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2-(3-Methyl-4,5-Dihydro-1H-1,2,4-Triazol-5-One-4-yl-Azomethine)-Phenyl Cinnamate: Theoretical and Experimentical Properties

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Abstract: In this study, theoretically spectral values of 2-(3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate was calculated according to Gaussian G09W software. These theoretical values were compared with experimental values and obtained the results are interpreted. For this purpose, firstly, 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate molecula were optimized using B3LYP/6-311G(2d,p) basis set. Bond angles, bond lengths, dihedral angles, dipole moments, the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) energy, mulliken charges and total energy of the molecule were calculated with B3LYP/6-311G(2d,p) basis set. UV-vis values in ethanol were calculated. In addition, Theoretically calculated IR values of this compound were calculated in gas phase. The calculated IR values are multiplied with appropriate scale factors and the values obtained according to B3LYP method is obtained using theoretical infrared spectrum. The identification of calculated IR values were used veda4f program. Finally, ^{1}H-NMR and ^{13}C-NMR spectral values according to GIAO method was calculated in gas phase and in DMSO solvent. Theoretically and experimentally values were inserted into the graphic according to equitation of δexp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. The calculated and experimental results were exhibited a very good agreement.

Keywords: 1.2.4-Triazol-5-one, Gaussian 09W, GIAO, B3LYP, Dihedral.

Introduction

1,2,4-Triazole and 4,5-dihydro-1H-1,2,4-triazol-5-one derivatives have been found to have a broad spectrum of biological activities (Bahçeci et al., 2016; Kardaş et al., 2016; Bahçeci et al., 2017; Aktaş Yokuş et al., 2017; Çiftçi et al., 2018; Beytur et al., 2019; Koç et al., 2020; Beytur, 2020; Boy et al, 2021). In the past years, by increasing development of computational chemistry, theoretically properties of Schiff bases were investigated. Quantum chemical calculation methods have widely been used to theoretically predict the structural, spectroscopic, thermodynamic and electronic properties of molecular systems. The quantum chemical calculation methods provide support for experimental structural and spectroscopic studies (Uğurlu et al., 2007; Beytur et al., 2019; Irak & Beytur, 2019; Uğurlu, 2019; Kotan et al., 2020; Uğurlu, 2020; Uğurlu and Beytur, 2020; Beytur & Avinca, 2021). In the present study, 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate molecula (Gürsoy Kol et al., 2020) were optimized using B3LYP/6-311G(2d,p) basis set (Figure 1). Bond angles, bond lengths, dihedral angles, dipole moments, the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) energy, mulliken charges and total energy of the molecule were calculated with B3LYP/6-311G(2d,p) basis set. Theoretical UV calculations were made with the TD-DFT/ B3LYP method based on an optimized structure. UV-vis absorption spectra of titled

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compound were obtained in ethanol solvent. To determine the stimulation contributions to UV-visible transitions, the GaussSum3.0 software was utilized. The calculated IR data of titled compound were calculated in gas phase. The assignments of fundamental vibrational modes of the title molecule were performed on the basis of total energy distribution (TED) analysis by using VEDA 4f program (Jamroz, 2004). ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of GIAO. All quantum chemical calculations were carried out by using Gaussian 09W (Wolinski et al., 1990; Frisch et al., 2009) program package and the GaussView molecular visualization program (Frisch et al., 2003).

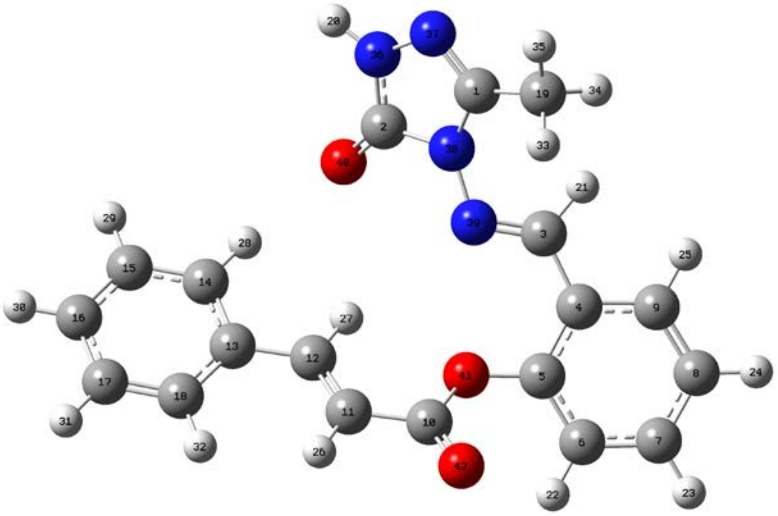

Figure 1. The optimized molecular structure (Gaussview Appearance) of titled molecule with B3LYP/6-311G(2d,p) basis set.

