A CHARACTERIZATION STUDY ON 4-AMINO-3,5-DIALKYL-1-TRIAZOLE BY DENSITY FUNCTIONAL THEORY AND AB INITIO HARTREE–FOCK CALCULATIONS

Yusuf ZALAOGLU[1] Gürcan YILDIRIM[2] Asaf Tolga ULGEN[2,3] Barış GUNER[4] Cabir TERZIOGLU[2]

[1]Osmaniye Korkut Ata University, Department of Physics, Osmaniye–Turkey, 80000
[2]Abant Izzet Baysal University, Department of Physics, Bolu–Turkey, 14280
[3]Sirnak University, Electrical and Electronics Engineering Faculty, Sirnak–Turkey, 73000
[4]Rize University, Department of Physics, Rize–Turkey, 53100

Özet

4-Amino-3,5-Dialkyl-1-Triazole molekülünün karakterizesi için, bağ uzunluklarını ve açılarını içeren temel haldeki optimize moleküler yapısı, 6–31G (d,p) temel setli yoğunluk fonksiyon metodu (DFT) ve ab initio Hartree–Fock (HF) kuantum hesaplama yöntemleri ile incelenmiştir. Hesaplanan bağ uzunlukları ve bağ açıları birbirleriyle ile iyi bir uyum içinde olduğu gözlenmiştir. Molekülün kimliği için ayrıca; atomik yükler, termodinamik nicelikler, nükleer magnetik rezonans ve mor ötesi spektrumları belirlendi ve yorumlandı. Teorik ^{13}C and ^{1}H kimyasal kaymalar mevcut deneysel verileri ile iyi bir uyuma sahip olduğunu görüldü. Buna ek olarak da hem sınır orbital (FMO) ve elektrostatik potansiyel enerji değerleri (MEP) simüle edildi, hem de enerji geçiş durumları ve bant enerjileri değerlendirildi.

Anahtar Kelimeler: 4-Amino-3,5-Dialkyl-1-Triazole, FMO, MEP, HF, DFT

4-AMİNO-3,5-DİALKYL-1-TRİAZOLE MOLEKÜLÜNÜN AB İNİTİO HARTREE-FOCK (HF) VE YOĞUNLUK FONKSİYON TEORİSİ (DFT) HESAPLAMALARI İLE KARAKTERİZE EDİLMESİ

Abstract

The optimized molecular structures including bond lengths and angles of 4-Amino-3,5-Dialkyl-1-Triazole molecule were investigated using Density Functional Theory (DFT) and ab initio Hartree–Fock (HF) quantum mechanical calculation methods at 6–31G (d,p) basis set in order to characterize the molecule. All the calculated bond lengths and bond angles were found to be in good agreement with each other. Moreover atomic charges, thermodynamic properties, nuclear magnetic resonance (NMR) spectra and ultraviolet visible (UV–Vis) spectra were determined and interpreted for the identification of the molecule. Theoretical ^{13}C and ^{1}H chemical shifts were shown to have a good agreement with available experimental determines. Furthermore, we not only simulated frontier molecular orbitals (FMO) and the molecular electrostatic potential (MEP) but evaluated the transition state and energy band gap.

