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Theoretical Investigation of Vibration and Electronic Properties of (E)-3-(Benzylideneamino)-4H-1,2,4-Triazol-4-Amine

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Abstract: In this study, the important application areas of triazoles have increased the interest in studies related to them. In this study, the structural parameters, vibrational frequency, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), hyper polarizability (β) and the potential energy curves (PEC) of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule were calculated at Hartree-Fock (HF) and Density Functional Theory (DFT) with B3LYP (Becke 3 Parameter Lee-Yang-Parr) model using the different basis set in gas phase. The potential energy curves of the studied molecule were performed as a function the θ[C3-N5-C2-N3] torsion angle varying from -180º to 180º at 10º intervals using both B3LYP/6-31+G(d) and HF/6-31+G(d) level of theory. The dipole moment value of the molecule was calculated as 5.43 Debye by the B3LYP/6-311++G(2d,2p) method and as 5.73 Debye by the HF/6-311++G(2d,2p) method, respectively. The obtained vibrational wave numbers were scaled with appropriate scale factors and the assigning of these vibrational wavenumbers was made according to the potential energy distribution (PED) using the VEDA 4f program. Also, by using HOMO-LUMO energies, energy gap values, ionization energy, electron affinity, chemical potential, electronegativity, hardness and softness indices were obtained. The approximate geometry of the molecules in three dimensions was drawn in the Gauss View 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords: (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine, Vibration analysis, Potential energy curve (PEC), HOMO-LUMO.

Introduction

Heterocyclic organic compounds are cyclic compounds in which at least one of the intra-ring atoms is a heteroatom (O, N, S) (Çiftçi et al., 2018; Koç et al., 2020; Beytur et al., 2019; Beytur, 2020; Boy et al., 2021). Triazoles are heterocyclic compounds with a five-member ring and as regards the position of N atoms, they are two types which are 1,2,3- and 1,2,4-triazole (Bahçeci et al., 2016; Kardaş et al., 2016; Bahçeci et al., 2017; Aktaş Yokuş et al., 2017; Çiftçi et al., 2018; Koç et al., 2020; Boy et al., 2021) These triazoles and their substituted-derivatives possess important biological activity in a wide variety of fields like analgesic (Khanage et al., 2013), antidiabetic (Hichri et al., 2019), anxiolytic (Navidpou et al., 2021) antimicrobial (Sahoo et al., 2013; Al-Khuzaie et al., 2014), antiviral (Abdullah et al., 2012; Pandey et al. 2012), anticancer (Grytsai et al., 2020; Boraei et al., 2019), anticonvulsant (Kapro et al., 2020; Jess et al. 2014), antibacterial (Rode et al., 2017; Mahmoud et al., 2014), antifungal (Karaca et al., 2017; Appna et al., 2019), antitubercular (Meenaxi et al., 2011), antioxidant (Peng et al., 2021; Abdul Hameed et al., 2014, antitubulin (Mustafa et al., 2019) and inflammatory (Mousa et al., 2012; Li et al., 2020). In 1855, The name triazole was first named by Bladin for the compound consisting of a carbon nitrogen ring system, $C_2H_3N_3$ (Agrwal et al., 2011). It has been determined that Schiff-based derivatives of 1,2,4-triazole compounds have important biological properties and various applications (Bekircan et al., 2006). Since (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule was

modeled for the first time in this study, there is no theoretical or experimental study of the molecule in the literature (Beytur et al., 2019; Irak and Beytur, 2019; Kotan et al., 2020; Uğurlu, 2020; Uğurlu and Beytur, 2020; Beytur and Avinca, 2021). Because the studied molecule has more than one rotatable dihedral angle, it is a structurally flexible molecule. The physical and chemical properties of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule have been investigated details. In this work, molecular structure, dipole moment, relative energies, rotational barriers, polarizability, first static hyper polarizability, potential energy curve, the electronic structure and HOMO-LUMO energies of above-mentioned molecule have been studied. Also, by using HOMO-LUMO energies, energy gap values were obtained. The molecular structure using numbering scheme of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-
amine molecule is given in Figure 1.

