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Experimentical and Gaussian Calculations of 3-Ethyl-4-(2-Benzenesulfonyloxy)-Benzylideneamino-4,5-Dihydro-1H-1,2,4-Triazol-5-One

Fevzi AYTEMIZ
Kafkas University

Murat BEYTUR
Kafkas University

Haydar YUKSEK
Kafkas University

Abstract: 3-Ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one has been optimized using the DFT/B3LYP and B3PW91 methods with the 6-311G(d,p) basis set in the ground state. The vibrational (IR) frequencies, ^{1}H and ^{13}C NMR chemical shift values (in gas phase and in DMSO solvent), nonlinear optical properties (NLO), HOMO−LUMO analysis and molecular electrostatic potential surfaces of 3-Ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one have been calculated using the DFT/B3LYP and DFT/B3PW91 methods with the 6-311G(d,p) basis set. IR absorption frequencies of titled molecule were calculated by same methods. Theoretically calculated IR data are multiplied with appropriate adjustment factors. The data obtained according to DFT/B3LYP and DFT/B3PW91 are formed using theoretical infrared spectrums. The veda4f program was used in defining IR data which were calculated data. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W. Experimental and theoretical values were inserted into the grafic according to equatation of δ exp=a+b. δ calc. The spectroscopic and structural data of titled molecule has been calculated by using 6-311G(d,p) basis set with DFT/B3LYP and DFT/B3PW9. The values obtained were compared with experimental values.

Keywords: Gaussian 09W, 1.2.4-Triazol-5-one, GIAO, B3PW91, B3LYP.

Introduction

Heterocyclic aromatic compounds containing nitrogen and oxygen have gained great importance globally not only because of their prevalence in natural products, but also because of their biological, photochemical, optoelectronic, theoretical, pharmacological properties and industrial importance (Kardas et al., 2016; Bahçeci et al., 2017a; Bahçeci et al., 2017b; Yüksek et al., 2018; Beytur et al., 2019a; Beytur et al., 2019b; Beytur, 2020; Koç et al., 2020; Sertçelik, 2020; Sertçelik & Durman, 2020; Boy et al., 2021). Computational chemistry is the atomic and molecular modeling of chemistry in computer environment by using theoretical chemistry methods derived from physics principles such as quantum mechanics, molecular mechanics and molecular Dynamics (Uğurlu et al., 2007; Irak & Beytur, 2019; Uğurlu, 2019; Kotan et al., 2020; Uğurlu, 2020; Uğurlu & Beytur, 2020; Beytur & Avinca, 2021). 3-Ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one (Kol et al., 2020) was optimized by using the B3LYP/6-311G(d,p) and B3PW91/6-311G(d,p) basis set (Frisch et al., 2009; Wolinski, et al., 1990) (Figure 1). Vibrational frequencies, ^{1}H-NMR and ^{13}C-NMR spectroscopic parameters, atomic charges and frontier molecule orbitals (HOMO and LUMO) of the title compound have been calculated by using same methods with same basis set from the optimized molecular

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structure. Titled compound has been calculated the ground state geometrical parameters, the dipole moment (μ), polarizability (α), the hyperpolarizability (β).