Key Words: 4-Amino-3,5-Dialkyl-1-Triazole, FMO, MEP, HF, DFT

1. INTRODUCTION

As it is well known, triazole one of a pair of isomeric chemical compounds has a five-membered ring of two carbon atoms and three nitrogen atoms. Derivatives of this compound were thought that it undertook some vital assignments to continue the biological activity. Thus, the researches on triazole derivatives increase in the last decades due to the fact that the increased interest in not only the fundamental researches in heterocyclic chemistry and biology but the application in industry of these derivatives in the last decades stems from its pharmacological, insecticidal, fungicidal, herbicidal (Joshi et al., 1962; Hartwell and Abbot,1969; Kubota et al., 1978; Ikizler et al., 1996; Costales et al., 1998; Liu et al., 2000; Varma, 2000; Demirbas et al., 2002; Holla et al., 2002; Almasirad et al., 2004). In order to support the experimental evidences, the scientists use computational methods which are reliable to characterize the molecule because of their efficiency and accuracy with respect to the evaluation of a number of molecular properties (Ravikumar et al., 2008). A suitable quantum chemical study is helpful to predict compound properties economically and to clarify some experiment phenomena insightfully (Sun et al., 2010). In this respect, the computational researches on compound properties tend to increase (Fang et al., 2008 ; Avci et al., 2009; Karakurt et al., 2010). In this study, we calculated the molecular structures including bond lengths and angles, atomic charges, thermodynamic properties, NMR spectra and UV–Vis Spectra. Furthermore; after frontier orbitals and the molecular electrostatic potential were visualized, transition states and energy band gap were determined and interpreted for the 4-Amino-3,5-Dialkyl-1-Triazole molecule by using quantum mechanical methods. The aim of this study is to not only clarify the characterization of 4-Amino-3,5-Dialkyl-1-Triazole but show the way to future studies of this molecule, as well.

2. COMPUTATIONAL DETAILS

In order to predict compound properties economically and obtain the characterization of the 4-Amino-3,5-Dialkyl-1-Triazole molecule, the optimized molecular structures, atomic charges, thermodynamic properties, NMR Spectra, UV spectra, translation energy (HOMO–LUMO) and molecular electrostatic potential (MEP) were investigated by means of HF (Young, 2001) and B3LYP (Becke, 1992) methods at 6–31G(d,p) (Francl et al., 1982) basis set and then compared with each other. All the computations were performed by using Gaussian 09 package program with molecular visualization program (Gaussview et al., 2003 ; Frisch, M. J., et. al, 2009) on the personal computer.

3. RESULT AND DISCUSSION

We determined the molecular geometry, thermodynamic properties, atomic charges, NMR spectra UV–Vis spectra, electrostatic potential and translation energy $\left|\Delta E\right|$ for the identification of 4-Amino-3,5-Dialkyl-1-Triazole.

3.1. Molecular Geometry

Essentially two internal rotating groups are present in the molecule. The first one is the amine group NH_2, which can rotate about the bond N–H (N_{20}–H_{21} and N_{20}–H_{22} for amine group connected to N_{19} atom). The other rotate group is the methyl groups CH_3, which can rotate about C–C (C_{16}–C_{23} for methyl groups C_{16}–CH_3 and C_{23}–CH_3, respectively). Therefore, there are many more possible conformers of the molecule. In this study, in order to find the most

optimized geometry, the molecular energies of these tautomeric forms were calculated at different methods and various basis sets. The energy obtained in this study is minimum for the most optimized geometry. The most optimized molecular structures including bond lengths and bond angles of 4-Amino-3,5-Dialkyl-1-Triazole are shown in Figure 1 along with labeling and symbolizing by using schema. Geometric properties of structure were calculated by B3LYP/6–31G(d,p) and HF/6–31G(d,p) levels of calculation and depicted in Table 1. As can be seen from the table, all calculated data are in good agreement with each other. The largest difference of the calculated geometries was found to be about 0.04 Å (C_{15}-N_{17}) for the bond lengths and 1.49° (C_5-C_6-C_{15}) for the bond angles.

Table 1. Calculations of the optimized geometric parameters of 4-Amino-3,5-Dialkyl-1-Triazole

	Bond Length (Å)	
	B3LYP/6–31G(d,p)	HF/6–31G(d,p)
C_1-C_2	1.39	1.38
C_1-C_6	1.41	1.39
C_1-H_7	1.08	1.07
C_2-C_3	1.40	1.39
C_2-H_8	1.09	1.08
C_3-C_4	1.40	1.39
C_3-C_{11}	1.51	1.51
C_4-C_5	1.40	1.39
C_4-H_9	1.09	1.08
C_5-C_6	1.40	1.39
C_5-H_{10}	1.08	1.08
C_6-C_{15}	1.47	1.48
C_{11}-H_{12}	1.10	1.09
C_{11}-H_{13}	1.09	1.08
C_{11}-H_{14}	1.10	1.09
C_{15}-N_{17}	1.32	1.28
C_{15}-N_{19}	1.39	1.37
C_{16}-N_{18}	1.31	1.28
C_{16}-N_{19}	1.38	1.36
C_{16}-C_{23}	1.49	1.49
N_{17}-N_{18}	1.38	1.37
N_{19}-N_{20}	1.4	1.38
N_{20}-H_{21}	1.02	1.00
N_{20}-H_{22}	1.02	1.00
C_{23}-H_{24}	1.09	1.08
C_{23}-H_{24}	1.09	1.08
C_{23}-H_{25}	1.10	1.08
	B3LYP/6–31G(d,p)	HF/6–31G(d,p)
C_2-C_1-C_6	120.72	120.49
C_2-C_1-H_7	120.87	120.46

