

## Kabul Edilmiş Araştırma Makalesi (Düzenlenmemiş Sürüm)

## Accepted Research Article (Uncorrected Version)

### Makale Başlığı / Title

Vibrational, geometrical and HOMO/LUMO/MEP analyses by using DFT/B3LYP and DFT/M06-2X methods: 3-Amino-1,2,4-triazole

DFT/B3LYP ve DFT/M06-2X metotları ile titreşimsel, geometriksel ve HOMO/LUMO/MEP analizleri: 3-Amino-1,2,4-triazole

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Abstract

The theoretically calculated modes and optimized structure parameters of 3-amino-1,2,4-triazole have been computed with Density Functional Theory (for two important methods) by using 6-311++G(d,p) basis level. We have calculated all data by using Gaussian 09W. The theoretical structure values and vibrational frequencies of investigated compound have been found to be consistent with the experimental data. We concluded that the optimized molecular geometric parameters (bond lengths and bond angles) and theoretical frequencies are deviated from the experimental values. Because, in the calculations we have assumed that isolated molecule is in gas phase, in experiments in fact, molecule is solid phase. Sandri et al. molecular interactions have been isolated from real situation. In summary, this study will provide support in future spectroscopy and other related studies.

Keywords: Triazole, IR, Vibration, DFT

Özet

3-amino-1,2,4-triazole için teorik olarak hesaplanan modlar ve optimize edilmiş yapı parametreleri yoğunluk fonksiyonu teorisi (iki önemli yöntem için) 6-311++G(d,p) temel seviyesiyle hesaplanmıştır. Tüm verileri Gaussian 09W kullanılarak hesapladık. İncelenen bileşiğin teorik yapı ve titreşim frekansları deneysel verilerle tutarlı bulundu. Sonuç olarak optimize edilmiş moleküler geometrik parametreleri (bağ uzunlukları ve açıları) ve teorik frekansların deneysel değerlerden farklı olduğunu gördük. Çünkü hesaplamalarda izole edilmiş moleküler yapıyı gaz ortamında varsaydık, deneyde ise moleküler katı fazdadır. Sandri et al. moleküler etkileşimleri gerçek durumdan izole etmişlerdir. Özetle, bu çalışma gelecekteki spektroskopik ve diğer ilgili çalışmalar için destek sağlayacaktır.

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1 Introduction

Triazole is a five-membered ring with three nitrogen atoms along with two carbons. It exists in two isomeric forms known as 1,2,3 and 1,2,4-triazoles in which the latter one is most common. Various heterocycles containing triazole moiety show a range of biological activities. Triazole is one of the most important and common heterocycles among five-membered heterocyclic compounds. In recent years, heterocycles containing 1,2,4-triazole moiety show very interesting applications. They show various biological and pharmacological activities in which many derivatives act as antimicrobials, antivirals, anticonvulsants, antidepressants, and antioxidant [1-7]. However, the theoretical analysis of the vibrational modes of such simple heterocycles (3-amino-1,2,4-triazole) has not been detected up until now. Generally, the specified experimental data weaker than computed values. To this situation can be caused by many factors. Rauhut and Pulay have concluded that the B3LYP technique provides optimized geometric values that are well consistent with the experimental data. Such conclusion was based on the experimental data for twenty simple organic compounds [8]. We want to determine optimized molecular geometry, vibrational theoretical frequencies, dipole moments and highest/lowest molecular orbitals for 3-amino-1,2,4-triazole. That is real goal. The electron density and MEP clouds associated with the title compound were also investigated.

2 Computational Details

The calculated modes, optimized structure parameters and related properties of 3-amino-1,2,4-triazole in the ground state (stable situation) have been computed via a aforementioned methods videlicet DFT/B3LYP and DFT/M06 methods with 6-311++G(d, p) grade. Whole computations have been done by utilizing visually based Gaussian 5.0 [9] and Gaussian 09W [10] programs. We have used correlation factors or scales factors of 0.9614 for B3LYP and, of 0.9489 for M06 methods with 6-311++G(d,p) basis level, according to references [11], [12]. These scale factors allow us to much closer to the experimental data. Different scales can be used for different regions, but we have used same scale factors in all regions.

3 Results and Discussions

3.1 Geometric Structure

Table 1 shows the bond lengths and bond angles for the optimized theoretical and experimental structures (Figure 1). As can be seen from Table 1, the optimized parameters calculated at both DFT levels differ slightly from the experimental values, and small variations are to be expected since the calculations correspond to the gas phase rather than the solid state. For example, in triazole important bond lengths are N-N, C-N4 and C-N4. By Starova et al. [13] ° ¤ j - j ' ÿ ¥ " ° ş a œ j - " 3 ş " © « ± a ÿ ş " ( ¤ j - j ' ¤ ş 2 j ' > j j a œş " œ ± " ş ° j ÿ ş " ş a ÿ " 6 -2X) by us, respectively for similar structure, 3-amino-5-mercapto-1,2,4-triazole [14], N6

1.3633 (B3LYP-6-311G(d,p)), 1.3747 (B3LYP-6-311G(d,p)) and 1.3232 (B3LYP-6-311G(d,p)). C1-N bond lengths have been observed [14] as 1.3602-1.3698 (B3LYP-6-311G(d,p)).