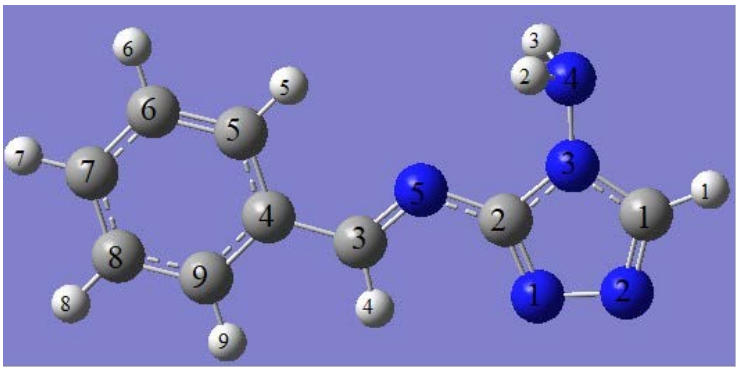

Figure 1. (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule numbering scheme

Method

Quantum-mechanical calculations on the (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule was performed by the aid of Gaussian 09W program package and Gauss view 5.0 molecular visualization programs (Frisch et al., 2010; Dennington et al., 2009) in the gas phase. The structural parameters, vibrational frequency, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), hyperpolarizability (β) and the potential energy curves (PEC) of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule were calculated at Hartree-Fock (HF) and Density Functional Theory (DFT) with B3LYP (Becke 3 Parameter Lee-Yang-Parr) (Becke et al., 1988;Lee et al., 1988; Becke, 1993) model using the 6-311++(2d,2p) basis set in gas phase. In order to obtain the best stable structures, Conformational analysis of the molecule was performed as a function of dihedral angle θ[C3-N5-C2-N3] which was varied between -180º and 180º with increments of 10º both HF/6-31+G (d) and B3LYP/6-31+G(d)level of theory. The computed harmonic frequencies at B3LYP/6-311++G(2d,2p) level of theory were scaled by 0.963 (Kashinski et al., 2017). Also, by using HOMO-LUMO energies, energy gap values, ionization energy, electron affinity, chemical potential, electronegativity, hardness and softness indices were obtained. Also, the calculated vibrational assignments of the normal modes were performed on the basis of the Potential Energy Distribution (PED) and it has been calculated using the Vibrational Energy Distribution Analysis VEDA 4 program (Jomroz 2004).

Results and Discussion

Conformational Analysis

The dihedral angle was defined as: Φ[C3-N5-C2-N3]. The dihedral angle Φ is the N5-C2 single bond about which internal rotation forms clearly different conformations. The potential energy curves of the (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule have been calculated at both HF/6-31+G(d) and B3LYP/6-31G+(d) level is shown Figure 2. The minimum of potential energy curves (PEC) was referred to as zero. Rotational barriers at 0º [ΔE0 =E (θ =0º)-E (equilibrium)], at 90º [ΔE90 =E (θ=90º)-E (equilibrium)] and at 180º [ΔE180 =E (θ=180º)-E (equilibrium)] were calculated by using the energies of the respective optimized structures. The low-energy conformers were obtained at = -180 and 180º conformer. As seen in figure 2., maxima energy conformer was seen at 0º dihedral angle at HF/6-31+G (d) and B3LYP/6-31G+ (d,) level of theory. The relative energy value at dihedral angle of 0º calculated HF/6-31+G (d) is bigger than that of B3LYP/6-31+G (d) by 2.473kcal/mol. The interesting thing in this study is that the minimum and maximum

energy values correspond to the planar form of the molecule. In general, the maximum energy values of the cyclic molecules correspond to their orthogonal comfort. From our previous work, conformation analysis of 4-(Methoxycarbonyl) phenylboronic acid and conformational analysis of 3-phenylthiophene and its fluoro derivatives, maximum potential energy barrier was shown at the orthogonal conformation (Uğurlu et al., 20017; Uğurlu et al., 2020).

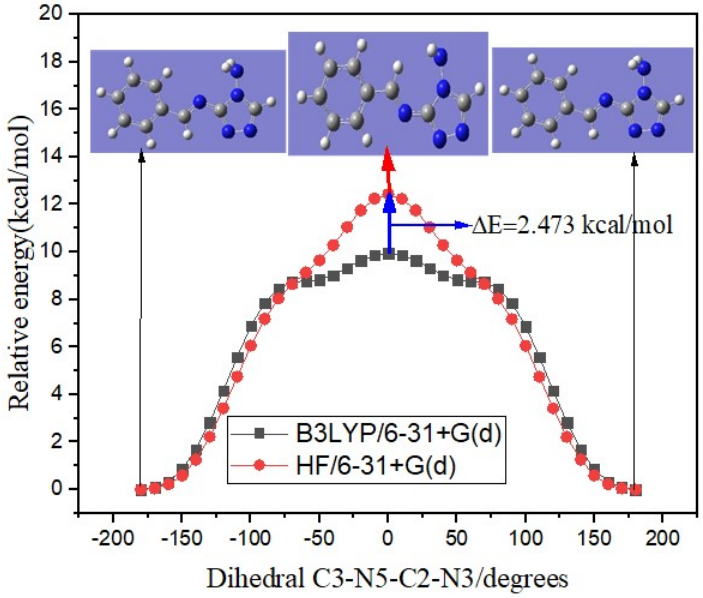

Figure 2. The potential energy curves of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule

