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Quantum Chemical Calculations of 2-Methoxy-4-[(3-*p*-Methylbenzyl-4,5-Dihydro-1*H*-1,2,4-Trıazol-5-One-4-YL)Azomethine] Phenyl-2-Methylbenzoate Molecule

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Abstract: 2-Methoxy-4-[(3-*p*-methylbenzyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl) azomethine] phenyl-2-methylbenzoate was optimized by using Density Functional Theory (DFT/B3LYP, B3PW91) methods (Frisch et al., 2009; Wolinski et. al., 1990). ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 (Wolinski et al., 1990). Theoretical and experimental values were inserted into the grafic according to equatation of δ exp$_{=}$a+b. δ calc. Experimental data obtained from the literature (Yüksek et al., 2018). The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Furthermore, the veda4f program was used in defining of IR data theoretically (Jamróz, 2004). Theoretically calculated IR data are multiplied with appropriate adjustment factors (Merrick et al., 2007) and the data obtained according to DFT(B3LYP, B3PW91) method are formed using theoretical infrared spectrum. Also, dipole moments, the HOMO-LUMO energy, ΔE_g, total energy of the molecule, bond lengths and Mulliken charges, the molecular surfaces such as molecular electrostatic potential (MEP) and MEP contour maps, the total density, the electron density and the electrostatic potential were calculated with same method and functions.

Keywords: 1,2,4-Triazol-5-one, DFT, Gaussian G09, HOMO-LUMO.

Introduction

Schiff bases are formed by the condensation of activated carbonyl and amino groups. These compounds contain an imine group (Puchtler, 1981). Organic compounds derived from 1H-1,2,4-Triazol-5-one have great importance in the synthesis of organic substances, pharmaceutical chemistry, medicine, food industry, antibacterial, antioxidant, and anti-inflammatory materials (Fan, et al., 2018; Chu, et al., 2019; Samuel, et al., 2017; Yüksek, et al., 2011; Yüksek, et al., 2020; Murtaza, et al., 2017). Besides, many heterocyclic compounds with 1,2,4 triazole derivatives; It has many biological activities such as antioxidant, antifungal, antimalarial, anti-analgesic, anticancer, anti convulsant, anti-viral (Zhang, et al., 2017; Ikizler, et al., 1998; Hashem, et al., 2007; Pandey, et al., 2012; Uddin, et al., 2020; Nilkanth, et. al., 2020; Jarrahpour, et al., 2015; Kotan, et al; 2020). Recently, the properties such as electronic, geometric, spectroscopic, conductivity and thermodynamics of Schiff bases and many organic compounds containing 1,2,4-triazole have been investigated theoretically and have taken their place in the literature (Kotan, et al., 2021; Beytur,et al., 2021; Ulaş, et al., 2021). In article in the literature, the molecular structure analysis, other all theoretical properties have been studied effectively with the Density Function Theory (DFT) method. In this study, all theoretical calculations were performed with the DFT (B3LYP and B3PW91) method and the 6-311G(d,p) basis set of Gaussian 09W program (Frisch, et al.,

2009) and the obtained results were evaluated. The scaled values (Merrick, et al., 2007) of infrared vibration frequencies were reached by using the Veda 4f program (Jamróz, 2004).