$C_6-C_1-H_7$	118.40	119.05
$C_1-C_2-C_3$	121.39	121.20
$C_1-C_2-H_8$	119.22	119.25
$C_3-C_2-H_8$	119.39	119.55
$C_2-C_3-C_4$	117.74	118.07
$C_2-C_3-C_{11}$	120.87	120.52
$C_4-C_3-C_{11}$	121.39	121.41
$C_3-C_4-C_5$	121.34	121.01
$C_3-C_4-H_9$	119.46	119.75
$C_5-C_4-H_9$	119.19	119.23
$C_4-C_5-C_6$	120.71	120.65
$C_4-C_5-H_{10}$	118.57	118.89
$C_6-C_5-H_{10}$	120.70	120.42
$C_1-C_6-C_5$	118.09	118.57
$C_1-C_6-C_{15}$	117.85	118.86
$C_5-C_6-C_{15}$	124.04	122.55
$C_3-C_{11}-H_{12}$	111.20	110.95
$C_3-C_{11}-H_{13}$	111.50	111.36
$C_3-C_{11}-H_{14}$	111.36	111.03
$H_{12}-C_{11}-H_{13}$	107.55	107.87
$H_{12}-C_{11}-H_{14}$	107.02	107.49
$H_{13}-C_{11}-H_{14}$	108.00	107.98
$C_6-C_{15}-N_{17}$	124.26	125.23
$C_6-C_{15}-N_{19}$	127.07	125.61
$N_{17}-C_{15}-N_{19}$	108.61	109.13
$N_{18}-C_{16}-N_{19}$	109.58	109.60
$N_{18}-C_{16}-C_{23}$	126.42	126.38
$N_{19}-C_{16}-N_{23}$	124.00	124.02
$C_{15}-N_{17}-N_{18}$	108.45	108.31
$C_{16}-N_{18}-N_{17}$	107.82	108.02
$C_{15}-N_{19}-C_{16}$	105.53	104.93
$C_{15}-N_{19}-N_{20}$	131.14	130.53
$C_{16}-N_{19}-N_{20}$	123.01	124.03
$N_{19}-N_{20}-H_{21}$	108.67	109.98
$N_{19}-N_{20}-H_{22}$	109.32	110.56
$H_{21}-N_{20}-H_{22}$	108.20	109.64
$C_{16}-C_{23}-H_{24}$	108.32	108.39
$C_{16}-C_{23}-H_{25}$	111.29	110.97
$C_{16}-C_{23}-H_{26}$	111.64	111.06
$H_{24}-C_{23}-H_{25}$	109.44	109.44
$H_{24}-C_{23}-H_{26}$	108.78	109.24
$H_{25}-C_{23}-H_{26}$	107.32	107.73

3.2. Charge Analysis

Atomic charges not only are very much dependent on how the atoms are defined but also play an important role in the application of quantum chemical calculations to molecular

systems. Atomic charges of 4-Amino-3,5-Dialkyl-1-Triazole, calculated by Mulliken (Olsen et al., 1985; Buyukuslu et al., 2010) method were shown in Figure 1. The magnitudes of the carbon atomic charges were found to be either positive or negative at the computational methods. These magnitudes are changing between –0.38 and 0.45. The maximum charge magnitude (C_{15}) was found 0.45 at B3LYP/6–31G(d,p) calculation levels, respectively. On the other hand, the minimum charge (C_{11}) was obtained to be –0.38 at the level of calculation. In addition, the magnitudes of charges calculated on N atoms are noted to be only negative value. These magnitudes are found to change from –0.32 to –0.46. N_{19} atom was determined to be the minimum charge value (–0.46) at B3LYP/6–31G(d,p) level of theory. Moreover, the magnitudes of the hydrogen atomic charges are arranged in an order from 0.05 to 0.29. The charge on H_{22} connected with N_{20} was calculated to be maximum at the calculation levels. The results show that:

    *All the hydrogen atoms in molecule lost electrons.
    *All nitrogen atoms in molecules accepted electrons.
    *Charge migration to heavy atoms can be related to molecular interactions.
    *HF basis set has more negative magnitudes than the others.
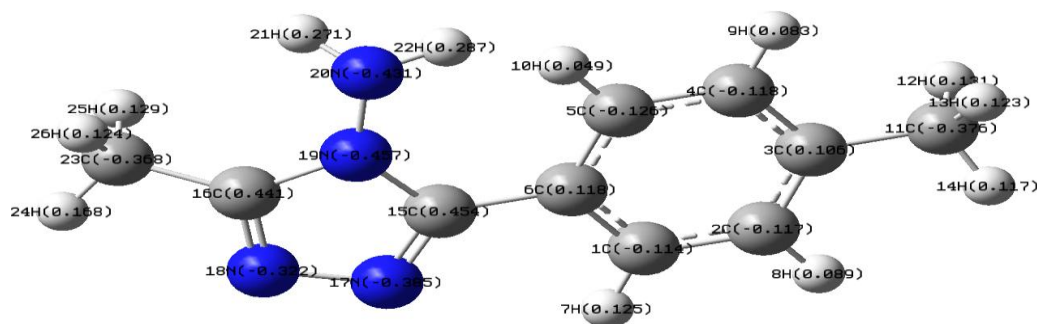   *All the computations are in good agreement with each other.

Figure 1. The molecular structure of 4-Amino-3,5-Dialkyl-1-Triazole (The values within parentheses indicate Mulliken atomic charges obtained from DFT method)

3.3. UV–Vis Spectra Analysis

These spectra analyses 4-Amino-3,5-Dialkyl-1-Triazole were investigated by various theoretical results. Absorption maxima (λmax) of the molecule were calculated by ZINDO (Zerner, 1991) and TD (Bauernschmitt and Ahlrichs, 1996) methods. The calculated visible absorption maxima of λ which are a function of the electron availability were reported in Table 2. The visible absorption maxima of the title molecule were corresponded to the electron transition between frontier orbitals (such as translation from HOMO to LUMO; or from HOMO–2 to LUMO+1) by using calculations of molecular orbital geometry. As can be seen from the table, the calculated absorption maxima values were found to be 266, 281 and 299 nm at ZINDO calculation level. Moreover, λmax were arranged in an order from 257 to 301 nm at TD–B3LYP/6–31G(d,p) while they were obtained to change from 201 to 240 nm (the smallest values in the all levels) at TD–HF/6–31G(d,p) calculation level. The results indicate the computations of ZINDO and TD–B3LYP/6–31G(d,p) were noted to be close to each other. Oscillator strength values were also depicted in the Table 2. It was found that the maximum strength value was found to be about 0.4056 at 299 nm for ZINDO calculation level while the

maximum computation at TD–HF (TD–B3LYP) method was calculated to be 0.3865 at 240 nm
(0.374 at 264 nm).

Table 2. Theoretical electronic absorption spectra values of 4-Amino-3,5-Dialkyl-1-Triazole

Calculated, λ_{cal} (nm)					
ZINDO		TD–B3LYP/6–31G(d,p)		TD–HF/6–31G(d,p)	
Wave Length (nm)	Oscillator Strength	Wave Length (nm)	Oscillator Strength	Wave Length (nm)	Oscillator Strength
299	0.4056	301	0.081	240	0.3865
281	0.0068	264	0.374	216	0.0001
266	0.0266	257	0.0059	201	0.0247