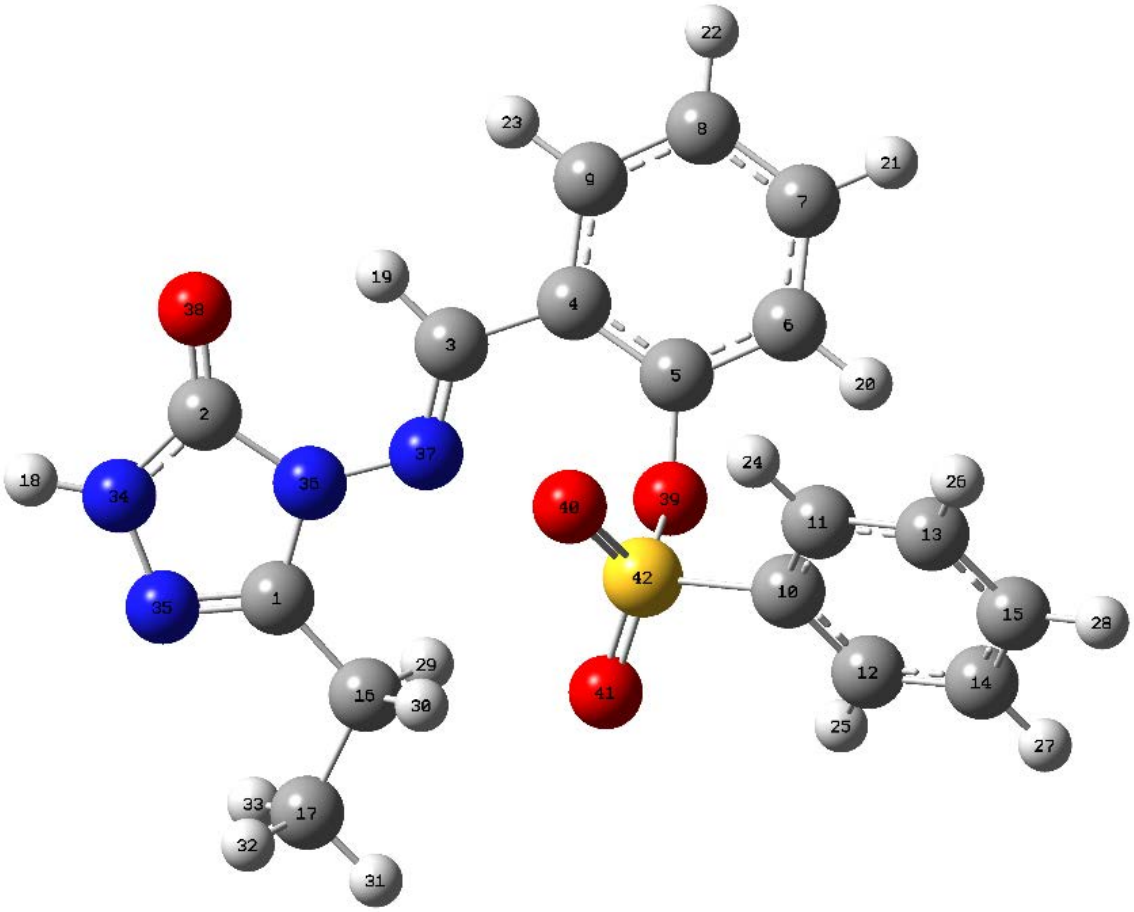


Figure 1. Optimized structure of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one with DFT/B3PW91/6-311G(d,p) level.

Computational Methods

The 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one (Kol et al., 2020) was optimized both the density functional theory (DFT)/B3LYP and the density functional theory (DFT)/B3PW91 methods (Lee et al.,1988; Becke, 1993) at 6-311G(d,p) level. ^{1}H NMR and ^{13}C NMR chemical shifts are calculated within GIAO approach (Ditchfield, 1974; Wolinski et al., 1990 Shirani et al., 2015) which is one of the most common approaches for calculating nuclear magnetic shielding tensors (Atalay et al., 2008; Avcı & Atalay, 2009; Beytur & Avinca, 2021). In the present study, ^{1}H and ^{13}C NMR chemical shifts were calculated within GIAO approach applying B3LYP and B3PW91 methods with 6-311G(d,p) basis set. Furthermore, All calculations were obtained by using Gaussian 09W program (Frisch et al., 2009), and the visualization parts were visualized with GaussView program (Dennington et al.,2009) employing B3LYP and B3PW91 methods with 6-311G(d,p) basis set. DFT levels were also used to calculate the dipole moment, the mean polarizability, the anisotropy of the polarizability and the total first static hyperpolrizability.

