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The Investigation of Spectroscopic and Electronic Properties of 3-Ethyl-4-(4-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one Compound Using Density Functional Theory and Hartree-Fock Basis Sets

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Abstract: In this study, we reported a combined experimental and theoretical study on 3-n-propyl-4-(3-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one compound. The title compound was prepared and characterized by Uv-Vis, FT-IR spectra, ^{1}H and ^{13}C NMR. UV-visible absorption spectra and the stimulation contributions in UV-visible transitions were obtained with TD-DFT/B3LYP and TD-FF methods and 6-311G(d) polarizer set based on optimized structure. Calculated absorption wavelengths (λ), oscillator power (f) and excitation energies were compared with experimental values. The calculated IR data of compound were calculated in gas phase by using of 6-31G(d) basis set of B3LYP and HF methods and are multiplied with appropriate scala factors. Theoretical infrared spectrums are formed from the data obtained according to B3LYP method. In the identification of calculated IR data was used the veda4f program. The molecular geometry, gauge including atomic orbital (GIAO), Experimental and theoretical 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. Obtained results indicate that there is a good agreement between the experimental and theoretical data. Also, HOMO-LUMO analyses properties, Mulliken's atomic charges, dipole moment and total energy of the title compound in the ground state were investigated by using Hartree-Fock (HF) and density functional theory (DFT/B3LYP) methods with 6-31G(d) basic set.

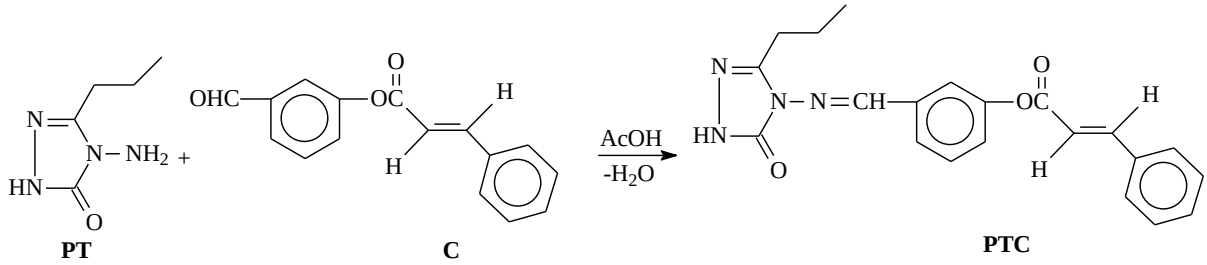
Keywords: 1,2,4-Triazol-5-one, DFT, Hartree-Fock, HOMO-LUMO, Gaussian G09

Introduction

Intense studies have been carried out in recent years on many properties of heterocyclic compounds (Aktaş Yokuş et al., 2017; Bahçeci et al., 2016; Bahçeci et al., 2017; Beytur et al., 2019; Koç et. al., 2019; Beytur et. al., 2021; Beytur, 2020; Uğurlu et al., 2020). Triazole is an unsymmetrical heterocyclic organic compound having three nitrogen atoms in the five-membered ring. 1,2,4-Triazole and derivatives are reported to possess a broad spectrum of biological activities such as antimicrobial, antifungal, antitumor, anti-HIV, antiviral, anticancer, anti-inflammatory, analgesic and antioxidant properties (Alkan et al., 2007; Boy et al., 2021; Bayrak et al., 2010; Çiftçi et al., 2018; Gürsoy-Kol et. al., 2010; Güzeldemirci et. al., 2010; Hashem et al., 2007; Tozkoparan et al., 2007; Turhan-Irak et. al., 2019). Also, several articles reporting the synthesis of some 1,2,4-triazol-5-one compounds and derivatives have been published (Bahçeci et al., 2002; Yüksek et al., 2005; Yüksek et al., 2006).

In this paper, 3-n-propyl-4-(3-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one (**PTC**) was obtained from the reaction of compound (**PT**) with 4-cinnamoyloxybenzaldehyde (**C**) (Vasavado et. al., 2003)

which was synthesized by the reaction of 4-hydroxybenzaldehyde with cinnamoyl chloride by using triethylamine (Scheme 1).