Method

The molecular structure of the title compound in the ground state is computed by performing the density functional theory (DFT) (Lee et al.,1988; Becke, 1993; Lee, 1998) at 6-311G(2d,p) level. Density functionals for all studies reported in this paper have been in the following form

$$E_{XC} = (1-a_0)E_X^{LSDA} + a_0 E_X^{HF} + a_X \Delta E_X^{B88} + a_C E_C^{LYP} + (1-a_C)E_C^{VWN}$$

where the energy terms are the Slater exchange, the Hartree-Fock exchange, Becke’s exchange functional correction, the gradient corrected correlation functional of Lee, Yang and Parr, and the local correlation functional of Vosko et al. (1980). The theoretical geometric structure of the title compound is given in Figure 1. Molecular geometry is restricted and the optimized geometrical parameters of the title compound in this study are carried out by using Gaussian 09W program package (Frisch et al., 2009) and the visualization parts were done with GaussView program (Dennington et al., 2009) on personal computer employing 6-311G(2d,p) basis set (Figure 1). Additionally, harmonic vibrational frequencies for the title compound are calculated with these selected methods and then scaled by 0.9905 (Avcı & Atalay, 2008) and these results were compared with the experimental data.

Results and Discussion

Molecular Structures

In the study, in order to see the compatibility of the bond lengths of titled compound with experimental data, the C-C bond lengths of the benzene ring and the C-H bond lengths compared with the experimental data recorded in the literature (Table 1). In the literature, all C-H bonds in the benzene ring are of equal length and measured as 1.084 A^{0} (Gökçe et al., 2014). The C-H bond lengths measured as 1.083 A^{0} according to the DFT calculated for the benzene ring found in the studied molecule. When the results examined, it seen that the average C-C bond lengths calculated according to the DFT of the benzene ring were almost the same as the measured length in the literature and very close to the experimental value (Gürsoy Kol et al., 2020) in the literature (Gökçe et al., 2014; Beytur et al., 2019). In addition, the calculated lengths of the C-C bonds in the benzene ring showed to have partial double bond character. The C-C single bond length is 1.54 A^0 in ethane and the C=C double bond length is 1.34 A^0 in ethylene (Gökçe et al., 2014). The calculated and found C-C bond lengths of the phenyl ring are between these two values. These results revealed that the calculated bond lengths were in full agreement with the experimental values (Gürsoy Kol et al., 2020). Another interesting result obtained from the examination of the theoretical bond lengths. When the bond lengths calculated according to the B3LYP method of the investigated compound examined, C2-N-H bond length found to be 1.371 A^0 according to B3LYP. It has been revealed that the values given in the literature are between C-C single bond length and C=C double bond length (Table 1). This showed that the electron pair remaining on the N atom and the carbonyl group delocalized because of resonance. The fact that the average length of the C2-N-H bond is shorter than that of B3LYP can be explained by the following resonance structures (Figure 2).