3.4. NMR Spectrum Analysis

Whereas no electron correlation effects are taken into account in HF methods, DFT
methods treat the electronic energy as a function of the electron density of all electrons
simultaneously and thus include electron correlation effect (Avci et al., 2009). In this study,
GIAO ^{13}C and ^{1}H NMR chemical shifts of 4-Amino-3,5-Dialkyl-1-Triazole have been
calculated and depicted in Table 3. These calculations obtained at HF/6–31G(d,p) and
B3LYP/6–31G(d,p) levels for the optimized geometry were observed to be in good agreement
with experimental results. ^{1}H isotropic chemical shift values were observed at 2.35–7.92 (in
2007) parts per million (ppm) while these values were found at 2.15–9.22, 1.43–8.51, 2.33–9.41
and 1.61–8.70 ppm at HF/6–31G(d,p)//HF/6–31G(d), HF/6–31G(d,p)//B3LYP/6–311+G(2d,p),
B3LYP/6–31G(d,p)//HF/6–31G(d) and B3LYP/6–31(d,p)//B3LYP/6–311+G(2d,p) calculation
levels, respectively. In addition, H_{13} has the minimum chemical shift of H atoms and this value
was observed at 2.35 ppm and obtained to change from 1.43 to 2.33 ppm at different basis sets.
The average chemical shift values of H atoms, observed to be 4.72 ppm (in 2007), were
calculated to be 4.69, 3.97, 4.89 and 4.17 ppm at HF/6–31G(d,p)//HF/6–31G(d), HF/6–
31G(d,p)//B3LYP/6–311+G(2d,p), B3LYP/6–31G(d,p)//HF/6–31G(d) and B3LYP/6–
31G(d,p)//B3LYP/6–311+G(2d,p) basis sets, respectively. In addition, ^{13}C isotropic chemical
shifts with regard to TMS calculated at the same basis sets were given in the same table. ^{13}C
chemical shift values were observed at 9.80–153.06; however, they were found at 9.94–179.52
and 0.2–162.00 ppm at HF/6–31G(d,p)//HF/6–31G(d) and HF/6–31G(d,p)//B3LYP/6–
311+G(2d,p) basis sets whereas these values were observed at 18.62–180.91and 1.10–163.40 at
B3LYP/6–31G(d,p)//HF/6–31G(d) and B3LYP/6–31G(d,p)//B3LYP/6–311+G(2d,p)
calculation levels, respectively. C_{23} atom has the minimum chemical shift changing between
0.10 and 18.62 ppm. Moreover, the average chemical shift values of C atom, observed to be
111.19 ppm (in 2007), were found to be 116.33, 100.46, 120.86 and 103.29 ppm at HF/6–
31G(d,p)//HF/6–31G(d), HF/6–31G(d,p)//B3LYP/6–311+G(2d,p), B3LYP/6–
31G(d,p)//B3LYP/6–311+G(2d,p) and B3LYP/6–31G(d,p)//HF/6–31G(d) calculation levels,
respectively. The results show that B3LYP/6–31G(d,p)//B3LYP/6–311+G(2d,p) calculations
for ^{1}H chemical shifts were obtained to be largest values in the calculation levels while the
HF/6–31G(d,p)//B3LYP/6–311+G(2d,p) ones were noted to be smallest values. On the other
hand, HF/6–31G(d,p)//HF/6–31G(d) computations for ^{13}C chemical shifts were noticed to be
largest values in the basis sets whereas B3LYP/6–31G(d,p)//HF/6–31G(d) ones were found to
be smallest values.

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3.5. Thermodynamic Properties

Several thermodynamic parameters have been calculated by using DFT and HF at 6–31G(d,p) basis set and semi empirical models and have been given in Table 4. Scale factors have been recommended (Minnesota Computational–Chemistry, 2009) for an accurate prediction in determining the zero–point vibration energies for HF and DFT calculation. The total energies and the change in the total entropy of the molecule at room temperature at different theoretical methods have been presented. Table 4 demonstrates several thermodynamic parameters of the molecule without results of experimental. Calculations of HF/6–31G(d,p) basis set for energy parameters and rotational constant are slighter larger than B3LYP/6–31G(d,p) ones. In contrast, HF entropy values are smaller than DFT values.