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

No	Exp.	B3LYP/ Vacuum	Differ/ Vacuum	B3LYP/ DMSO	Differ B3LYP	B3PW91/ Vacuum	Differ B3PW91/ Vacuum	B3PW91 /DMSO	Differ B3PW91/DMSO
C1	146.33	152.25	-5.92	153.18	-6.85	146.53	-0.20	147.39	-1.06
C2	151.24	152.64	-1.4	153.62	-2.38	147.61	3.63	148.51	2.73
C3	153.53	152.08	1.45	152.79	0.74	147.96	5.57	148.63	4.90
C4	128.66	133.11	-4.45	132.51	-3.85	128.00	0.66	127.34	1.32
C5	112.99	125.99	-13	126.08	-13.09	122.02	-9.03	122.03	-9.04
C6	121.25	126.2	-4.95	126.67	-5.42	122.18	-0.93	122.72	-1.47
C7	152.42	160.9	-8.48	161.53	-9.11	155.48	-3.06	156.16	-3.74
C8	139.7	145.8	-6.1	145.82	-6.12	140.36	-0.66	140.42	-0.72
C9	128.66	133.66	-5	133.98	-5.32	129.61	-0.95	129.90	-1.24
C10	30.74	34.58	-3.84	34.37	-3.63	30.43	0.31	30.18	0.56
C11	130.7	138.42	-7.72	138.39	-7.69	133.18	-2.48	133.20	-2.50
C12	128.09	133.04	-4.95	133.18	-5.09	128.94	-0.85	129.80	-1.71
C13	128.9	132.43	-3.53	132.86	-3.96	128.55	0.35	128.99	-0.09
C14	135.66	142.08	-6.42	143.37	-7.71	136.94	-1.28	138.35	-2.69
C15	128.9	132.83	-3.93	133.06	-4.16	128.88	0.02	129.12	-0.22
C16	127.99	131.87	-3.88	131.65	-3.66	127.90	0.09	127.68	0.31
C17	20.53	21.53	-1	21.14	-0.61	18.35	2.18	17.94	2.59
C18	56.22	59.09	-2.87	59.81	-3.59	55.08	1.14	55.74	0.48
C19	164.69	170.39	-5.7	171.45	-6.76	165.11	-0.42	166.11	-1.42
C20	126.43	130.84	-4.41	130.34	-3.91	125.79	0.64	125.26	1.17
C21	132.72	136.63	-3.91	136.92	-4.20	132.42	0.30	132.75	-0.03
C22	126.26	129.21	-2.95	129.89	-3.63	125.29	0.97	126.00	0.26
C23	133.02	137.41	-4.39	138.89	-5.87	133.38	-0.36	134.91	-1.89
C24	131.86	135.72	-3.86	136.19	-4.33	131.85	0.01	132.33	-0.47
C25	139.77	151.45	-11.68	151.44	-11.67	146.15	-6.38	146.16	-6.39
C26	21.06	25.21	-4.15	24.77	-3.71	21.87	-0.81	21.00	0.06
H27	11.92	7.61	4.31	8.14	3.78	7.71	4.21	8.25	3.67
H28	9.65	10.71	-1.06	10.68	-1.03	10.93	-1.28	10.89	-1.24
H29	7.73	8.83	-1.1	8.91	-1.18	9.01	-1.28	9.10	-1.37
H30	7.3	7.86	-0.56	8.08	-0.78	8.02	-0.72	8.18	-0.88
H31	7.44	7.68	-0.24	7.86	-0.42	7.86	-0.42	8.04	-0.60
H32	4.05	4.46	-0.41	4.53	-0.48	4.59	-0.54	4.67	-0.62
H33	4.05	4.58	-0.53	4.72	-0.67	4.75	-0.70	4.90	-0.85
H34	7.19	8.12	-0.93	8.31	-1.12	8.28	-1.09	8.48	-1.29
H35	7.07	7.93	-0.86	8.10	-1.03	8.07	-1.00	8.26	-1.19
H36	7.07	7.95	-0.88	8.10	-1.03	8.10	-1.03	8.26	-1.19
H37	7.19	8.19	-1	8.20	-1.01	8.36	-1.17	8.38	-1.19
H38	2.21	3.14	-0.93	3.16	-0.95	3.23	-1.02	3.26	-1.05
H39	2.21	2.69	-0.48	2.79	-0.58	2.80	-0.59	2.91	-0.70
H40	2.21	2.91	-0.7	2.99	-0.78	3.01	-0.80	3.10	-0.89
H41	3.87	4.15	-0.28	4.19	-0.32	4.48	-0.61	4.66	-0.79
H42	3.87	5	-1.13	5.08	-1.21	5.07	-1.20	5.15	-1.28
H43	3.87	4.41	-0.54	4.58	-0.71	4.21	-0.34	4.25	-0.38
H44	8.09	9.31	-1.22	9.36	-1.27	9.48	-1.39	9.54	-1.45
H45	7.68	8.07	-0.39	8.26	-0.58	8.24	-0.56	8.43	-0.75
H46	7.71	8.2	-0.49	8.43	-0.72	8.37	-0.66	8.61	-0.90
H47	7.46	8.06	-0.6	8.25	-0.79	8.22	-0.76	8.42	-0.96
H48	2.61	2.7	-0.09	3.44	-0.83	3.61	-1.00	3.56	-0.95
H49	2.61	3.79	-1.18	2.89	-0.28	3.92	-1.31	3.77	-1.16
H50	2.61	3.49	-0.88	3.63	-1.02	2.83	-0.22	3.03	-0.42

In addition, ^{13}C NMR and ^{1}H NMR chemical shift values were determined by DFT (B3LYP/B3PW91) method and 6-311G(d,p) base set according to GIAO method (Wolinski, et. al., 1990). The results of these spectral calculations and the experimental results from the literature (Yüksek, et al., 2018) were compared. Also, all theoretical calculations of the molecule have been done.

Method

In this study, the Gaussian 09W package program, which is a very comprehensive program, was used. First of all, with the B3LYP/6-311G(d,p) basis set of DFT, the most stable low-energy optimized structure of atoms and molecules has been established. Each atom of molecule was then given a number. From this optimized structure, spectroscopic, thermodynamic, geometric, electronic properties of the molecule were calculated (Frisch et al., 2009). IR vibration frequency values were calculated with the Veda 4f program (Jamróz., 2004). The ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the GIAO method using the Gaussian G09 package program (Wolinski et al., 1990). These values were compared with the experimental values (Yüksek, et al., 2018) and the difference values were found, and these values were δ exp=a+b. δ calc. plotted according to the equation. The regression coefficient was found using the Sigmaplot program. The HOMO-LUMO energy, total energy, bond angle, bond length, Mulliken atomic charges, dipole moment of the target molecule was calculated. In addition, MEP surface maps were visualized.