Scheme 1. Synthesis method of compound PTC

Method

Synthesis

The compound **PT** (10 mmol) was dissolved in acetic acid (20 mL) and treated with 3-cinnamoyloxybenzaldehyde **(C)** (10 mmol). The mixture was refluxed for 2 hour. Several recrystallizations of the residue from ethanol gave pure compound 3-n-propyl-4-(3-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one (PTC) was preparated. m.p. 195 °C; Yield 97 %. IR: (NH) 3166; C=CH 3064; C=O 1709; C=C 1633; C=N 1611; COO 1203; 1,3–disubstituted aromatic ring 846 and 721; monosubstituted aromatic ring 763 and 681 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ 0.97 (t, 3H, $CH_2CH_2C\underline{H}_3$; *J*=7.60 Hz), 1.70 (sext, 2H, $CH_2C\underline{H}_2CH_3$; *J*=7.60 Hz), 2.67 (t, 2H, $C\underline{H}_2CH_2CH_3$; *J*=7.20 Hz), 6.94 (d, 1H, =CH; *J*=16.00 Hz), 7.40-7.43 (m, 1H, ArH), 7.48-7.51 (m, 3H, ArH), 7.61 (t, 1H, ArH; *J*=8.00 Hz), 7.70-7.72 (m, 1H, ArH), 7.75-7.77 (m, 1H, ArH), 7.83-7.85 (m, 2H, ArH), 7.92 (d, 1H, =CH; *J*=16.00 Hz), 9.78 (s, 1H, N=CH), 11.90 (s, 1H, NH). ^{13}C-NMR (100 MHz, DMSO-d_6): δ 13.46 ($CH_2CH_2\underline{C}H_3$), 18.84 ($CH_2\underline{C}H_2CH_3$), 26.62 ($\underline{C}H_2CH_2CH_3$), 116.99 and 146.76 (CH=CH), 128.70 (2C); 129.01 (2C); 130.96; 133.82 (Monosubstitued Ar-C), 120.26; 124.90; 125.55; 130.26; 135.21; 151.26 (1,3-Disubstitued Ar-C), 146.91 (Triazole C_3), 150.93 (N=CH), 152.66 (Triazole C_5), 164.84 (COO). UV [Etanol, λ_{max}, nm (ε, $L.mol^{-1}.cm^{-1}$)]: 286 (18657), 264 (18187), 224 (16199).

Computational Properties

The molecular structure of the title compound in the ground state is computed by performing both the Density Functional Theory (DFT) and Hartree-Fock (HF) (Becke, 1993; Lee, 1998) at 6-31G(d) level. The theoretical geometric structure of the compound **PTC** 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 G09 program package (Frisch et al., 2009) and the visualization parts were done with GaussView program (Dennington et al., 2009) on personal computer employing 6-31G(d) basis set. Additionally, harmonic vibrational frequencies for the title compound are calculated with these selected methods and then scaled by 0.9516 and 0.9905, respectively (Avcı and Atalay, 2008) and these results were compared with the experimental data.

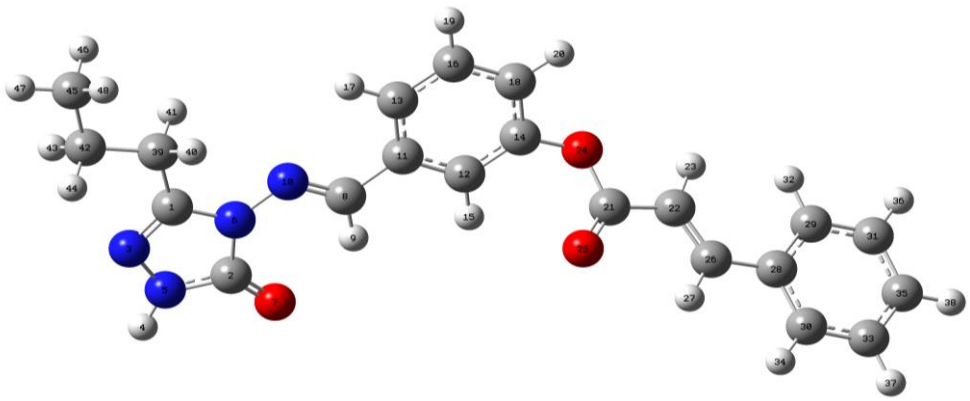


Figure 1. The optimized molecular structure of titled molecule PTC with DFT/HF 6–31G(d) level