Table 3. Theoretical ^{13}C and ^{1}H isotropic chemical shifts (with respect to TMS, all values in ppm) for 4-Amino-3,5-Dialkyl-1-Triazole ($C_{10}H_{13}N$)

Calculated Chemical Shift (ppm)				
Atom	HF/6–31G (d,p)// HF/6–31G(d)	HF/6–31G (d,p)// B3LYP / 6–11+G(2d,p)	B3LYP/6–31G(d,p)// HF/6–31G(d)	B3LYP/6–31G (d,p)// B3LYP /6–311+G(2d,p)	[a]Experimental
C_{23}	9.94	0.20	18.62	1.10	9.80
C_{11}	17.32	8.51	28.40	10.88	20.83
C_5	125.39	107.86	128.89	110.87	124.71
C_1	126.54	109.02	130.5	112.98	127.57
C_4	127.29	109.78	130.7	113.18	127.57
C_2	128.78	111.26	133.97	116.45	128.81

C$_6$	129.32	111.8	134.07	116.55	128.81
C$_3$	142.38	124.86	145.96	128.44	138.67
C$_{16}$	176.87	159.35	176.55	159.02	152.10
C$_{15}$	179.52	162.00	180.91	163.40	153.06
H$_{10}$	9.22	8.51	9.41	8.70	7.92
H$_7$	9.15	8.44	9.08	8.36	7.92
H$_8$	8.14	7.42	8.18	7.46	7.30
H$_9$	7.90	7.18	7.95	7.24	7.30
H$_{22}$	5.72	5.00	5.93	5.21	6.05
H$_{21}$	2.48	1.76	3.01	2.29	6.05
H$_{25}$	2.45	1.74	2.78	2.06	2.35
H$_{12}$	2.40	1.68	2.71	2.00	2.35
H$_{26}$	2.24	1.52	2.56	1.84	2.35

H_{14}	2.22	1.51	2.37	1.66	2.35
H_{24}	2.19	1.48	2.34	1.62	2.35
H_{13}	2.15	1.43	2.33	1.61	2.35

[a]Taken from (Gumrukcuoglu ve ark., 2007)

Table 4. Theoretically computed energies (a.u.), zero–point vibrational energies (kcal mol^{-1}), rotational constants (GHz) , entropies (cal mol^{-1} K^{-1}) and dipole moment (Debye)

Parameters	B3LYP/6–31G(d,p)	HF/6–31G(d,p)
Total energy	−607.28	−603.44
Zero–point energy	130.63	131.29
Rotational constant	0.31	0.32
	0.35	0.36
	2.14	2.18
Entropy		
Total	114.87	113.26
Translational	41.60	41.60
Rotational	31.59	31.54
Vibrational	41.68	40.13
Dipole Moment	5.69	6.27

3.6. HOMO and LUMO Analysis

Highest Occupied Molecular Orbital and Lowest Unoccupied Molecular Orbital are very important parameters for quantum chemistry. We can determine the way the molecule interacts with other species; hence, they are called the frontier orbitals. HOMO, which can be thought the outermost orbital containing electrons, tends to give these electrons such as an electron donor. On the other hand; LUMO can be thought the innermost orbital containing free places to accept electrons (Gece, 2008). Owing to the interaction between HOMO and LUMO orbital of a structure, transition state transition of π–π^* type is observed with regard to the molecular orbital theory (Fukui, 1975). Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures (Lewis et al., 1994) and given in Table 5. In addition, 3D plots of highest occupied molecular orbitals and lowest unoccupied molecular orbitals are shown in Fig. 2. According to B3LYP/6–31G(d,p) calculation level, HOMO – LUMO energy band gap (ΔE) of this molecule is about 0.19 a.u. while the band gap is about 0.42 at HF/6–311G(d,p) calculation level. The

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highest occupied molecular orbitals were localized mostly on the molecule; however, no translation appears on the amino group. On the other hand, the lowest unoccupied molecular orbitals were mainly localized on the molecule except for methyl group. Moreover, the HOMO–1 and HOMO–2 orbitals were partially localized on different parts of the title molecule. The HOMO–1 orbitals were only delocalized on the Triazole ring and amino group, while the HOMO–2 orbitals were only delocalized on the benzene ring. Likewise, the LUMO+1 and LUMO+2 orbitals were partially delocalized on different parts of the molecule. The LUMO+1 orbitals were partially delocalized on the benzene ring and slightly localized on the amino group whereas the LUMO+2 orbitals were mainly delocalized on the molecule except for hydrogen atoms. In addition, Lowest MO Eigen value was calculated −15.65 and −14.42 (a.u.) at B3LYP/6–31G(d,p) and HF/6–31G(d,p) basis sets, respectively. Highest MO Eigen value was also found to be about 5.30 (a.u.) at B3LYP/6–31G(d,p) and 4.86 (a.u.) at HF/6–31G(d,p) calculation level. The HOMO–1, HOMO–2, LUMO+1 and LUMO+2 Eigen values of the molecule were also depicted in the same table.