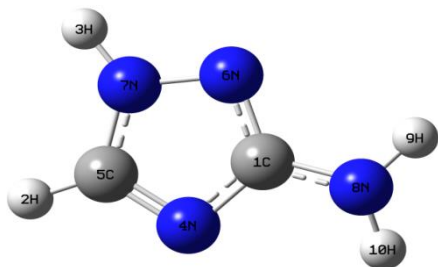


Figure 1: The optimized molecular structure of amino-1,2,4-triazole

Other related bond lengths are of amino group. For N8H9 and N8H10 respectively. These bond angles have been calculated as 101.7/101.8, 110.3/110.2, 110.2/110.2, respectively.

If we see important bond angles N4C1-N4, N6N7-C5, N7C5-N4, C1N4-C5 and within the amino group N8H9 bond angle have been observed as 103.21, 109.98, 111.23, 102.01 respectively. These bond angles have been calculated as 101.7/101.8, 110.3/110.2, 110.2/110.2, respectively.

In order to quantify the level of agreement between the experimental and computational results, the relationship factors between them have been calculated (last row in each section of Table 1). These values are 0.9906/0.9900 for the bond lengths and 0.9841/0.9859 for the bond angles for B3LYP/MO62X methods. These values show that the calculated bond lengths at B3LYP level are slightly closer to the experimental data, but the calculated bond angles at MO6 level are marginally closer to the data obtained experimentally.

### 3.2 Vibrational Spectra

The molecular structure of amino-1,2,4-triazole ( $C_2H_4N_4$ ) belong to  $C_s$  symmetry. It has 32(N7) in plane mode and others 13 (7) in out of plane mode. Additionally, the calculated vibrational modes were cleared up through the medium of Potential Energy Distribution (PED) investigations for primary vibration modes with VEDA4 program package [15], [16]. Table 2 shows the resulting scaled vibrational frequencies and proposed vibrational assignments of the optimized molecule. Table 2 also shows the experimental vibrational modes. The experimental observed IR data has been obtained from the Sigma Aldrich Cooperation, 2016 [17] as shown in Figure 2. The calculated IR spectrum has been given in Figure 3, and the important vibrational modes have been examined as discussed below.

3.2.1 Triazole Ring Vibrations  
It is not so easy to define the C-N and C=N vibrational bands, exactly. Because there are mixed band structures in this area. By Gokce et al. [6], the stretching vibrations in their

Table 1 The observed and calculated optimized structural parameters of 3-amino-1,2,4-triazole

Optimized Structure: $\angle$	Observed values	Calculated parameters	
		B3LYP	MO62X
C1-N4	1.363	1.368	1.363
C1-N6	1.319	1.326	1.319
C1-N8	1.401	1.378	1.379
H2-C5	-	1.079	1.079
H3-N7	0.930	1.007	1.007
N4-C5	1.336	1.320	1.315
C5-N7	1.339	1.341	1.339
N6-N7	1.398	1.367	1.357
N8-H9	0.863	1.009	1.009
N8-H10	0.867	1.009	1.009
$R^2$ values $\gamma$		0.9906	0.9900
Bond Angles $\delta$			
N4-C1-N6	114.89	115.1	115.1
N4-C1-N8	120.02	121.8	121.8
N6-C1-N8	123.14	123.1	123.1
C1-N4-C5	102.01	102.9	102.6
H2-C5-N4	-	126.2	126.3
H2-C5-N7	-	123.6	123.5
N4-C5-N7	111.23	110.2	110.2
C1-N6-N7	103.21	101.7	101.8
H3-N7-C5	128.38	129.8	129.7
H3-N7-N6	121.42	119.9	120.1
C5-N7-N6	109.98	110.3	110.2
C1-N8-H9	114.98	114.9	114.1
C1-N8-H10	113.21	114.1	113.3
H9-N8-H10	114.34	114.2	113.4
$R^2$ values		0.9841	0.9859

<sup>a</sup>Values are taken from Ref. [13]

molecular structure of (3-pyridyl)-4H-1,2,4-triazole-3-thiol have been applied to the bands observed at 1033(Ra) and 1041

(IR)-1046 (Ra) cm<sup>-1</sup> for thioflavin T structure. These modes have been calculated at 1032.79 and 1051.97 with 39% and 40% contributions of PED, respectively [6] and [18].