Results and Discussion

Computational Details

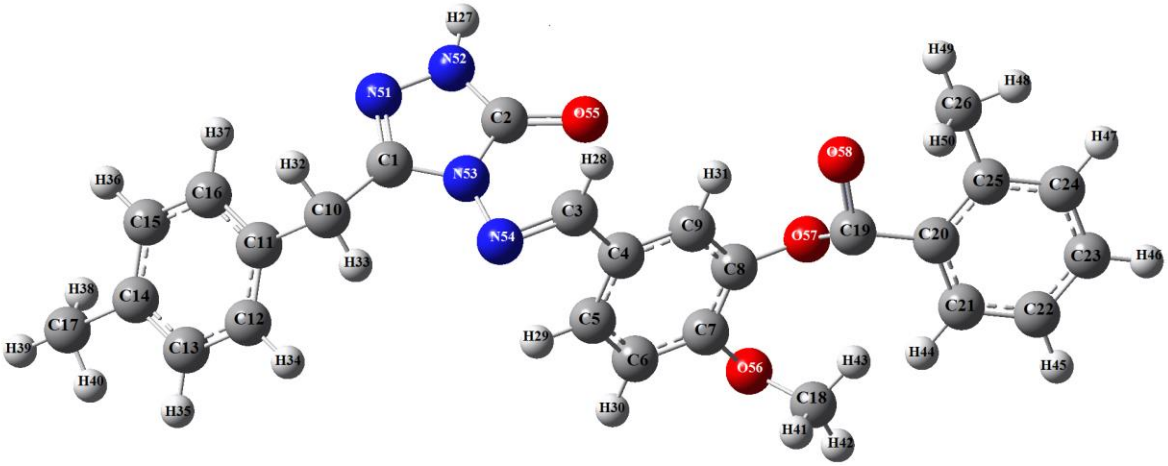


Figure 1. The Gaussview structure of the molecule.

The Relation between R Values of the Compound

There is such a relationship between R^2-values of the compound. B3LYP(DMSO): ^{1}H: 0.8702, ^{13}C: 0.9951; B3PW91(DMSO)6-311G(d,p) ^{1}H: 0.8674,^{13}C: 0.9955; B3LYP(vacuum): ^{1}H: 0.8433, ^{13}C: 0.9948; B3PW91(vacuum)6-311G(d,p) ^{1}H: 0.8403,^{13}C: 0.9953. These values for compound were seen in the Table 2. Theoretical and experimental carbon/proton chemical shifts ratios between according to R^2 lineer a correlation were observed (Figure 2).

Table 2. The correlation data for chemical shifts

	^{13}C-NMR/ R^2	^{1}H-NMR /R^2
B3LYP(DMSO)	0.9951	0.8702
B3PW91(DMSO)	0.9955	0.8674
B3LYP	0.9948	0.8433
B3PW91	0.9953	0.8403