Results and Discussion

Infrared Vibretional Frequenciens

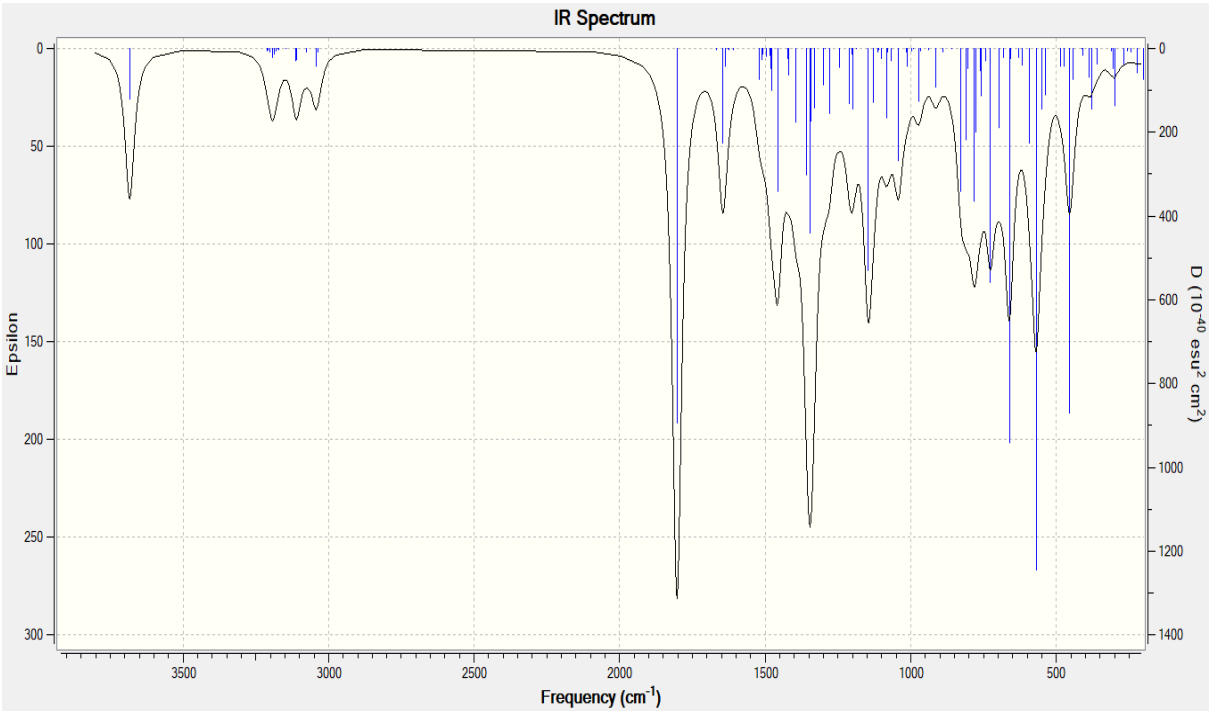
The vibration spectra of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one were simulated to predict the presence of functional groups and their vibrational modes. Vibrational wavenumbers were calculated based on the optimized geometries by using B3LYP and B3PW91 methods with the 6-311G(d,p) basis set. According to the data obtained by B3LYP and B3PW91 methods, vibration types were determined in detail by VEDA 4 program. The related compound has 42 atoms and has 120 vibrations.

The experimental and calculated vibrational frequencies, the calculated IR intensities and assignments of vibrational frequencies for title compound were summarized in Table 1 and Figure 2.

Table 1. The selected frequencies values of the 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one