Results and Discussion

UV–visible Spectroscopy

The title molecule allow strong $\pi \rightarrow \pi^*$ and $\sigma \rightarrow \sigma^*$ transitions in UV–vis region with high extinction coefficients (Silverstein, et al., 1991). The experimental absorption wavelengths of the compound **PTC** in ethanol solvent have been observed at 300, 262 and 214 nm. The absorption wavelengths (λ) excitation energies, and oscillator strengths (*f*) of UV–vis absorption spectroscopy of the compound **PTC** has been calculated in ethanol solvents by using TD–DFT/B3LYP and TD–HF method (Figure 2 and Table 1).

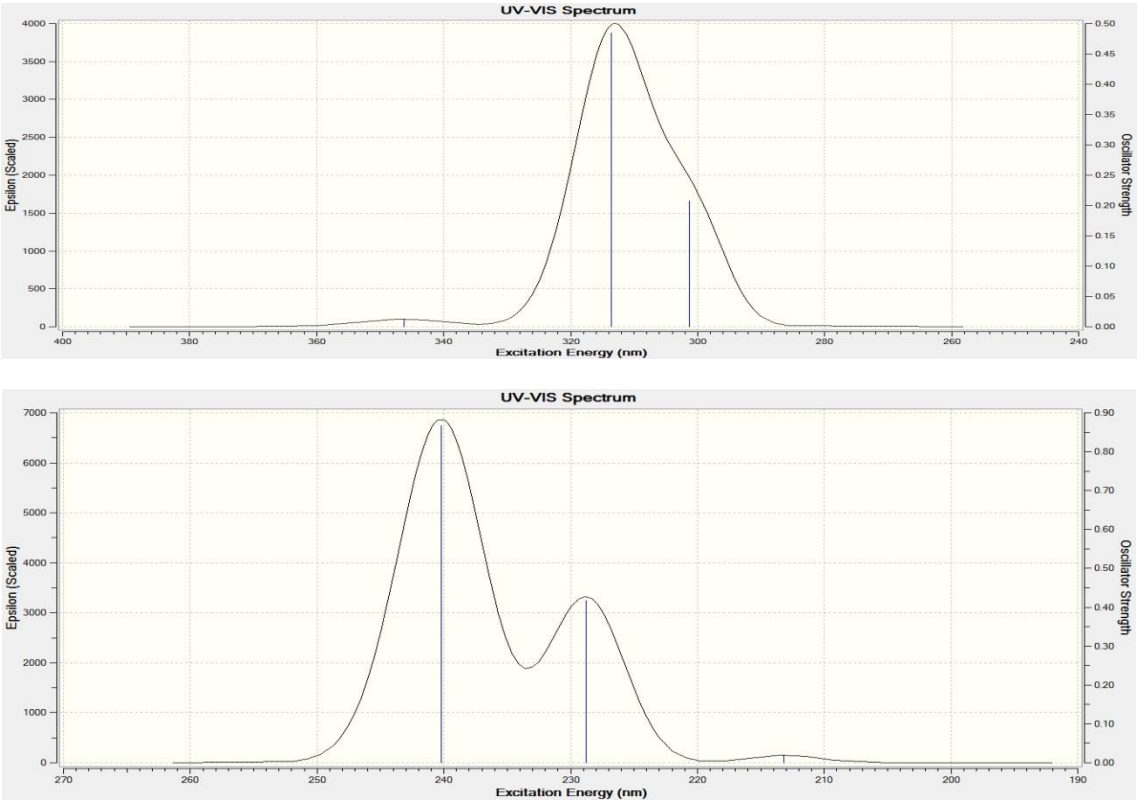


Figure 2. UV-Visible spectra experimental and simulated with DFT/B3LYP/6-31G(d) and HF/6-31G(d) levels of the compound PTC, respecvtively.