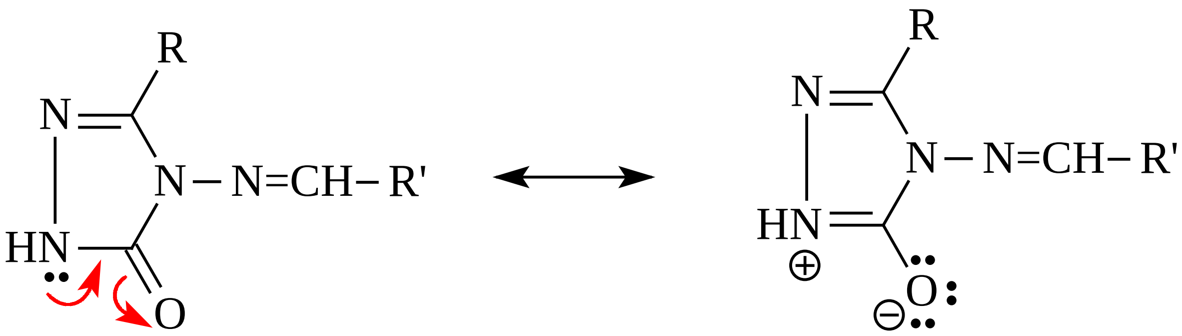

Figure 2. Resonance structures of 4,5-dihydro-1H-1,2,4-triazol-5-one

Table 1. The bond lengths of the 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate compound calculated according to the B3LYP method

Bond Lengths		B3LYP (A^0)	Bond Lengths		B3LYP (A^0)
1	C1-C19	1.4878	23	C10-O42	1.2042
2	C1-N37	1.2964	24	C11-C12	1.3428
3	C1-N38	1.3922	25	C11-H26	1.0824
4	C2-N36	1.3691	26	C12-13	1.4619
5	C2-N38	1.4103	27	C12-H27	1.0853
6	C2-O40	1.2129	28	C13-C14	1.4026
7	C3-C4	1.4596	29	C13-C18	1.4042
8	C3-2H1	1.0919	30	C14-C15	1.3892
9	C3-N39	1.2796	31	C14-H28	1.0837
10	C4-C5	1.4093	32	C15-C16	1.3896
11	C4-C9	1.4039	33	C15-H29	1.0836
12	C5-C6	1.3906	34	C16-C17	1.3941
13	C5-O41	1.3719	35	C16-H30	1.0838
14	C6-C7	1.3884	36	C17-C18	1.3845
15	C6-H22	1.0789	37	C17-H31	1.0837
16	C7-C8	1.3906	38	C18-H32	1.083
17	C7-H23	1.0833	39	C19-H33	1.0921
18	C8-C9	1.3832	40	C19-H34	1.0921
19	C8-H24	1.0826	41	C19-H35	1.0887
20	C9-H25	1.0843	42	H20-N36	1.0049
21	C10-C11	1.4622	43	N36-N37	1.3768
22	C10-O41	1.3854	44	N38-N39	1.3864

The molecular geometrical parameters such as bond angles and dihedral angles of the 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate are listed using in Table 2 and Table 3. It was observed that the bond angles obtained by the B3LYP method were close to the expected values. Bond angle is an important factor in the geometry of molecules, because the plane angle occurs in the equilibrium state of the two interacting forces in the molecule.

Table 2. The bond angles of the 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate compound calculated according to the B3LYP method (^{0})

	Bond Angles	B3LYP (^{0})		Bond Angles	B3LYP (^{0})
1	C19-C1-N37	123.13	36	C13-C12-H27	115.6044
2	C19-C1-N38	125.9073	37	C12-C13-C14	118.3926
3	N37-C1-N38	110.8561	38	C12-C13-C18	123.0971
4	N36-C2-N38	101.4299	39	C14-C13-C18	118.51
5	N36-C2-O40	130.1743	40	C13-C14-C15	120.5951
6	N38-C2-O40	128.3751	41	C13-C14-H28	119.1157
7	C4-C3-H21	114.2009	42	C15-C14-H28	120.284
8	C4-C3-N39	125.0841	43	C14-C15-C16	120.2368
9	H21-C3-N39	120.706	44	C14-C15-H29	119.6618
10	C3-C4-C5	125.6881	45	C16-C15-H29	120.1013
11	C3-C4-C9	116.3561	46	C15-C16-C17	119.7512
12	C5-C4-C9	117.9547	47	C15-C16-H30	120.2404
13	C4-C5-C6	120.3749	48	C17-C16-H30	120.008
14	C4-C5-O41	117.6201	49	C16-C17-C18	120.205
15	C6-C5-O41	121.8841	50	C16-C17-H31	119.9923
16	C5-C6-C7	120.1461	51	C18-C17-H31	119.8023
17	C5-C6-H22	119.2838	52	C13-C18-C17	120.7011
18	C7-C6-H22	120.5681	53	C13-C18-H32	120.0489
19	C6-C7-C8	120.5651	54	C17-C18-H32	119.2466
20	C6-C7-H23	119.2427	55	C1-C19-H33	111.1482
21	C8-C7-H23	120.1918	56	C1-C19-H34	112.5671
22	C7-C8-C9	119.1739	57	C1-C19-H35	107.7895
23	C7-C8-H24	120.5649	58	H33-C19-H34	107.9611
24	C9-C8-H24	120.2608	59	H33-C19-H35	108.9834
25	C4-C9-C8	121.7843	60	H34-C19-H35	108.3069
26	C4-C9-H25	118.4798	61	C2-N36-H20	125.2109
27	C8-C9-H25	119.7358	52	C2-N36-B37	114.0035
28	C11-C10-O41	112.1974	63	H20-N36-N37	120.2674
29	C11-C10-O42	124.5826	64	C1-N37-N36	105.1228
30	O41-C10-4O2	123.2197	65	C1-N38-C2	108.3967
31	C10-C11-C12	125.0121	66	C1-N38-N39	131.0926
32	C10-C11-H26	112.456	67	C2-N38-N39	119.2082
33	C12-C11-H26	122.5012	68	C3-N39-N38	115.9559
34	C11-C12-C13	126.2106	69	C5-O41-C10	121.3439
35	C11-C12-H27	118.1717			