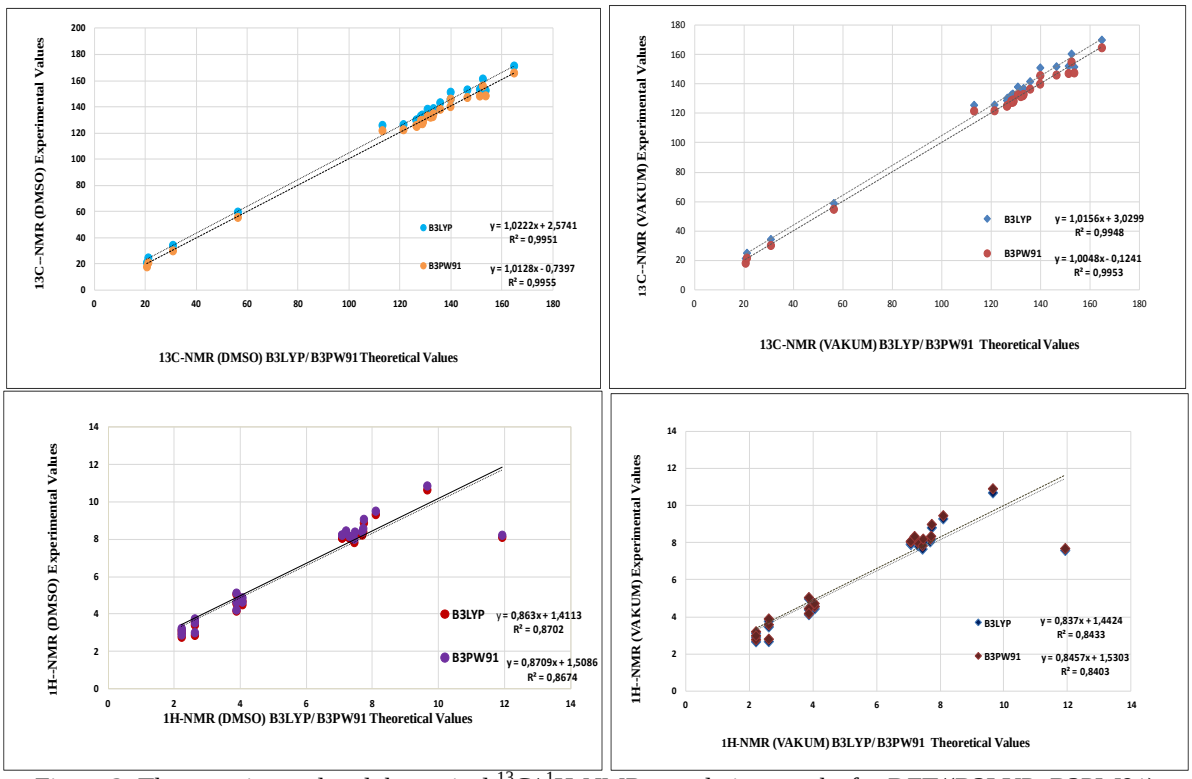


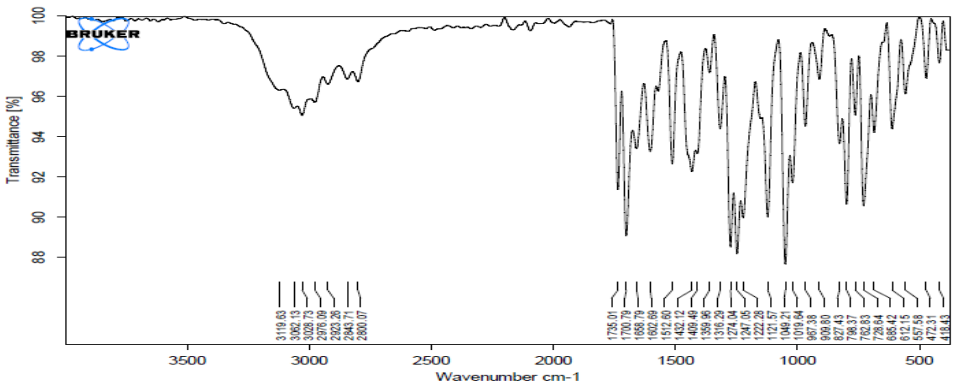
Figure 2. The experimental and theoretical ^{13}C/ ^{1}H-NMR correlation graphs for DFT/(B3LYP, B3PW91) methods chemical shifts

The Vibration Frequency of the Compound

Theoretically IR values were calculation Veda 4f program and scala values were obtain. The calculated harmonic vibrational frequency values were scaled with 0.9671 for B3LYP 3-21 G level, 0.9688 for 6-311G(d,p) level (Merrich et al., 2007). The positive frequency in the data was found. IR spectrums were drawn with obtained values according to DFT method. Theoretically IR values were compare with experimentally IR values and found corresponding with each other of values.

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

Experimental IR	Scaled B3LYP	Scaled B3PW91	Experimental IR
ν (NH)	3169	3514	3565
ν (C=O)	1739. 1700	1708. 1664	1737. 1750
ν (C=N)	1589	1577	1613
ν (COO)	1231	1248	1259