Selected Vibration Frequencies	Exper.	B3LYP	B3PW91
τ $H_{24}C_{11}C_{13}C_{15}$, $H_{25}C_{12}C_{14}C_{15}$, $H_{26}C_{13}C_{15}C_{14}$, $H_{27}C_{14}C_{15}C_{13}$ (38)	680	690	663
ν $S_{42}C_{10}$ (25)	716	719	696
τ $H_{24}C_{11}C_{13}C_{15}$, $H_{25}C_{12}C_{14}C_{15}$, $H_{26}C_{13}C_{15}C_{14}$, $H_{27}C_{14}C_{15}C_{13}$ (47)	736	750	720
τ $H_{20}C_6C_5C_4$, $H_{21}C_7C_8C_9$, H_{22},$C_8C_9C_4$, $H_{23}C_9C_4C_3$ (67)	760	776	747
ν $S_{42}O_{40}$, $S_{42}O_{41}$ (22)	1182	1073	1045
ν $S_{42}O_{40}$, $S_{42}O_{41}$ (59)	1182	1135	1109
ν $S_{42}O_{40}$, $S_{42}O_{41}$ (29)	1356	1329	1296
ν $S_{42}O_{40}$, $S_{42}O_{41}$ (60)	1356	1344	1315
ν $N_{35}C_1$, $N_{37}C_3$ (17)	1595	1622	1574
ν $N_{35}C_1$, $N_{37}C_3$ (54)	1595	1631	1583
ν $N_{35}C_1$, $N_{37}C_3$ (59)	1595	1651	1602
ν $O_{38}C_2$ (73)	1690	1786	1737
ν C_3H_{19}, C_6H_{20}, C_7H_{21}, C_8H_{22} (99)	3056	3118	2999
ν C_3H_{19}, C_6H_{20}, C_7H_{21}, C_8H_{22} (98)	3056	3140	3027
ν $C_{11}H_{24}$, $C_{12}H_{25}$, $C_{13}H_{26}$, $C_{14}H_{27}$ (98)	3056	3143	3030
ν C_3H_{19}, C_6H_{20}, C_7H_{21}, C_8H_{22} (67), ν C_9H_{23} (32)	3056	3149	3037
ν $C_{11}H_{24}$, $C_{12}H_{25}$, $C_{13}H_{26}$, $C_{14}H_{27}$ (98)	3056	3155	3042
ν C_3H_{19}, C_6H_{20}, C_7H_{21}, C_8H_{22} (98)	3056	3172	3058
ν $C_{11}H_{24}$, $C_{12}H_{25}$, $C_{13}H_{26}$, $C_{14}H_{27}$ (98)	3056	3177	3061
ν C_3H_{19}, C_6H_{20}, C_7H_{21}, C_8H_{22} (88), ν C_9H_{23} (11)	3056	3181	3064
ν $N_{34}H_18$ (100)	3167	3648	3522
ν, stretching; δ, bending; δs, scissoring; ρ, rocking; γ, out-of-plane bending; τ, torsion			

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.



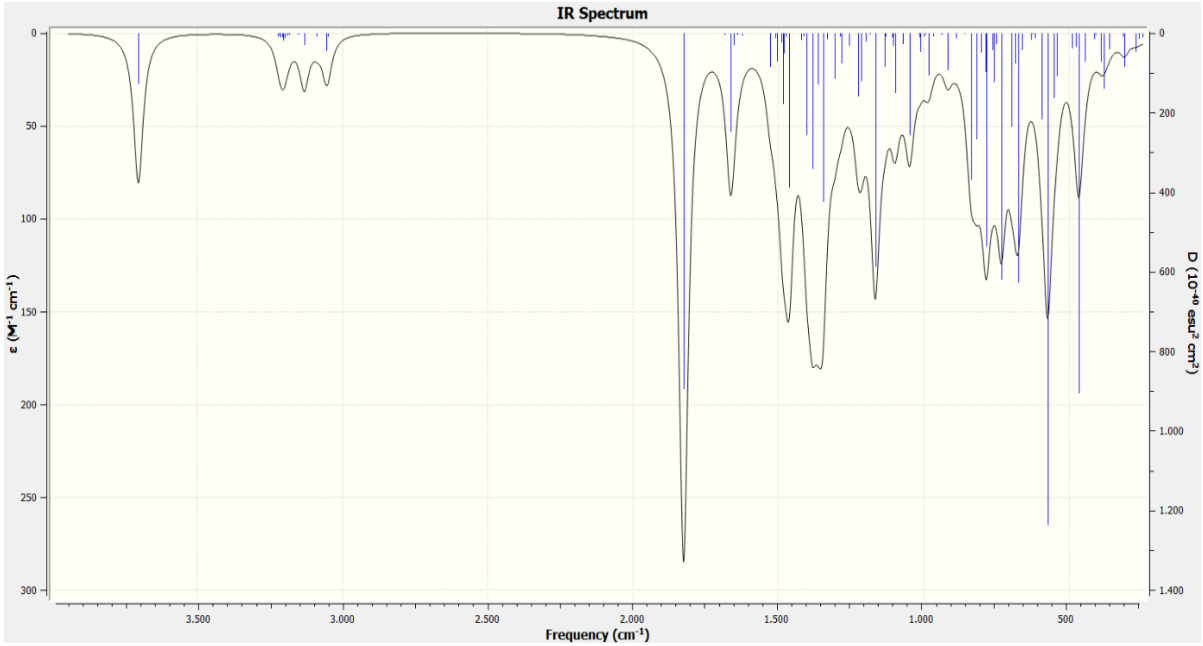


Figure 2. Theoretical (B3LYP) (a) and theoretical (B3PW91) (b) IR spectra of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one