Table 1. The experimental and calculated absorption wavelength (λ), excitation energies and oscillator strengths (*f*) the compound PTC.

λ (nm)B3LYP/HF	Uyarma Enerjisi (eV) B3LYP/HF	*f* (osilatör gücü) B3LYP/HF
346.29/240.22	3.5804/5.1614	0.0125/0.8667
313.54/228.79	3.9543/5.4192	0.4849/0.4176
301.36/213.21	4.1142/5.8151	0.2077/0.0198

Analysis of Vibrational Modes

The vibrational spectra of substituted benzene derivatives have been greatly investigated by various spectroscopic, since the single substitution can have a tendency to put greater changes in vibrational wavenumbers of benzene (Turhan-Irak et. al., 2017; Beytur et al., 2019; Uğurlu et. al., 2020). In other words, molecular system of benzene is greatly affected by the nature of substituents. The number of potentially active fundamentals of non-linear molecule which have N atoms is equal to (3N-6) apart from three translational and three rotational degrees of freedom. The molecule contains 48 atoms and 138 normal vibration modes have C1 symmetry (Table 2 and Figure 3).

Table 2. The calculated frequencies values of the titled compound (PTC).

Selected Vibrational Types	B3LYP	HF	Selected Vibrational Types	B3LYP	HF
τ HNNC, τ NNCN	630	640	ν NC, δ HCN, τ HCCN	1332	1351
τ CCCO, τ OCOC	665	676	δ NNC	1350	1385
τ HCCC, τ CCCC	671	680	δ HCH, τ HCCC	1462	1462
τ HCCC, τ OCOC	690	695	ν NC, ν CC	1589	1615
τ ONNC	693	713	ν NC, ν CC	1593	1620
δ OCO, δ COC	729	750	ν NC	1615	1670
τ HCCC, τ CCCC, τ OCOC	750	759	ν CC, δ HCC	1631	1703
δ CCC	754	771	ν OC	1740	1761
ν NC, δ CNN	774	781	ν OC, ν NC	1754	1788
τ HCCC, τ CCCC	784	805	ν CH	3075	3024
ν NN, δ NNC, δ NCC	818	828	ν CH	3105	3046
τ HCCN, τ HCCC	1098	1097	ν CH	3118	3048
ν CC, ν OC, δ OCO	1118	1103	ν NH	3540	3520
ν OC, δ HCC	1140	1108			