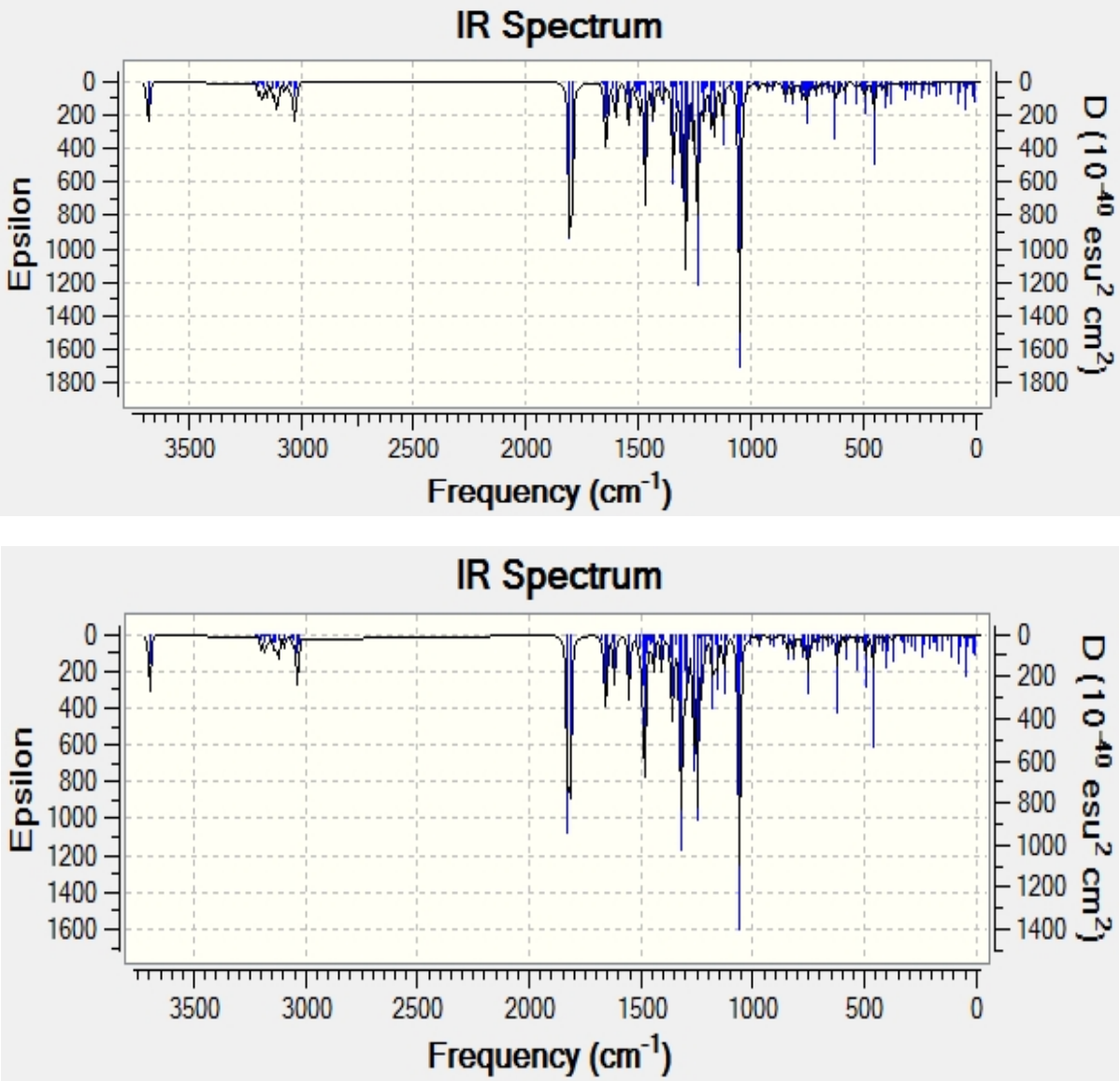


Figure 3. Experimental and theoretical IR spectrums simulated with DFT/(B3LYP, B3PW91)

Molecular Geometry

The bond angle and length are geometric parameters of the structure. To calculate these two parameters, 6-311 G(d,p) basis set and B3LYP and B3W91 functions are used. According to this calculations result, the highest bond length is between C(1)-C(10) atoms that this values are 1.49/1.48 Å for B3LYP/ B3PW91 6-311G(d,p). Besides, respectively, the bond lengths in the triazole ring N51-N52, N51-C1, C2-O55, C2-N52, N53-C1 are calculated 1.37/1.36; 1.29/1.29; 1.21/1.21;1.36/1.36, 1.38/ 1.38 Å for B3LYP 3-21G(d,p)/ 6-311G(d,p) basis sets (table 4). In the literature, the N-N, N=C, C=O bond lengths are measured as 1.40 , 1.28, 1.21 Å (Sudha et al. 2018). The calculated bond length values are consistent with literature values.

The highest bond angle is between N(52)-C(2)-O(55) atoms, which is $129.86/129.84^0$ for B3LYP/ B3PW91 6-311G(d,p) basis sets (table 5). The calculated Mulliken atomic charges (Mulliken, 1955) calculated by using the B3LYP, B3PW91 method with 6-311G(d,p) basis sets. The electronegative oxygen (O) and nitrogen (N) atoms have negative atomic charge values. The carbon atoms surrounded by electronegative atoms have negative atomic charge values. The C1 atom surrounded by two electronegative atoms (N51, N53) and C2 atom which is surrounded by three electronegative atoms (N52, N53, O55) have negative charges values. All hydrojen atoms of the compound (H27-50) have positive atomic charge values (table 6).

Table 4. The calculated bond lengths with B3LYP/B3PW91 6-311G(d,p)

Bond	Length	B3LYP	B3PW91	Bond	Length	B3LYP	B3PW91
1	C(1)-N(51)	1.297	1.296	35	C(20)-C(21)	1.404	1.401
2	C(1)-N(53)	1.387	1.383	36	C(23)-H(46)	1.084	1.085
3	C(1)-C(10)	1.492	1.487	37	C(23)-C(24)	1.390	1.388
4	N(51)-N(52)	1.379	1.369	38	C(24)-H(47)	1.084	1.085
5	N(52)-H(27)	1.005	1.005	39	C(24)-C(25)	1.398	1.396
6	N(52)-C(2)	1.369	1.365	40	C(25)-C(26)	1.508	1.502
7	C(2)-O(55)	1.216	1.214	41	C(26)-H(48)	1.091	1.092
8	C(2)-N(53)	1.419	1.414	42	C(26)-H(49)	1.091	1.091
9	N(53)-N(54)	1.371	1.363	43	C(26)-H(50)	1.091	1.092
10	N(54)-C(3)	1.285	1.284	44	C(8)-C(9)	1.389	1.387
11	C(3)-H(28)	1.086	1.088	45	C(9)-C(4)	1.396	1.394
12	C(3)-C(4)	1.461	1.457	46	C(10)-H(32)	1.093	1.094
13	C(4)-C(5)	1.405	1.402	47	C(10)-H(33)	1.091	1.092
14	C(4)-C(9)	1.396	1.394	48	C(10)-C(11)	1.522	1.517
15	C(5)-H(29)	1.082	1.083	49	C(11)-C(12)	1.394	1.392
16	C(5)-C(6)	1.379	1.377	50	C(12)-H(34)	1.085	1.085
17	C(6)-H(30)	1.083	1.084	51	C(12)-C(13)	1.393	1.391
18	C(6)-C(7)	1.405	1.402	52	C(13)-H(35)	1.085	1.086
19	C(7)-O(56)	1.357	1.351	53	C(13)-C(14)	1.396	1.394
20	O(56)-C(18)	1.433	1.425	54	C(14)-C(17)	1.509	1.504
21	C(18)-H(41)	1.089	1.090	55	C(17)-H(38)	1.095	1.095
22	C(18)-H(42)	1.090	1.091	56	C(17)-H(39)	1.092	1.092
23	C(18)-H(43)	1.093	1.093	57	C(17)-H(40)	1.093	1.093
27	C(7)-C(8)	1.401	1.399	58	C(14)-C(15)	1.399	1.397
28	C(8)-O(57)	1.396	1.390	59	C(15)-H(36)	1.085	1.086
29	O(57)-C(19)	1.380	1.373	60	C(15)-C(16)	1.390	1.388
30	C(19)-O(58)	1.203	1.201	61	C(16)-H(37)	1.085	1.086
31	C(19)-C(20)	1.487	1.483	62	C(16)-C(11)	1.398	1.395
32	C(21)-C(22)	1.387	1.385				
33	C(22)-H(45)	1.083	1.084				
34	C(22)-C(23)	1.392	1.390				