Molecular Structure

Since the molecule (E)-3-(benzylideneamino)-4H-1,2,4-triazole-4-amine was modeled theoretically for the first time, there are no molecular and crystal structures in the literature. The calculated parameter studied molecule of both at the B3LYP/6-311++G (2d, 2p) and the HF/6-311++ G (2d,2p) methods in the ground state are tabulated in the Table 1.

Table 1. Selected structural parameters of (E)-3-(benzylideneamino)-4H-1,2,4-triazole-4-amine molecule

	Bond length (Å)			Bond angle (˚)	
Atoms	B3LYP	HF	Atoms	B3LYP	HF
C1-N2	1.3087	1.2795	N1-C2-N3	109.32	109.84
C1-N3	1.3598	1.3547	N1-C2-N5	130.82	130.21
C2-N1	1.3148	1.2836	N3-C2-N5	119.85	119.95
C2-N3	1.3774	1.3582	C4-C3-N5	122.75	122.80
C2-N5	1.3768	1.3837	C1-N3-C2	105.08	104.42
C3-C4	1.4589	1.4712	C1-N3-C4	125.46	125.76
C3-N5	1.2834	1.2610	C2-N3-C4	129.46	129.82
C4-C5	1.4027	1.3945	C2-N5C3	118.62	117.74
C4-C9	1.4003	1.3888		Dihedral angle (˚)	
C5-C6	1.3848	1.3794	N1-C2-N3-C1	0.00	0.00
C6-C7	1.3959	1.3907	N1-C2-N3-N4	179.98	180.00
C7-C8	1.3906	1.3827	N5-C2-N3-C1	-179.99	-180.00
C8-C9	1.3894	1.3866	N5-C2-N3-N4	-0.02	0.00
N1-N2	1.3780	1.3632	N1-C2-N5-C3	0.02	0.02
N3-N4	1.4019	1.3817	N3-C2-N5-C3	-179.98	-179.98
			N5-C3-C4-C5	0.01	0.00
			N5-C3-C4-C9	-179.99	-180.00
			C4-C3-N5-C2	180.00	180.00

The equilibrium state structures of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule obtained by the HF/6-311++ G (2d,2p) and DFT/6-311++G (2d,2p) methods are compiled The calculated values of the electronic, dipole moment, polarizability, hyperpolarizability, HOMO, LUMO energy and energy gap (Eg) at the ground-state equilibrium geometry of studied molecules are listed in Table 2. The dipole moment value of the molecule was calculated as 5.43 Debye by the B3LYP/6-311++G(2d,2p) method and as 5.73 Debye by the HF/6-311++G(2d,2p) method, respectively.

Table 2. The electronic, HOMO, LUMO energy, dipole moment, polarizability, hyperpolarizability, and energy gap (ΔEg) of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine

B3LYP/6-3111++G(2d,2p)						
Electronic Energy (a.u)	μ (D)	α (a.u)	β(a.u)	EHOMO (a.u)	ELUMO (a.u)	Eg(eV)
-622.257742790	5.43	161,43	1113,28	-0.242422	-0.090555	4.13
HF/6-3111++G(2d,2p)						
-618.381993944	5.73	138,61	203,08	-0.321382	0.031610	9.61

Molecular electrostatic potential (MEP) surface values of the optimized geometry of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule by the HF/6-311++ G (2d,2p) and DFT/6-311++G (2d,2p) level of theory and the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) obtained both methods are presented Figure 3.