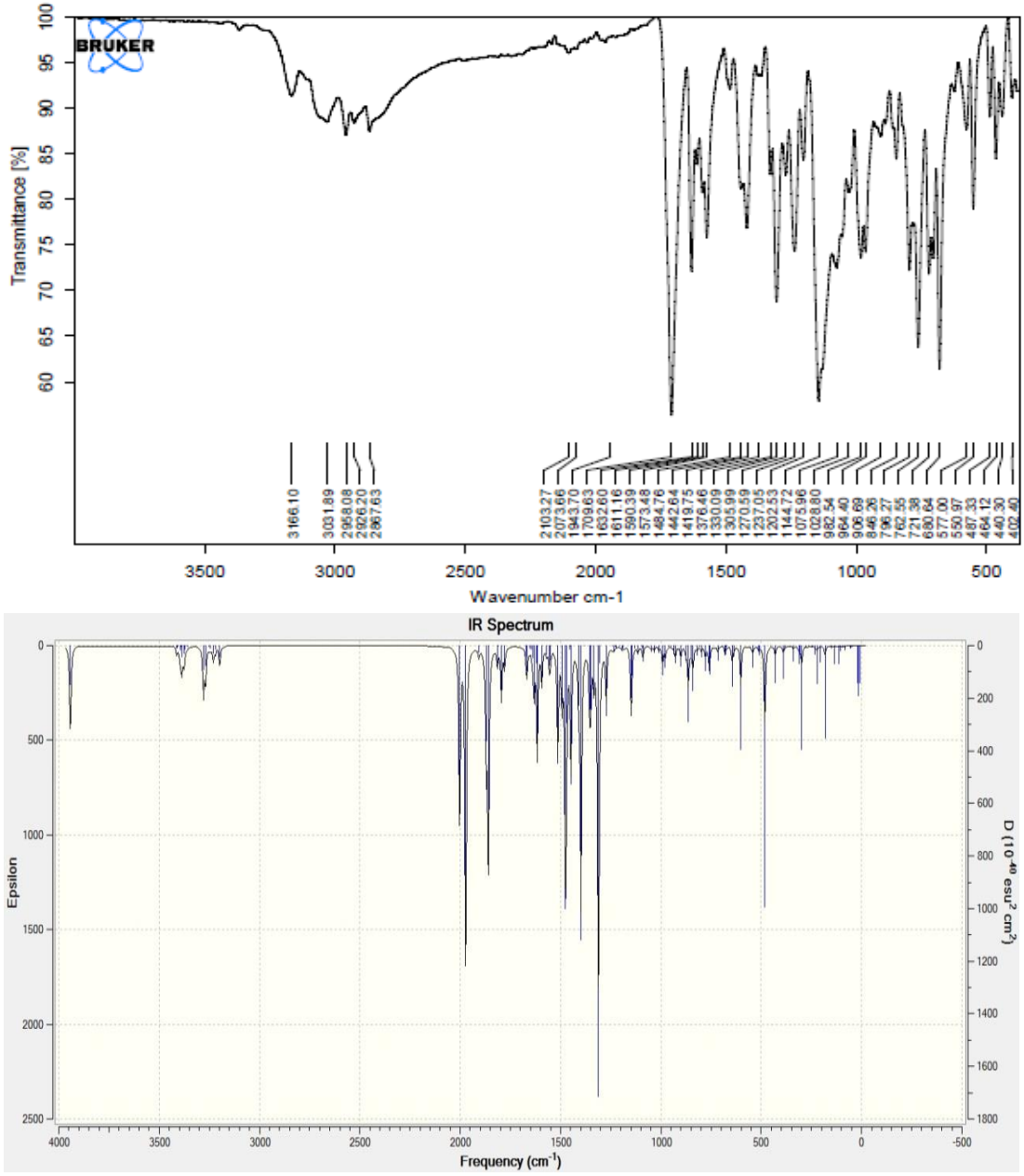


Figure 3. IR spectra experimental and simulated with DFT/B3LYP/6–31G(d) levels of the compound PTC.

NMR Spectral Analysis

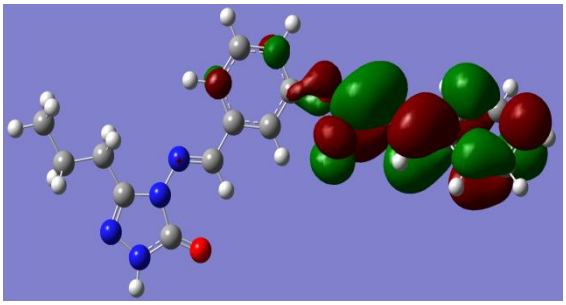
In the NMR spectroscopy, the isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties in nuclear magnetic resonance (NMR) spectroscopy which provide the accurate predictions of molecular geometries (Rani, et al., 2010; Subramanian et al., 2010; Wade, 2006). For this purpose, the optimized molecular geometry of the compound **PTC** 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 compound **PTC** the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital method (Table 3). Theoretically and experimentally 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. The correlation graphics are given Figure 4 and the linear correlation data of the compound **PTC** by considering the results are given in Table 3.

Table 3. The calculated and experimental 13C and 1H NMR isotropic chemical shifts of the compound PTC (with respect to TMS, all values in ppm).