Table 3. The dihedral angles of the 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate compound calculated according to the B3LYP method (^{0})

	Dihedral Angles	B3LYP (^{0})		Dihedral Angles	B3LYP (^{0})
1	N37-C1-C19-H33	130.1083	8	N37-C1-N38-N39	-168.9207
2	N37-C1-C19-H34	-108.6386	9	N36-C2-N38-N39	172.3401
3	N38-C1-C19-H33	-45.7879	10	O40-C2-N38-N39	-9.1986
4	N38-C1-C19-H34	75.4652	11	C4-C5-O41-C10	-137.4737
5	N38-C1-C19-H35	-165.1561	12	C6-C5-O41-C10	46.5133
6	C19-C1-N38-C2	173.9174	13	C1-N38-N39-C3	-51.1342
7	C19-C1-N38-N39	7.4022	14	C2-N38-N39-C3	143.5507

Dipole Moments

Theoretical dipole moments of 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate have been given in Tables 4.

Table 4**.** The calculated dipole moment values of the molecule

Dipole Moment	μ_x	μ_y	μ_z	μ_{Toplam}
B3LYP (a.u.)	2.2670	1.7798	0.1816	2.8879

Electronic Properties

The energies of two important molecular orbitals of the title molecule; the second highest and highest occupied MO’s (HOMO), the lowest and the second lowest unoccupied MO’s (LUMO) were calculated by using DFT/B3LYP method with 6-311G+(d,p) level. In these chemical reactions, HOMO energy is defined as electron donor tendency (π-donor), and LUMO energy is defined as electron acceptor tendency (π-acceptor). The energy gap is a critical parameter in determining molecular electrical transport properties (Fukui, 1982). The HOMO-LUMO energy gap of the title molecule found to 4.110 eV. (Figure 3). The HOMO is located almost over the carbon atoms, oxygen atoms and slightly delocalized in hydrogen atom and the LUMO is mainly delocalized in carbon atoms of benzene ring.

