
C4	0.117	-0.034	**C28**	-0.144	-0.132	**H52**	0.172	0.209
C5	-0.197	-0.226	**C29**	-0.144	-0.143	**H53**	0.114	0.134
C6	0.350	0.394	**C30**	-0.145	-0.132	**H54**	0.149	0.178
C7	-0.158	-0.227	**C31**	-0.303	-0.286	**H55**	0.134	0.164
C8	-0.143	-0.204	**H32**	0.212	0.299	**H56**	0.152	0.184
C9	-0.154	-0.191	**H33**	0.165	0.251	**H57**	0.135	0.179
C10	0.617	0.832	**H34**	0.144	0.225	**H58**	0.448	0.164
C11	-0.214	-0.349	**H35**	0.139	0.212	**H59**	0.168	0.201
C12	-0.146	-0.112	**H36**	0.151	0.235	**H60**	0.114	0.135
C13	0.166	0.012	**H37**	0.153	0.225	**H61**	0.147	0.165
C14	-0.186	-0.211	**H38**	0.171	0.250	**H62**	0.146	0.166
C15	-0.131	-0.204	**H39**	0.143	0.218	**H63**	0.124	0.134
C16	-0.123	-0.191	**H40**	0.140	0.212	**N64**	-0.370	-0.580
C17	-0.131	-0.205	**H41**	0.139	0.212	**N65**	-0.341	-0.339
C18	-0.170	-0.198	**H42**	0.139	0.211	**N66**	-0.433	-0.645
C19	-0.437	-0.410	**H43**	0.137	0.214	**N67**	-0.313	-0.327
C20	0.184	0.051	**H44**	0.182	0.218	**N68**	-0.386	-0.587
C21	-0.168	-0.208	**H45**	0.181	0.217	**N69**	-0.367	-0.559
C22	-0.129	-0.197	**H46**	0.127	0.204	**O70**	-0.549	-0.672
C23	-0.128	-0.203	**H47**	0.130	0.202	**O71**	-0.550	-0.720
C24	-0.129	-0.198	**H48**	0.129	0.201	**O72**	-0.478	-0.586

Table 5. Electronic properties of the molecule

	DFT (kcal/mol)	**HF (kcal/mol)**
Ionization Potential	186.64	191.04
Electron Affinity	143.42	141.82
Electronegativity	165.03	166.43
Chemical hardness	21.61	24.61
Chemical softness	0.02314	0.02032
Energy	-11010.83	-10942.34

Table 6. The calculated dipole moment values of the molecule

Dipole Moment	B3LYP (a.u.)	HF (a.u.)
μ_x	-1.3559	-1.7535
μ_y	-1.1907	-1.7096
μ_z	-1.0108	-1.0467
μ_{Toplam}	2.0683	2.6633

Discussion

The vibrational frequencies, ^{1}H and ^{13}C NMR chemicals shifts, HOMO and LUMO analyses and atomic charges of 1-(4-methylpiperazine-1-yl-methyl)-3-benzyl-4-(3-cinnamoyloxybenzyliden-amino)-4,5-dihydro-1H-1,2,4-triazol-5-one have been calculated by using DFT/B3LYP and HF methods. ^{13}C and ^{1}H NMR chemical shifts parameters were obtained theoretically are in a very good agreement with the experimental data.

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