NMR Spectral Analysis

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 (Wade, 2006; Rani et al., 2010; Subramanian et al., 2010). In this study, the optimized molecular structure of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one was obtained by using B3LYP and B3PW91 methods with 6-311G(d,p) level in DMSO solvent (Table 2). The related compound the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level according to Gauge-Independent Atomic Orbital (GIAO) method. Theoretical and experimental values (Kol et al., 2020) 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 (Figure 3).

Table 2**.** The experimental and calculated ^{13}C and ^{1}H NMR isotropic chemical shift values of the molecule DFT/B3LYP (a) and DFT/B3PW91 (b) methods

No	Experimental	B3LYP/DMSO	Fark/DMSO	B3PW91/DMSO	Fark/DMSO
C1	148.35	155.10	-6.75	149.35	-1.00
C2	151.21	153.80	-2.59	148.73	2.48
C3	146.19	154.54	-8.35	150.39	-4.20
C4	127.25	135.23	-7.98	130.22	-2.97
C5	147.81	153.16	-5.35	147.35	0.46
C6	123.40	129.44	-6.04	125.50	-2.10
C7	128.10	135.51	-7.41	131.65	-3.55
C8	126.42	132.41	-5.99	128.37	-1.95
C9	133.56	139.66	-6.10	135.64	-2.08
C10	135.23	145.76	-10.53	138.71	-3.48
C11	128.43	131.53	-3.10	127.89	0.54
C12	128.43	131.04	-2.61	127.27	1.16
C13	129.71	132.79	-3.08	128.82	0.89
C14	129.71	134.78	-5.07	130.83	-1.12
C15	132.65	139.52	-6.87	135.59	-2.94
C16	18.38	22.31	-3.93	18.01	0.37
C17	10.05	7.61	2.44	4.14	5.91
H18	11.91	7.40	4.51	7.49	4.42
H19	9.78	10.30	-0.52	10.52	-0.74

H20	7.76	7.62	0.14	6.45	1.31
H21	7.59	7.56	0.03	7.50	0.09
H22	7.49	7.33	0.16	7.74	-0.25
H23	7.30	6.35	0.95	7.80	-0.50
H24	7.58	7.46	0.12	7.60	-0.02
H25	7.93	8.09	-0.16	8.28	-0.35
H26	7.60	7.65	-0.05	7.82	-0.22
H27	7.85	7.90	-0.05	8.09	-0.24
H28	7.86	7.94	-0.08	8.12	-0.26
H29	2.62	2.70	-0.08	2.80	-0.18
H30	2.62	3.67	-1.05	3.72	-1.10
H31	1.21	1.26	-0.05	1.36	-0.15
H32	1.21	1.25	-0.04	1.34	-0.13
H33	1.21	1.27	-0.06	1.37	-0.16