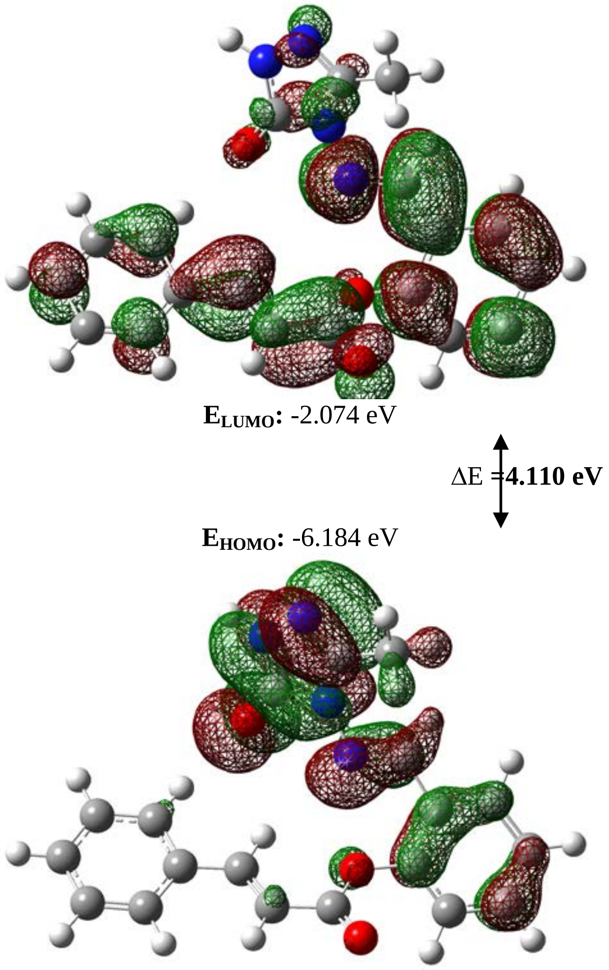

Figure 3. Calculated HOMO-LUMO shapes of the molecula by B3LYP method 6-311G(2d.p) basis set

UV-vis Properties

Theoretical UV calculations were made with the TD-DFT/B3LYP method based on an optimized structure. UV-vis absorption spectra of 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate compound (Gürsoy Kol et al., 2020) were obtained in ethanol solvent (Figure 4). Table 5 displays the predicted excitation energies, absorption wavelengths (λ), and oscillator power (*f*) in the ethanol of the titled compound.

To determine the stimulation contributions to UV-visible transitions, the GaussSum3.0 software was utilized (Rani et al., 2010). The computed absorption wavelengths listed in Table 5. Absorption modes are produced by imine group n->π* transitions between 300 and 400 nm (Tanal, 2011). For TD-DFT calculations (B3LYP), the primary transition contribution from HOMO to LUMO (95%) was calculated as n->π* transitions at 357.30 nm and the primary transition contribution from HOMO to LUMO-1 (92%) was identified as n->π* transitions at 330.81 nm for titled compound. Furthermore, the primary transition contribution from HOMO-1 to LUMO (83%) was identified at 306.65 nm and can be caused in the benzene ring and azomethine group π>π* transitions.

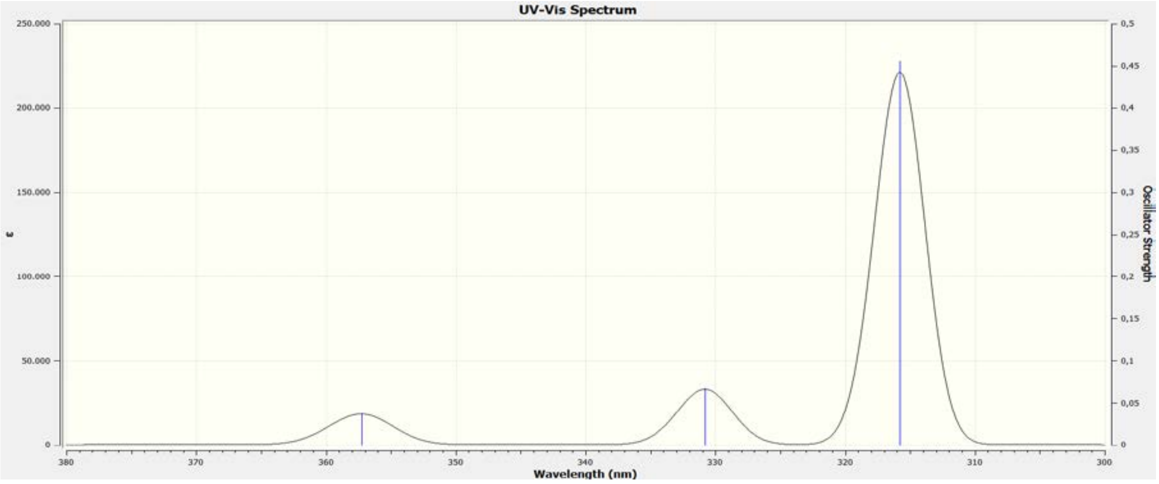

Figure 4. The generated (DFT/B3LYP) UV-vis spectra graphic for 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate

Table 5. The theoretical UV-vis, oscillator power and the primary transition contribution values with TD-DFT/ B3LYP level of titled compund