Table 5. The calculated bond angles with B3LYP/B3PW91 6-311G(d,p)

Bond Angles	B3LYP	B3PW91	Bond Angles	B3LYP	B3PW91
N(51)-C(1)-N(53)	111.440	111.370	C(4)-C(5)-H(29)	119.157	119.118
N(51)-N(52)-C(2)	114.366	114.511	H(29)-C(5)-C(6)	120.495	120.560
N(51)-N(52)-H(27)	120.514	120.497	C(4)-C(5)-C(6)	120.348	120.321
H(27)-N(52)-C(2)	125.101	124.977	C(5)-C(6)-H(30)	121.362	121.367
N(52)-C(2)-O(55)	129.862	129.840	H(30)-C(6)-C(7)	117.095	117.063
O(55)-C(2)-N(53)	128.893	128.963	C(5)-C(6)-C(7)	121.542	121.569
N(52)-C(2)-N(53)	101.245	101.196	C(6)-C(7)-O(56)	115.798	115.862
N(51)-C(1)-C(10)	124.504	124.651	C(7)-O(56)-C(18)	120.475	120.156
C(1)-C(10)-H(32)	106.336	106.336	O(56)-C(18)-H(41)	105.398	105.525
C(1)-C(10)-H(33)	109.020	108.990	O(56)-C(18)-H(42)	111.480	111.480
C(1)-C(10)-C(11)	113.862	113.635	O(56)-C(18)-H(43)	110.935	111.599
C(10)-C(11)-C(12)	120.942	120.965	O(56)-C(7)-C(8)	126.160	126.112
C(11)-C(12)-H(34)	119.560	119.553	C(7)-C(8)-O(57)	120.043	119.978
H(34)-C(12)-C(13)	119.566	119.585	C(8)-O(57)-C(19)	118.791	118.560
C(12)-C(13)-H(35)	119.388	119.406	O(57)-C(19)-O(58)	122.003	122.124
H(35)-C(13)-C(14)	119.513	119.479	O(57)-C(19)-C(20)	126.651	126.631
C(13)-C(14)-C(17)	121.265	121.266	C(19)-C(20)-C(21)	119.444	119.395
C(13)-C(14)-C(15)	117.797	117.778	C(20)-C(21)-H(44)	118.798	118.774
C(14)-C(17)-H(38)	111.067	111.440	H(44)-C(21)-C(22)	120.094	120.132
C(14)-C(17)-H(39)	111.415	111.414	C(21)-C(22)-H(45)	120.098	120.120
C(14)-C(17)-H(40)	111.398	110.981	H(45)-C(22)-C(23)	120.629	120.643
C(14)-C(15)-H(36)	119.427	119.412	C(22)-C(23)-H(46)	120.281	120.280
H(36)-C(15)-C(16)	119.345	119.354	H(46)-C(23)-C(24)	119.753	119.747
C(15)-C(16)-H(37)	119.823	119.875	C(23)-C(24)-H(47)	119.358	119.413

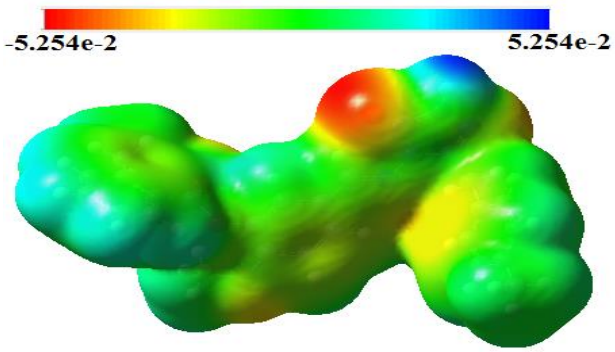
H(37)-C(16)-C(11)	119. 459	119. 411	H(47)-C(24)-C(25)	118.530	118.468
N(53)-N(54)-C(3)	118.850	118.752	C(24)-C(25)-C(26)	118.555	118.614
N(54)-C(3)-H(28)	121.955	121.928	C(25)-C(26)-H(48)	111.773	111.759
H(28)-C(3)-C(4)	117.627	117.746	C(25)-C(26)-H(49)	111.494	111.435
C(3)-C(4)-C(5)	123.074	123.061	C(25)-C(26)-H(50)	109.913	109.945