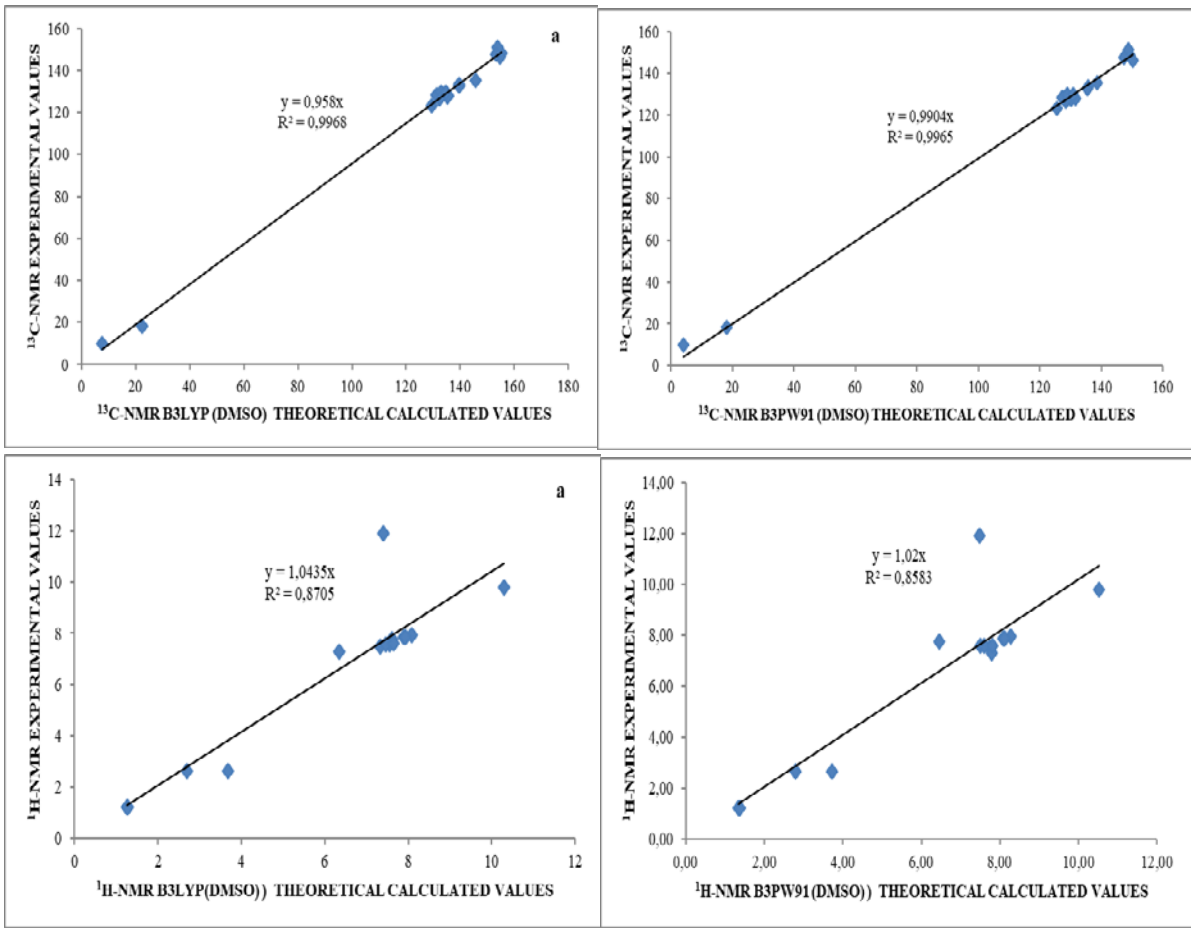


Figure 3. The correlation graphics of ^{13}C-NMR (DMSO), ^{1}H-NMR (DMSO) chemical shift values of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one DFT/B3LYP (a) and DFT/B3PW91 (b) methods

Electronic Properties

Electronic absorption is characterized by an electron transition from the most occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). It basically means the transition from the unexcited state to the first excited state. HOMO is orbital that acts as electron donor, LUMO is orbital that acts as electron acceptor. The energy values of HOMO (π donor) and LUMO (π acceptor) and the energy gaps obtained from these values determine the chemical activity of the studied molecules (Sagdinc & Pir, 2009). HOMO and LUMO energies of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1*H*-1,2,4-

triazol-5-one were calculated by using B3LYP and B3PW91 methods (Figure 4). From Fig 4, for B3LYP level, HOMO and LUMO energies were predicted as -6.082 and -1.896 eV.
The energy gap between the HOMO and LUMO orbitals was found as 4.185 eV. for B3PW91 level, HOMO and LUMO energies were predicted as -6.127 and -1.933 eV. The energy gap between the HOMO and LUMO orbitals was found as 4.194 eV.