λ (nm) B3LYP	Excitation Energy (cm^{-1}) B3LYP (eV)	Oscillator Power (*f*) B3LYP	Transition Contribution* B3LYP
357.30	3.47	0.0374	H->L (95%) / H->L+1 (3%)
330.81	3.7479	0.0676	H->L+1 (92%) / H->L (4%)
315.78	3.9263	0.0456	H-1->L (83%)/H-2->L (9%)/H-1->L+1 (4%)

*H: HOMO *L: LUMO

Vibrational Frequencies

2-(3-Methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate calculated vibration frequencies and vibration spectra to determine the functional groups. The harmonic vibrational frequencies were calculated by using B3LYP method with the 6-311G(2d,p) basis set. Theoretically found excess values can be adjusted by applying the scaling factors B3LYP (0.9905) (Foresman, 1996; Avcı & Atalay, 2008).

Table 6. The calculated frequencies values of the molecule.

Selected Vibrational Types	Experimental	scaled DFT
$C_4C_9C_8C_7$, $C_8C_7C_6C_5$, $C_9C_8C_7C_6$ (47)	707	713
$H_{22}C_6C_7C_8$, $H_{22}C_7C_8C_9$, $H_{24}C_8C_9C_4$ (21)	707	726
$C_1N_{38}N_{39}$, $C_2N_{36}N_{37}$ (23)	756	771
$C_5O_{41}C_{10}$, $O_{41}C_{10}C_{11}$ (10)	756	785
$O_{41}C_5$, $O_{41}C_{10}$ (14)	1299	1176
$O_{41}C_5$, $O_{41}C_{10}$ (17)	1299	1200
$N_{37}C_1$, $N_{39}C_3$ (44)	1597	1550
$N_{37}C_1$, $N_{39}C_3$ (64), $H_{21}C_3N_{39}$ (11)	1597	1586
C_6C_5, C_7C_6, $C_{11}C_{12}$, $C_{18}C_{17}$ (19)	1634	1590
$O_{40}C_2$ (75)	1694	1690
$O_{42}C_{10}$ (85)	1725	1718
C_3H_{21}, C_6H_{22}, C7H23, C_8H_{24} (96)	3064	2922
C_9H_{25} (85)	3064	3006
$C_{11}H_{26}$, $C_{12}H_{27}$, $C_{14}H_{28}$, $C_{15}H_{29}$ (49)	3064	3011
$C_{11}H_{26}$, $C_{12}H_{27}$, $C_{14}H_{28}$, $C_{15}H_{29}$ (80)	3064	3012
C_3H_{21}, C_6H_{22}, C7H23, C_8H_{24} (81)	3064	3019
C_3H_{21}, C_6H_{22}, C7H23, C_8H_{24} (86)	3064	3035
$C_{11}H_{26}$, $C_{12}H_{27}$, $C_{14}H_{28}$, $C_{15}H_{29}$ (96)	3064	3036
C_3H_{21}, C_6H_{22}, C7H23, C_8H_{24} (99)	3064	3073
$N_{36}H_{20}$ (100)	3172	3501

The titled compound has 42 atoms and the number of the normal vibrations are 120. The observed and calculated vibrational frequencies, the calculated IR intensities and assignments of selected vibrational frequencies for title compound are summarized in Table 6 and simulated IR spectra were given in Figure 5. It has been seen that the theoretical values and the experimental values are compatible (Gürsoy Kol et al., 2020).