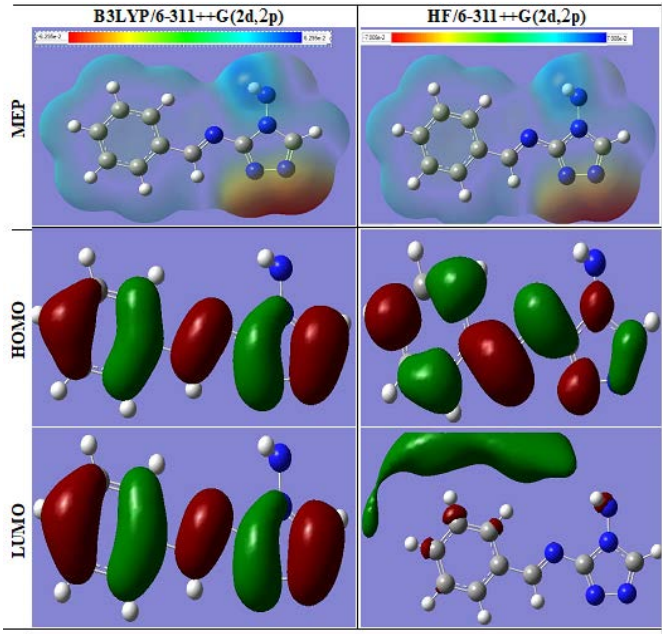

Figure 3. HOMO-LUMO and MEP) surface (PES) of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine

The electron affinity (A), global hardness (η)/softness (S), electronegativity (χ), chemical potential (μ), ionization potential (I), chemical potential (Pi) calculated by using HOMO-LUMO energies calculated the B3LYP/6-311++G (d, p) for the compound were given in Table 3.

Table 3. Electronic properties of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule

	property	a.u	eV	kcal/mol	kJ/mol
	LUMO	-0.091	-2.464	-56.824	-237.752
	HOMO	-0.242	-6.596	-152.121	-636.479
A	Electron affinity	0.091	2.464	56.824	237.752
I	Ionization potential	0.242	6.596	152.121	636.479
ΔE	Energy gap	0.152	4.132	95.297	398.727
χ	Electronegativity	0.166	4.530	104.472	437.116
Pi	Chemical potential	-0.166	-4.530	-104.472	-437.116
ω	Electrophilic index	0.001	0.029	0.660	2.763
IP	Nucleophilic index	-0.013	-0.344	-7.933	-33.192
S	Molecular softness	0.038	1.033	23.824	99.682
η	Molecular hardness	0.076	2.066	47.648	199.363

Vibrational Frequencies

(E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule consist of 23 atoms having 63 normal modes of vibrations. The calculated vibrational wavenumbers, FT-IR and FT-Raman intensity of the title compounds are given in Table 4.

Table 4. The obtained vibrational wave numbers were scaled with appropriate scale factors.