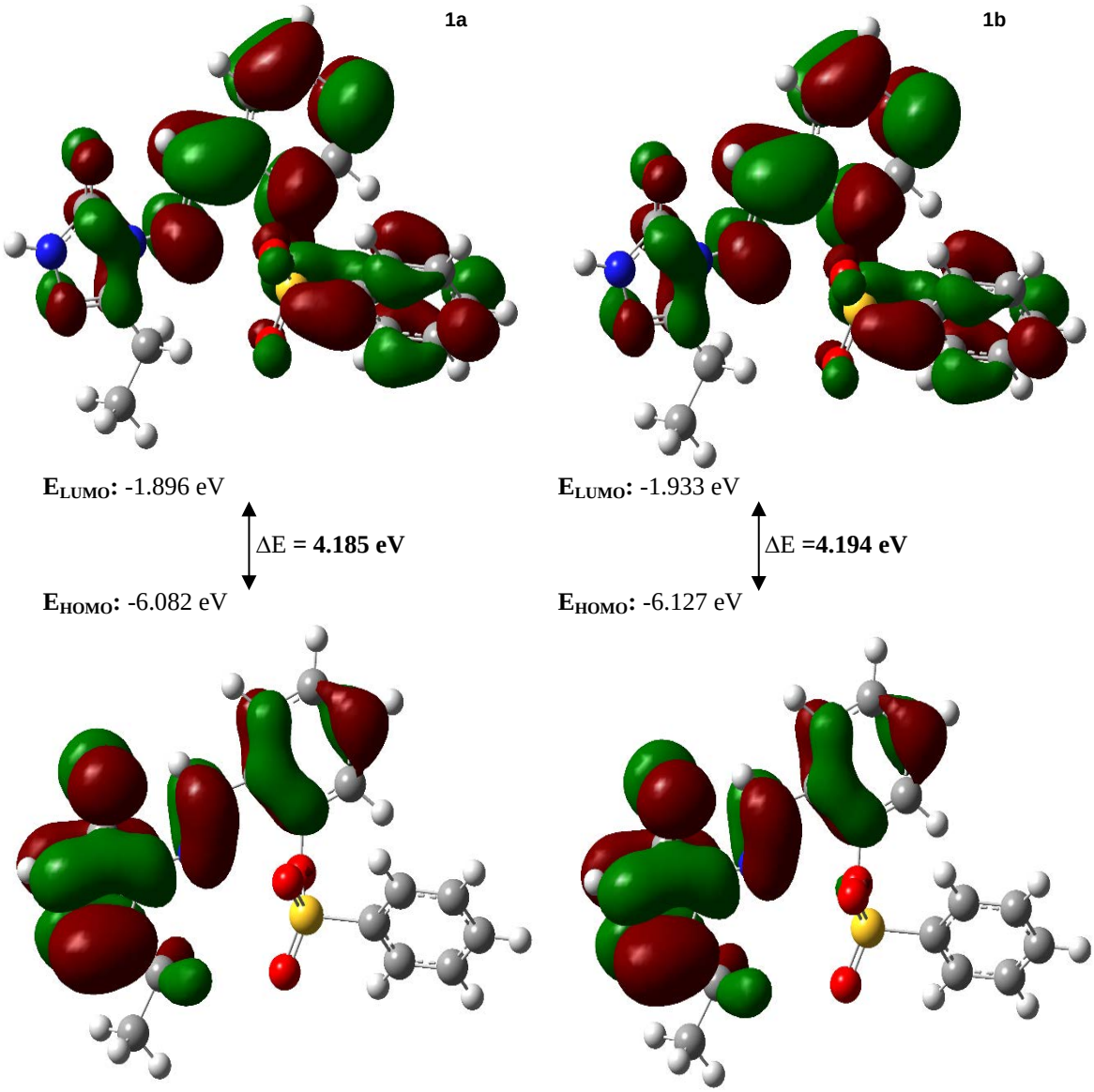


Figure 4. Calculated HOMO-LUMO values of the molecula calculated using the DFT/B3LYP and DFT/B3PW91 methods

Nonlinear Optical Properties

The nonlinear optical (NLO) property is the atomic-level response to the electric field received in a light beam. The diffusion of a light wave in a dielectric material differs in the spatial and temporal distribution of electric charges by interaction of electrons with the electromagnetic field of the light wave (Armstrong et al., 1962). The importance of polarizability and initial hyperpolarizability in molecular systems is associated with electronic communication between donor and acceptor groups due to intramolecular charge transfer (Prasad et al., 2010). The molecular electronic dipole moment, molecular polarizability, polarizability anisotropy and molecular initial hyperpolarizability of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one were calculated using B3LYP and B3PW91 methods and the results are given in Table 3.