Table 6. The calculated mulliken charges datas B3LYP/B3PW91 6-311G(d,p)

Atom	DFT	B3PW91	Atom	DFT	B3PW91
C1	0.354	0.393	H29	0.108	0.121
C2	0.533	0.576	H30	0.106	0.118
C3	0.129	0.157	H31	0.102	0.115
C4	-0.175	-0.217	H32	0.150	0.169
C5	0	0.003	H33	0.136	0.155
C6	-0.102	-0.119	H34	0.083	0.094
C7	0.208	0.218	H35	0.082	0.092
C8	0.125	0.114	H36	0.084	0.094
C9	0.084	0.007	H37	0.098	0.112
C10	-0.157	-0.195	H38	0.127	0.130
C11	-0.120	-0.139	H39	0.109	0.123
C12	-0.060	-0.070	H40	0.115	0.143
C13	-0.076	-0.082	H41	0.124	0.135
C14	-0.098	-0.110	H42	0.124	0.139
C15	-0.075	-0.082	H43	0.117	0.133
C16	-0.036	-0.033	H44	0.115	0.126
C17	-0.258	-0.288	H45	0.10	0.110
C18	0.134	-0.175	H46	0.101	0.111
C19	0.415	0.435	H47	0.091	0.101
C20	-0.202	-0.233	H48	0.094	0.145
C21	-0.012	-0.014	H49	0.136	0.109
C22	-0.094	-0.105	H50	0.127	0.155
C23	-0.067	-0.073	N51	-0.228	-0.241
C24	-0.075	-0.084	N52	-0.313	-0.332
C25	-0.070	-0.078	N53	-0.382	-0.417
C26	-0.206	-0.245	N54	-0.209	-0.231
H27	0.249	0.258	O55	-0.390	-0.406
H28	0.140	0.158	O56	-0361	-0.363

MEP Surface Analysis

By looking at the molecular electrostatic potential map, we can identify the electronegative and electropositive regions of the molecule. In the MEP map, the red regions were seen in the nucleophilic regions and the blue regions were seen in the electrophilic regions. In the MEP shape of this structure, the carbonyl group is around red, while the N-H acidic proton is blue around.



MEP

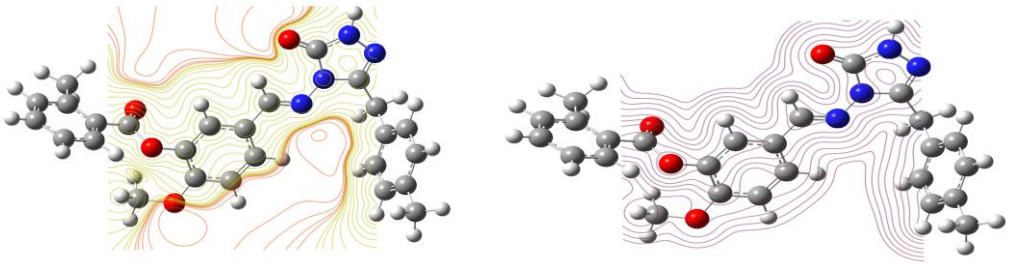


Figure 4. The calculated MEP and surface contour map of the molecule

Frontier Molecular Orbital Analysis

Frontier molecular orbitals (FMO) designated kinetic stability, the electronic transitions, electric and optical properties (Fukui, 1982). The HOMO-LUMO energy values was calculated as 4.17/4.20 eV for B3LYP and B3PW91 functionals in the 6-311G (d,p) basis set (figure 5). With the HOMO-LUMO energy gap electron affinity (A), global hardness (η), electronegativity (χ), chemical potential (μ), softness (S), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP) for the compound was calculated and we are seen in table 7.

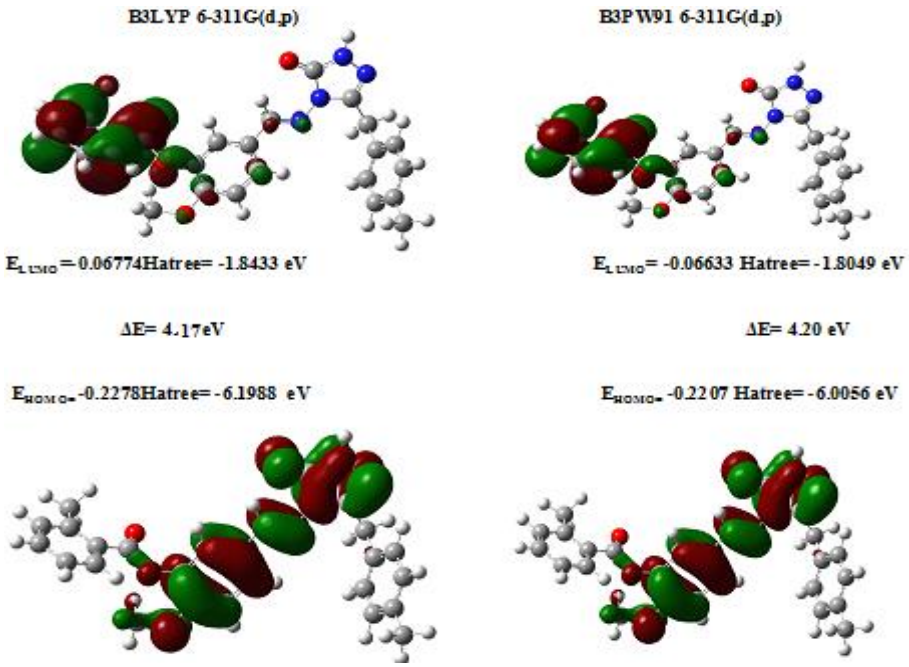


Figure 5. HOMO-LUMO energy of the molecule 6-311G(d,p)