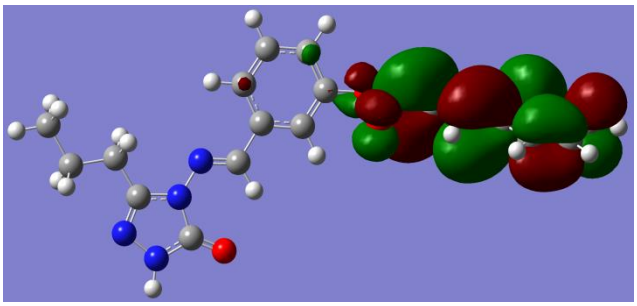
Nucleus	Experi-mental	B3LYP	B3LYP/ DMSO	Different	Different /DMSO	HF	HF/ DMSO	Different	Different /DMSO
C1	146,91	151,37	152,81	-4,46	-5,90	145,62	147,56	1,29	-0,65
C2	152,66	151,83	152,62	0,83	0,04	145,39	146,10	7,27	6,56
C3	150,93	154,94	155,30	-4,01	-4,37	148,49	149,06	2,44	1,87
C4	135,21	139,59	139,02	-4,38	-3,81	130,57	130,05	4,64	5,16
C5	125,55	131,57	130,85	-6,02	-5,30	125,66	125,11	-0,11	0,44
C6	151,26	155,23	154,99	-3,97	-3,73	144,23	143,54	7,03	7,72
C7	124,40	126,41	127,50	-2,01	-3,10	121,15	122,09	3,25	2,31
C8	130,26	132,54	133,78	-2,28	-3,52	125,36	126,37	4,90	3,89
C9	120,26	124,64	124,89	-4,38	-4,63	119,23	119,72	1,03	0,54
C10	164,84	166,16	167,57	-1,32	-2,73	156,83	158,68	8,01	6,16
C11	116,99	120,07	119,32	-3,08	-2,33	108,25	107,41	8,74	9,58
C12	146,76	152,73	154,13	-5,97	-7,37	147,63	149,12	-0,87	-2,36
C13	133,82	137,76	136,93	-3,94	-3,11	128,15	127,06	5,67	6,76
C14	129,01	137,87	138,39	-8,86	-9,38	130,15	130,77	-1,14	-1,76
C15	128,70	132,51	132,86	-3,81	-4,16	124,54	124,51	4,16	4,19
C16	130,96	134,70	136,13	-3,74	-5,17	128,05	129,34	2,91	1,62
C17	128,70	132,24	132,75	-3,54	-4,05	124,30	124,42	4,40	4,28
C18	129,01	129,53	129,84	-0,52	-0,83	123,02	123,61	5,99	5,40
C19	26,62	39,01	38,61	-12,39	-11,99	24,03	23,69	2,59	2,93
C20	18,54	29,60	29,72	-11,06	-11,18	14,32	14,46	4,22	4,08
C21	13,46	25,93	25,42	-12,47	-11,96	13,02	12,55	0,44	0,91
H22	11,90	6,98	7,46	4,92	4,44	6,19	6,62	5,71	5,28
H23	9,78	10,14	10,08	-0,36	-0,30	9,58	9,55	0,20	0,23
H24	7,71	7,81	7,81	-0,10	-0,10	7,26	7,39	0,45	0,32
H25	7,41	7,23	7,47	0,18	-0,06	7,12	7,39	0,29	0,02
H26	7,61	7,67	7,93	-0,06	-0,32	7,38	7,67	0,23	-0,06
H27	7,76	8,30	8,40	-0,54	-0,64	8,12	8,26	-0,36	-0,50
H28	6,94	6,70	6,86	0,24	0,08	6,19	6,37	0,75	0,57
H29	7,92	8,06	8,10	-0,14	-0,18	7,96	8,01	-0,04	-0,09
H30	7,83	7,61	7,77	0,22	0,06	7,36	7,56	0,47	0,27
H31	7,50	7,72	7,90	-0,22	-0,40	7,35	7,53	0,15	-0,03
H32	7,49	7,66	7,88	-0,17	-0,39	7,42	7,66	0,07	-0,17
H33	7,50	7,72	7,92	-0,22	-0,42	7,32	7,59	0,18	-0,09
H34	7,85	8,19	7,38	-0,34	0,47	7,95	8,10	-0,10	-0,25
H35	2,67	3,07	3,17	-0,40	-0,50	2,18	2,30	0,49	0,37
H36	2,67	3,12	3,22	-0,45	-0,55	2,20	2,34	0,47	0,33
H37	1,70	2,33	2,28	-0,63	-0,58	1,52	1,45	0,18	0,25
H38	1,70	2,33	2,28	-0,63	-0,58	1,52	1,45	0,18	0,25
H39	0,97	1,46	1,53	-0,49	-0,56	0,75	0,83	0,22	0,14
H40	0,97	1,45	1,52	-0,48	-0,55	0,74	0,83	0,23	0,14
H41	0,97	1,67	1,67	-0,70	-0,70	1,06	1,06	-0,09	-0,09