Table 3. Calculated polarizability and hyperpolarizability values of the molecule (B3LYP/6-311+G(d,p)) and (HF/6-311+G(d,p))

	B3LYP		B3PW91
α_{xx}	49.129 a.u.	α_{xx}	48.842 a.u.
α_{yy}	39.222 a.u.	α_{yy}	38.785 a.u.
α_{zz}	22.755 a.u.	α_{zz}	22.628 a.u.
α	$37.035x10^{-24}$ esu	α	$36.752x10^{-24}$ esu
$\Delta\alpha$	$23.075x10^{-24}$ esu	$\Delta\alpha$	$22.905x10^{-24}$ esu
β_x	11157.703 a.u.	β_x	11281.155 a.u.
β_y	2409.077 a.u.	β_y	2549.952 a.u.
β_z	-1623.633 a.u.	β_z	-1750.805 a.u.
β_{xxx}	8391.943 a.u.	β_{xxx}	8607.260 a.u.
β_{xxy}	1977.660 a.u.	β_{xxy}	1879.232 a.u.
β_{xyy}	788.101 a.u.	β_{xyy}	794.663 a.u.
β_{yyy}	2168.793 a.u.	β_{yyy}	2188.666 a.u.
β_{xxz}	538.547 a.u.	β_{xxz}	624.984 a.u.
B_{xyz}	-298.263 a.u.	B_{xyz}	-263.699 a.u.
B_{yyz}	-1010.880 a.u.	B_{yyz}	-1121.951 a.u.
β_{xzz}	277.644 a.u.	β_{xzz}	-289.840 a.u.
β_{yzz}	-335.110 a.u.	β_{yzz}	-339.014 a.u.
B_{zzz}	-654.400 a.u.	B_{zzz}	-644.478 a.u.
β	$11.530x10^{-30}$ esu	β	$11.698x10^{-30}$ esu

Dipole Moments

Theoretical dipole moments of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one have been given in Tables 4.

Table 4. The calculated dipole moment values of the molecule

Dipole Moment	B3LYP (a.u.)	B3PW91 (a.u.)
μ_x	6.1015	6.0061
μ_y	1.2346	1.2006
μ_z	-1.5448	-1.5468
μ_{Toplam}	6.4139	6.3172

Conclusion

In the present study, The molecular optimization of 3-ethyl-4-(2-benzenesulfonyloxy)-benzylideneamino-4,5-dihydro-1H-1,2,4-triazol-5-one was performed. The structure of the compound was optimized using the DFT/B3LYP and B3PW91 methods 6-311G(d,p) basis set. The vibrational values of the relevant molecule were investigated in detail with the help of potential energy distribution (PED). ^{1}H NMR and ^{13}C NMR chemical shifts are calculated within GIAO approach which is one of the most common approaches for calculating nuclear magnetic shielding tensors. The experimental values were compared with the theoretically calculated ^{1}H NMR and ^{13}C NMR chemical shift values, and it was determined that the values obtained by the B3PW91 method were approximate to the experimental values. The relatively small energy gap between HOMO and LUMO energies indicates that charge transfer occurs in the molecule. Due to the sulfonyl and carbonyl groups in the studied molecule, it shows significant polarizability and initial hyperpolarizability properties and can be used as an effective NLO material.

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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Author Information

Fevzi Aytemiz
Kafkas University
Kars, Turkey
Contact E-mail: *fevziaytemiz53@gmail.com*

Murat Beytur
Kafkas University
Kars, Turkey

Haydar Yuksek
Kafkas University
Kars, Turkey

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