Table 5. Some of the calculated energy values of 4-Amino-3,5-Dialkyl-1-Triazole in its ground state with singlet symmetry at computational models

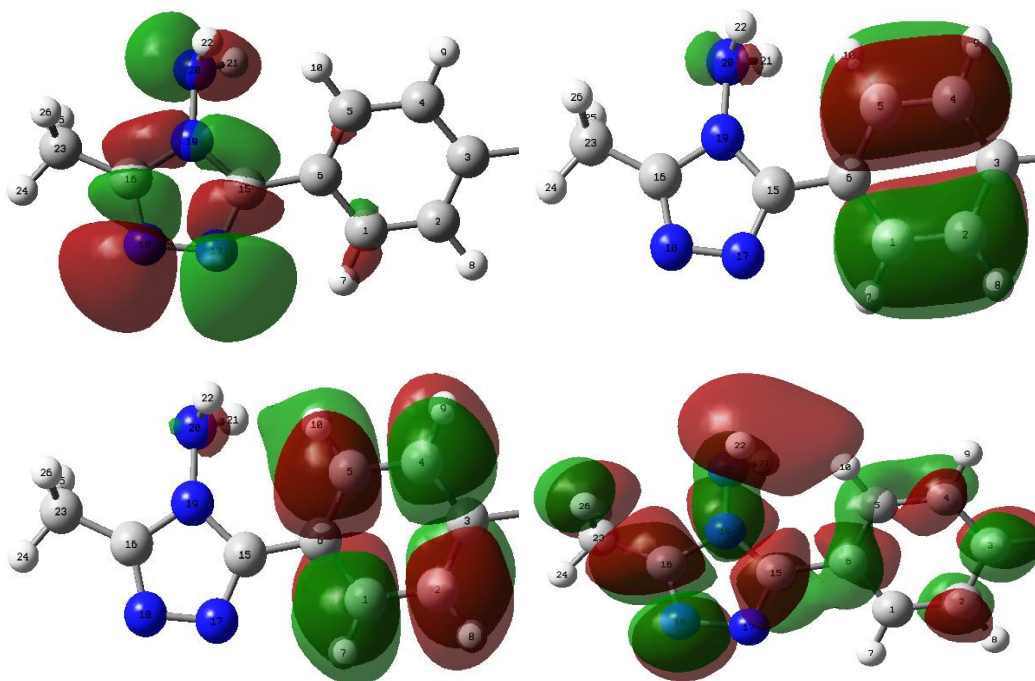| Quantity	HF Result	DFT Result
Lowest MO Eigen value (a.u.)	−15.65	−14.42
Highest MO Eigen value (a.u.)	5.30	4.86
The virial (−V/T)	2.0012	2.0096
HOMO (a.u.)	−0.31	−0.22
LUMO (a.u.)	0.11	−0.03
HOMO–LUMO gap, ΔE (a.u.)	0.42	0.19
HOMO–1	−0.35	−0.24
HOMO–2	−0.37	−0.29
LUMO+1	0.13	−0.01
LUMO+2	0.19	0.04
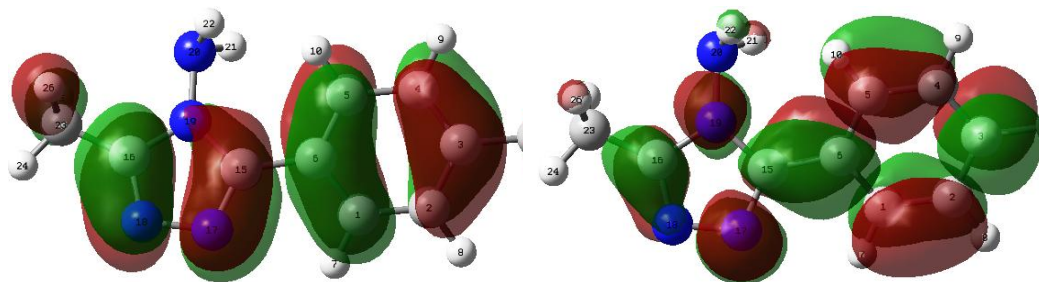
Figure 2. 3D plots of a) the HOMO; b) LUMO; c) HOMO–1; d) HOMO–2; e) LUMO+1 and f) LUMO+2 of 4-Amino-3,5-Dialkyl-1-Triazole obtained from DFT method. (Red regions show the positive phase while greens present the negative phase)