Electronic Properties

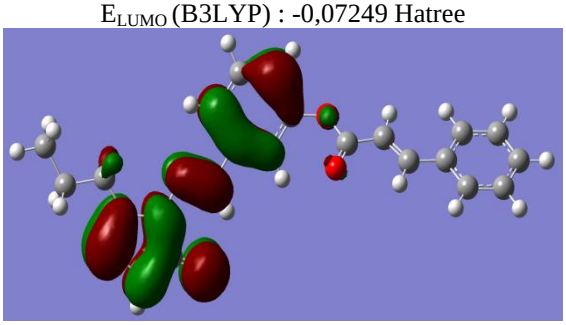
The energies of two important molecular orbitals of the molecule; the second highest and highest occupied MO's (HOMO), the lowest and the second lowest unoccupied MO's (LUMO) were calculated by using DFT/B3LYP and HF methods with 6-31G(d) level and are presented in Figure 4. The energy gap of the title molecule was calculated at DFT/B3LYP and HF level, which reveals the chemical reactivity and proves the occurrence of eventual charge transfer. The HOMO is located almost over the carbon atoms, oxygen atoms and also slightly delocalized in hydrogen atom and the LUMO is mainly delocalized in carbon atoms of benzene ring. The energy gap (energy difference between HOMO and LUMO orbital) is a critical parameter in determining molecular electrical transport properties (Fukui, 1982). The HOMO-LUMO energy gap of the title molecule is found to 0.11445/0.3863 a.u. obtained at DFT/HF method with 6-31G(d) levels.



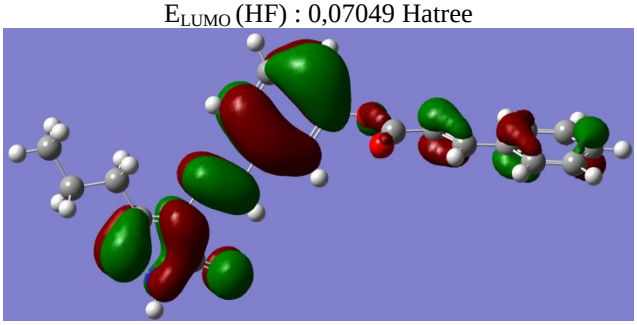
E_{LUMO} (B3LYP) : -0,07249 Hatree



E_{LUMO} (HF) : 0,07049 Hatree



E_{HOMO} (B3LYP) : -0,21698 Hatree



E_{HOMO} (HF) : -0,31579 Hatree

Figure 4. The calculated HOMO-LUMO energies of the molecule according to DFT/B3LYP/6–31G(d,p) and HF/B3LYP/6-311G(d,p) levels

Dipole moment and total energy

The energetic behavior of title molecule was investigated in vacum. Dipol moments and total energy values of title molecule were calculated by using B3LYP/6-31G(d), HF/6-31G(d) level. The calculated dipole moments and total energy values are given in Table 4.