B3LYP		HF		
Unsc	Sc.	Unsc.	Sc.	Assignments with PED (≥10 %)
3561	3383	3818	3429	νN4Ha(100)
3491	3316	3736	3355	νN4Hb(100)
3272	3108	3430	3081	νC1H(49) νC3H(50)
3206	3046	3368	3025	νC5H(24) νC8H(60)
3197	3037	3352	3011	νC5H(46) νC8H(35)
3186	3026	3340	3000	νC6H(83)
3175	3016	3328	2989	νC5H(24) νC7H(41) νC9H(32)
3169	3011	3321	2982	νC7H(39) νC9H(52)
3079	2925	3267	2934	νC1H(50) νC3H(50)
1704	1619	1857	1668	τHbN4Hb(71) βHaN4N3C1(24)
1659	1576	1843	1655	νN1C2(24) νN2C1(24) νC7C8(15)
1635	1553	1787	1605	νC7C8(30) νC9C4(16)
1611	1530	1761	1582	νC6C7(26) νC9C4(12) τHC6C7(11) τC8C9C4(10)
1535	1458	1721	1545	τHC5C6(31) τHC9C8(10) τC8C9C4(10)
1520	1444	1712	1537	νN5C3(11) νN3C2(16) τHC3C4(16) τC2N3C1(13)
1498	1423	1650	1482	νN1C2(13) νN5C2(21) τC2N3C1(17)
1485	1411	1617	1452	νN1C2(10) τHC5C6(12) τHC8C9(25)
1439	1367	1595	1432	νN1C2(10)N5C3(15) τHC1N2(21)
1400	1330	1539	1382	νN5C3(14) νN3C2(10) νN4N3(11) τHC1N2(15) τHC3C4(17)
1361	1293	1490	1338	τHC8C9(39) τHC9C8(19)
1350	1283	1467	1318	νC5C6(27) νN3C1(18)
1349	1282	1452	1304	τHaN4N3(99)
1328	1261	1356	1218	νC5C6(23) νC9C4(22)
1249	1186	1342	1205	νC4C3(27)
1222	1161	1333	1197	νN4N3(16) τHC1N2(13) τHC3C4(22) τN1C2N3(15)
1203	1143	1299	1167	νN5C3(24) τHC1N2(12) τHC3C4(13) τHC6C7(11)
1195	1135	1280	1150	νC7C8(13) τHC6C7(28) τHC9C8(25)
1185	1126	1215	1091	νC5C6(18) τHC7C8(69)
1104	1048	1188	1067	νC6C7(43) τHC5C6(15) τHC6C7(13) τHC9C8(10)
1061	1008	1169	1050	τN1C2N3(52)
1046	993	1153	1035	νC8C9(30) τC5C6C7(16) τHC5C6(15) τC8C9C4(14)
1028	977	1119	1005	βHC3N5C2(29) βHC6C7C8(22) βHC7C8C9(27)
1019	968	1114	1001	νC8C9(42) τC5C6C7(53)
1014	964	1108	995	βHC5C6C7(61) βC5C6C7C8(20)
999	949	1082	972	βHC3N5C2(27)βHC5C6C7(12)βHC9C8C7(42) βC6C7C8C9(10)
984	934	1071	962	νN3C2(21) τN1C2N3(28) βHaN4N3C1(25)
955	907	1048	941	νN3C1(21)τN1C2N3(11)βHbN4Hb(13)βHaN4N3C1(36)βHC9C8
945	897	1046	940	βHC3N5C2(15) βHC6C7C8(42) βHC8C9C4(12)
884	839	970	872	τC3N5C2(10) τC4C3N5(19)
860	817	952	855	βHC6C7C8(21) βHC7C8C9(29) βHC8C9C4(49)
841	799	951	854	βHC1N2N1(85)
812	771	870	781	νN3C2(11)N5C2(17)C4C3(11) τN1C2N3(13)
781	742	854	767	βHC3N5C2(17)βHC7C8C9(10)βHC8C9C4(14) βC8C9C4C3(21)
732	696	809	726	βC3N5C2N3(11)βN1C2N3C1(15)βN2C1N3C2(31)
703	667	766	688	βHC5C6C7(10)βHC7C8C9(18) βHC8C9C4(10) βC5C6C7C8(31)
700	665	756	679	τN4N3(36) τN1C2N3(11) τC2N3C1(25)
668	635	724	650	βHC1N2N1(14) βC3N5C2N3(20) βN1C2N3C1(45)
635	603	675	606	τC6C7C8(13) τC7C8C9(58) τC8C9C4(16)
616	586	657	590	τC6C7C8(45)
545	518	587	527	τC2N3C1(10) τN5C2N1(28) τN4N3C1(14)
506	481	547	491	βC5C6C7C8(29) βC7C8C9C4(20) βC8C9C4C3(15)

417	396	454	407	βHC9C8C7(15) βC6C7C8C9(45) βC8C9C4C3(21)
410	389	441	396	τC9C4C3(28) τN4N3C1(32)
362	344	394	354	βC3N5C2N3(11)βN2C1N3C2(12)βC7C8C9C4(35)
253	241	294	264	βC6C7C8C9(22) βC7C8C9C4(23) βC9C4C3N5(15)
238	226	268	240	τC4C3(13) τC3N5C2(15) τN4N3C1(26)
217	206	254	228	βN4C1C2N3(90)
203	193	221	198	τC3N5C2(10) τC9C4C3(27) τN5C2N1(25) τC4C3N5(10)
161	153	216	194	βHbN4N3C1(87)
130	123	118	106	βC3N5C2N3(25) βN2C1N3C2(17) βC9C4C3N5(30)
75	72	81	73	τC3N5C2(35) τC9C4C3(16) τ N5C2N1(16) τC4C3N5(28)
66	63	72	65	βC9C4C3N5(13) βC4C3N5C2(63) βN5N3N1C2(15)
26	25	19	17	βC3N5C2N3(13)βN1C2N3C1(14)βN2C1N3C2(16)

ν; stretching, τ; in plane bending, β; out of plane bending,

Conclusion

In this study, the equilibrium state structures, vibrational frequency, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), hyperpolarizability (β) and the potential energy curves (PEC) of (E)-3-(benzylideneamino)-4H-1,2,4-triazol-4-amine molecule were calculated the HF/6-311++ G (2d,2p) and DFT/6-311++G (2d,2p) methods in gas phase. As seen in figure 2., maxima energy conformer was seen at 0º dihedral angle at HF/6-31+G (d) and B3LYP/6-31G+ (d,) level of theory. The relative energy value at dihedral angle of 0º calculated HF/6-31+G (d) is bigger than that of B3LYP/6-31+G (d) by 2.473kcal/mol. The dipole moment value of the molecule was calculated as 5.43 Debye by the B3LYP/6-311++G(2d,2p) method and as 5.73 Debye by the HF/6-311++G(2d,2p) method, respectively.

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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