Table 7. The calculated electronic structure parameters of the molecule

		B3LYP 3-21G(d,p)		B3LYP 6-311G(d,p)	
		Hatree	ev	Hatree	ev
	LUMO	-0.0599	-1.62992	-0.06774	-1.84325
	HOMO	-0.2191	-5.96186	-0.2278	-6.1986
A	elektron ilgisi	0.0599	1.62992	0.06774	1.84325
I	İyonlaşma potansiyeli	0.2191	5.96186	0.2278	6.1986
ΔE	energy gap	0.1592	4.33194	0.16006	4.35534
χ	electronegativity	0.1395	3.79589	0.14777	4.02093
Pi	chemical potential	-0.1395	-3.79589	-0.14777	-4.02093
ω	electrophilic index	0.000774518	0.02108	0.000873766	0.02378
IP	Nucleophilic index	-0.0111042	-0.30215	-0.01182603	-0.32179
S	molecular softness	12.5628	341.843	12.4953	340.006
η	molecular hardness	0.0796	2.16597	0.08003	2.17767

Table 8. The calculated dipole moments datas of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
B3LYP	-1.6296	1.5316	-0.6621	2.3323
B3PW91	-2.5397	1.9737	-0.8065	3.3160

Table 9. The calculated total energy datas of the molecule

Energy(a.u.)	B3LYP	B3PW91
	-1525.48470748	-1524.88006830

Thermodynamics Properties

Thermodynamics parameters were calculated with the (B3LYP/ B3PW91) functionals of DFT method at 298.150 K and under 1 atm pressure and were summarized in the Table 10.

Table 10. The calculated thermodynamics parameters of the molecule

Parameters	B3LYP	B3PW91
Rotational temperatures (Kelvin)		
A	0.01000	0.01002
B	0.00226	0.00227
C	0.00203	0.00204
Rotational constants (GHZ)		
A	0.20833	0.20877
B	0.04710	0.04727
C	0.04225	0.04257
Thermal Energies E(kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	304.170	305.163
Total	305.948	306.940
Thermal Capacity CV(cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	110.899	110.650
Total	116.861	116.612
Entropy S(cal/mol-K)		
Translational	44.242	44.242
Rotational	37.892	37.879
Vibrational	129.652	128.917
Total	211.786	211.038
Zero-point correction (Hartree/Particle)	0.456549	0.458187
Thermal correction to Energy	0.487559	0.489140
Thermal correction to Enthalpy	0.488503	0.490085
Thermal correction to Gibbs Free Energy	0.387876	0.389814
Sum of electronic and zero-point Energies	-1525.028158	-1524.421882
Sum of electronic and thermal Energies	-1524.997149	-1524.390928
Sum of electronic and thermal Enthalpies	-1524.996205	-1524.389984
Sum of electronic and thermal Free Energies	-1525.096831	-1524.490254
Zero-point vibrational energy (Kcal/mol)	286.48894	287.51650

Conclusion

All quantum chemical calculations of 2-Methoxy-4-[(3-*p*-methylbenzyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl) azomethine] phenyl-2-methylbenzoate compound with B3LYP, B3PW91/6-311G(d,p) sets were theoretically investigated. As a result of the comprehensive and comparative calculations based on the optimized structure. The R^2 values for the ^{13}C-NMR data of the molecule are 0.9955 in the B3PW91 6-311G (d,p) basic set and in the DMSO solvent environment and the closest value to 1 when compared to the other sets. As can be seen from the graphs, a deviation was observed in the ^{1}H-NMR chemical shift results. The reason for this is the

N-H acidic proton in the structure. IR vibration frequencies were calculated theoretically with two different methods and the values compared with the experimental values, and it was concluded that the values calculated with the comprehensive set B3PW91/6-311G(d,p) were more compatible with the experimental. No negative values were found in the theoretical IR data, which showed us that the molecule was stable. Among the energy values of the HOMO-LUMO orbitals of the molecule, the highest ΔEg value is 4.20 eV obtained with B3PW91/ 6-311G((d,p) and this result tells us that the structure is stable. In addition, electron affinity using the HOMO-LUMO orbital energies, ionization potential, molecular hardness-softness, nucleophilic properties were calculated. The thermodynamic values of the molecule were found and, the geometric parameters were calculated and the bond lengths were compared with the values in the literature. The obtained data were found to be compatible with each other and with the experimental data. In addition, molecular surface maps were created and nucleophilic and electrophilic regions of the molecule were determined from the MEP map.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

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