Table 4. The calculated dipole moment values of the molecule

Dipole Moment	B3LYP (a.u.)	HF (a.u.)
μ_x	1.3544	2.5992
μ_y	3.1952	4.3845
μ_z	2.9544	3.8141
μ_{Toplam}	4.5576	6.3661

Mulliken's Atomic Charges

The Mulliken atomic charges at the HF/6-31 G(d) and B3LYP/6-31 G(d) level of compound 3 in gas phase are given in Table 7 (Mulliken, 1955). The electronegative N42, N43, N44, N45, O46, O47 and O48 atoms of compound PTC have negative atomic charge values. The Mulliken atomic charges (DFT/HF) of the mentioned atoms were calculated as -0.519 -0.659, -0.338/-0.348, -0.428 /-0.637, -0.311/-0.312, -0.540/-0.656, -0.549/-0.707 and -0.479/-0.568 a.u., respectively. The C1, C2, C3, C6, C10 and C13 carbon atoms bounded to the mentioned electronegative atoms in the molecule under study have positive atomic charge values. The values of

the positive charges of the mentioned carbon atoms were found as 0.556/0.627, 0.825/1.059, 0.037/0.094, 0.350/0.406, 0.618/0.811 and 0.166/0.016 a.u., respectively. Therefore the C1 atom surrounded with two electronegative N43 and N44 atoms, the C2 atom surrounded with the electronegative N42, N45 and O46 atoms and the C10 atom surrounded with two electronegative O47 and O48 atoms have the highest positive charge values. In the compound **PTC** the atomic charges of all hydrogen atoms have positive values.

Table 4. Mulliken atomic charges of the molecule

	DFT	HF		DFT	HF		DFT	HF
C1	0.556	0.627	C17	-0.131	-0.204	H33	0.139	0.209
C2	0.825	1.059	C18	-0.170	-0.202	H34	0.137	0.212
C3	0.037	0.094	C19	-0.323	-0.352	H35	0.170	0.200
C4	0.117	-0.032	C20	-0.251	-0.312	H36	0.169	0.199
C5	-0.199	-0.231	C21	-0.447	-0.486	H37	0.154	0.181
C6	0.350	0.406	H22	0.355	0.418	H38	0.153	0.181
C7	-0.159	-0.223	H23	0.212	0.290	H39	0.144	0.159
C8	-0.142	-0.204	H24	0.167	0.236	H40	0.143	0.159
C9	-0.155	-0.190	H25	0.144	0.224	H41	0.149	0.171
C10	0.618	0.811	H26	0.139	0.212	N42	-0.519	-0.659
C11	-0.215	-0.347	H27	0.152	0.234	N43	-0.338	-0.348
C12	-0.146	-0.120	H28	0.153	0.222	N44	-0.428	-0.637
C13	0.166	0.016	H29	0.171	0.247	N45	-0.311	-0.312
C14	-0.186	-0.215	H30	0.143	0.216	O46	-0.540	-0.656
C15	-0.131	-0.203	H31	0.140	0.210	O47	-0.549	-0.707
C16	-0.123	-0.192	H32	0.139	0.210	O48	-0.479	-0.568

Conclusion

In this paper, 3-*n*-propyl-4-(3-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one (PTC) was synthesized from the reaction of compound (PT) with 4-cinnamoyloxybenzaldehyde (C). The structure of the titled compound is characterized by using 1H, 13C NMR, FT-IR and UV spectroscopic methods. The molecular structures, vibrational frequencies, 1H and 13C NMR chemicals shifts, UV-vis spectroscopies, HOMO and LUMO analyses and atomic charges of 3-ethyl-4-(4-cinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one molecule (PTC) synthesized for the first time have been calculated by using DFT/B3LYP and HF methods. By considering the results of experimental works it can be easily stated that the ^{1}H and ^{13C} NMR chemical shifts, vibrational frequencies, and UV spectroscopic parameters obtained theoretically are in a very good agreement with the experimental data.

Acknowledgment

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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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