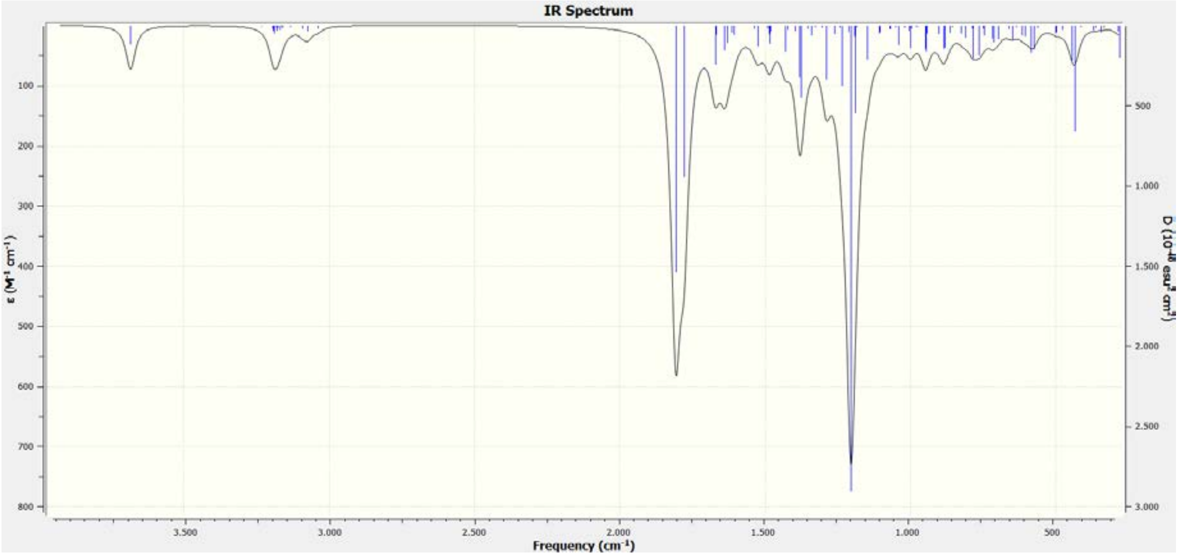

Figure 5. IR spectra simulated with DFT/B3LYP/6-311G(2d,p) level of the titled compound.

NMR Spectral Analysis

Nuclear magnetic resonance (NMR) spectroscopy allows us to identify the molecules under study and calculate the magnetic properties (Wade, 2006; Rani, et al., 2010; Subramanian et al., 2010). In the present study, the optimized the 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate was obtained in DMSO solvent by using B3LYP method with 6-311G(2d,p) basis level. The ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital method (Table 7) (Wolinski et al.,1990; Wade, 2006). The correlation graphics are given Figure 3 and the linear correlation data of the titled compound by considering the results are given in Table 7.

Table 7. Theoretically and experimentally ^{13}C and ^{1}H-NMR (B3LYP/(DMSO)) chemical shift values of the studied molecule according to the TMS standard (δ/ppm)

No	Experimental	DFT/DMSO	Diff./DMSO	No	Experimental	DFT/DMSO	Diff./DMSO
1C	147.08	155.48	-8.40	20H	11.82	7.55	4.27
2C	148.15	146.11	2.04	21H	9.92	8.56	1.36
3C	151.11	167.14	-16.03	22H	8.02	7.97	0.05
4C	123.48	127.46	-3.98	23H	7.62	7.83	-0.21
5C	149.70	156.38	-6.68	24H	7.46	7.59	-0.13
6C	125.99	127.63	-1.64	25H	7.38	7.82	-0.44
7C	130.98	136.68	-5.70	26H	6.95	6.59	0.36
8C	126.48	128.21	-1.73	27H	7.94	8.75	-0.81
9C	133.67	140.42	-6.75	28H	7.5	8.62	-1.12
10C	164.67	168.75	-4.08	29H	7.82	7.70	0.12
11C	116.42	118.10	-1.68	30H	7.48	7.71	-0.23
12C	144.15	156.08	-11.93	31H	7.82	7.68	0.14
13C	132.39	139.42	-7.03	32H	7.5	8.14	-0.64
14C	128.94	139.29	-10.35	33H	2.25	1.97	0.28
15C	128.69	132.64	-3.95	34H	2.25	2.43	-0.18
16C	126.91	135.96	-9.05	35H	2.25	2.13	0.12
17C	128.69	132.11	-3.42				
18C	128.94	128.73	0.21				
19C	11.01	13.53	-2.52				