3.7. Molecular Electrostatic Potential

At any given point r(x, y, z) in the vicinity of a molecule, the molecular electrostatic potential, V(r) is defined in terms of the interaction energy between the electrical charge generated from the molecule electrons and nuclei and a positive test charge (a proton) located at r (Politzer and Murray, 2002; Ozdemir et al., 2010; Parlak et al., 2011). The molecular electrostatic potential (MEP) is related to the electronic density and a very useful descriptor for determining sites for electrophilic attack and nucleophilic reactions as well as hydrogen–bonding interactions (Luque et al., 2000; Okulik and Jubert, 2005). In Figure 3, while negative (red) regions of MEP were related to electrophilic reactivity the positive (blue) regions were related to nucleophilic reactivity. As seen from the figure, whereas the red region was localized on the nitrogens and vicinity of these atoms the blue region was delocalized on the amino group. Hence, it was found that the compound is useful to both bond metallically and interact intermolecularly. This result also supports the evidences of charge analyses part.
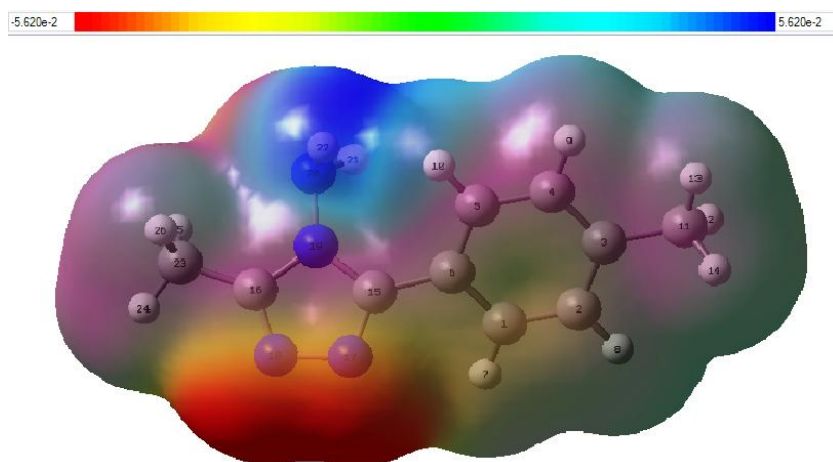
Figure 3. 3D plots of the molecular electrostatic potential map (in a.u.) of 4-Amino-3,5-Dialkyl-1-Triazole molecule (obtained from DFT method)

4. CONCLUSION

In this study, we tried to clarify the characterization of 4-Amino-3,5-Dialkyl-1-Triazole by means of computational methods. Bond lengths and angles were calculated by using DFT and HF methods and compared with each other. All compared data were shown to have in a good agreement with each other. This good agreement is well within the accuracy of computational results. Moreover, after frontier molecular orbitals and molecular electrostatic potential were visualized, electronic structure and energy band gap of the title molecule were investigated and interpreted. Atomic charges, thermodynamic properties, NMR spectra and UV–Vis spectra were also determined for the identification of the molecule. Theoretical ^{13}C and ^{1}H chemical shifts were found to be in good agreement with available experimental determines. In conclusion, all the calculated data and simulations not only show the way to the characterization of the molecule but also help for the application in industry and fundamental researches in heterocyclic chemistry and biology in the future.

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