The ^{1}H-NMR spectrum of the titled compound was observed belong to H20 proton peak at 11.82 ppm because acidic show feature (Yüksek, 1992; Yüksek et al., 2005; Yüksek et al., 2006; Gürsoy Kol et al., 2020). H21 protons were observed at 9.92 ppm. Theoretically, DMSO solvent these values for the mentioned proton atoms were found as 7.55/4.27 ppm. In Table 7, the ^{13}C chemical shift value of the molecule are observed at 164.67 ppm for the C10 carbon atom double bounded to the oxygen in carbonyl group (Anderson et al., 2004). DMSO solvent the calculated ppm values (DFT/B3LYP) for C11=C12 carbon atom were theoretically found as 116.42/144.15 ppm. Additionally, due to the electronegative property of nitrogen atoms in molecule, the experimental (Gürsoy Kol et al., 2020) NMR chemical shift values for C1 and C2 carbon atom the bounded to nitrogen atoms in 1,2,4-triazol ring and C3 carbon atom with sp^{2} hybride are observed at 147.08, 148.15 and 151.11 ppm, respectively. It has been seen that the theoretical values and the experimental values are compatible (Gürsoy Kol et al., 2020). ^{13}C-NMR and ^{1}H-NMR chemical shift values were calculated by regression analysis by analyzing experimental data using the least squares method. The obtained R^{2} value was found 0.9899 for ^{13}C-NMR data (Figure 6).

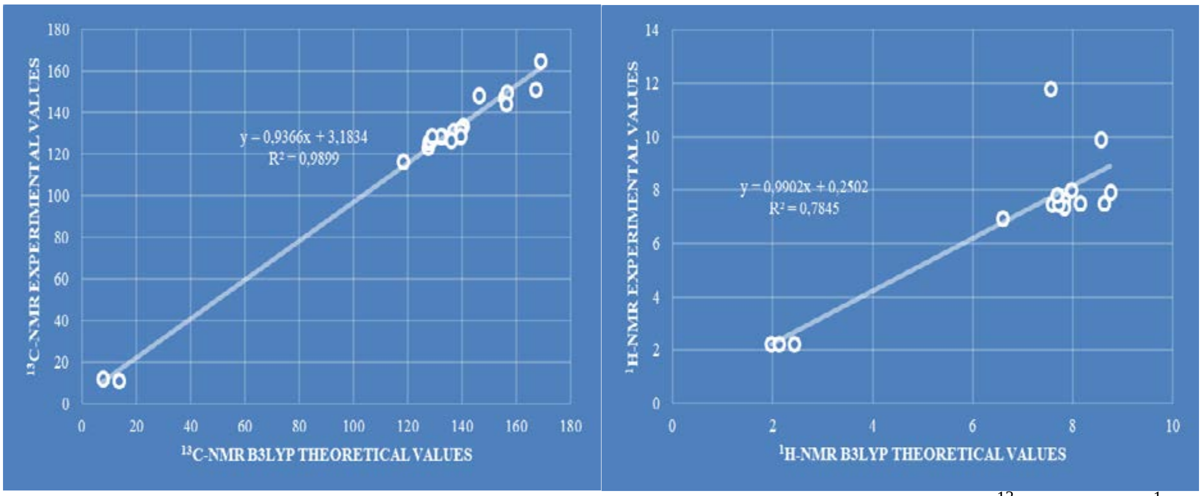

Figure 6. Regression analysis of the theoretical values calculated with experimental data of ^{13}C-NMR and ^{1}H-NMR chemical shift values by B3LYP method 6-311G(2d.p) basis set

Conclusion

In the theoretical paper, 2-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl-azomethine)-phenyl cinnamate was optimized by using Gaussian G09W software. The bond lengths obtained from the optimized structure were examined. The bond lengths of the compound named C-C bond lengths of the benzene ring and the d C-H bond lengths registered in the literature were compared. The molecular geometrical parameters such as bond angles and dihedral angles of the the compound were calculated. The energies of two important molecular orbitals of the title molecule; Dipole moment, HOMO and LUMO were calculated by using DFT/B3LYP method with 6-311G(2d,p) level. The HOMO-LUMO energy gap was found to be 4.110 eV. Theoretical UV calculations were made with the TD-DFT/B3LYP method based on an optimized structure. The GaussSum3.0 software was used to determine the stimulation contributions to the UV-visible transitions. The titled compound calculated vibration frequencies and vibration spectra to determine the functional groups. The ^{1}H and ^{13}C NMR chemical shift values were determined at the same level by using Gauge-Independent Atomic Orbital method. It has been found that the theoretical spectroscopic values and the experimental values are compatible.

Scientific Ethics Declaration

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

Acknowledgements or Notes

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