Table 2 The observed and calculated vibrational frequencies of the title compound at 6-31+G(d,p) level

Modes	Exp. FT-IR <sup>b</sup>	Calc. B3LYP	Calc. M062X	Assignments(%PED)
b <sub>1</sub>	-	3544	3532	" (99) asymmetric stretching
b <sub>2</sub>	-	3523	3513	" fl
b <sub>3</sub>	3420	3443	3428	" (99) symmetric stretching
b <sub>4</sub>	3130	3123	3114	" fl
b <sub>5</sub>	1593	1587	1586	fl " fl
b <sub>6</sub>	1540	1526	1536	" " fl " fl
b <sub>7</sub>	1466	1458	1463	" " " " fl "
b <sub>8</sub>	1420	1417	1433	fl " " " "
b <sub>9</sub>	1314	1330	1345	" " " " fl "
b <sub>10</sub>	1266	1247	1254	fl " " " "
b <sub>11</sub>	1153	1146	1159	" " fl " "
b <sub>12</sub>	1047	1066	1072	fl " " " fl "
b <sub>13</sub>	1026	1023	1038	" " fl " " fl "
b <sub>14</sub>	969	970	980	" " " "
b <sub>15</sub>	926	952	950	" " " "
b <sub>16</sub>	831	812	851	fl " " " " "
b <sub>17</sub>	768	744	753	" " " " " "
b <sub>18</sub>	731	712	711	" " " " -N6-N7 " "
b <sub>19</sub>	642	628	633	" " " " fl " " "
b <sub>20</sub>	568	552	583	fl " " " fl " fl "
b <sub>21</sub>	462	442	478	fl " " " " " "
b <sub>22</sub>	-	403	398	" " " " fl " " "
b <sub>23</sub>	-	314	316	" " " " fl " " "
b <sub>24</sub>	-	280	281	fl " " " " " "
R <sup>2</sup> values		0.9997	0.9996	

<sup>a</sup>Potential Energy Distribution (PED). less than 10% are not shown.

<sup>b</sup>Taken from (SigmaAldrich, 2016) [17].

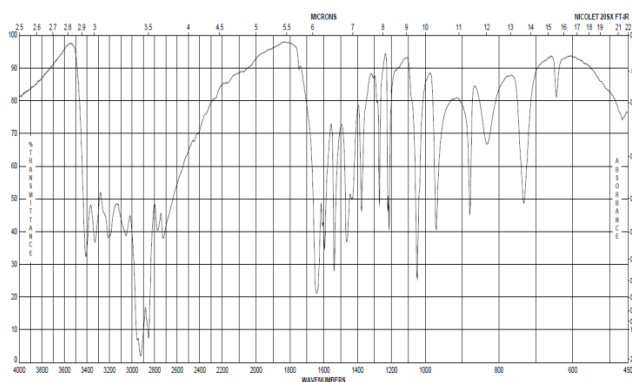


Figure 2: Experimental IR spectrum of 3-amino-1,2,4-triazole

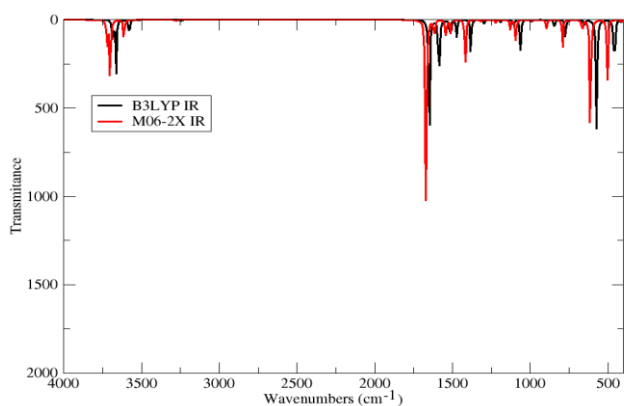


Figure 3: Theoretical IR spectrum of 3-amino-1,2,4-triazole

In our calculations these modes have been calculated at 1247/1254, 1146/1159, 1066/1072, 1023/1038 and 952/950  $\text{cm}^{-1}$  (B3LYP/M062X). These calculated frequencies have been assigned at 1266, 1153, 1047, 1026 and 926  $\text{cm}^{-1}$  (FT-IR), respectively. 1,4-Diphenyl-3-(phenylammonio)-1H-1,2,4-triazolium [19] shows a band at 1576  $\text{cm}^{-1}$  (C-N stretching vibration of 1,2,4-triazole moiety), and the computed one was appeared at 1557  $\text{cm}^{-1}$  in the current study, the C-N stretching vibration modes have been calculated at 1526/1536, 1458/1463, 1417/1433, 1330/1345, 1247/1254, 1146/1159, 1066/1072 and 952/950  $\text{cm}^{-1}$  (B3LYP/M062X), these vibrational frequencies have been identified in IR spectrum at 1540, 1466, 1420, 1314, 1266, 1153, 1047 and 969  $\text{cm}^{-1}$  respectively. In that study [19], the stretching vibration mode of triazole circle has been seen at 1441  $\text{cm}^{-1}$  and the computed vibration has been found as 1438  $\text{cm}^{-1}$  in this work, the C-N stretching modes have been observed at 1540, 1466, 1314 and 1266  $\text{cm}^{-1}$  and, calculated at 1526/1536, 1458/1463, 1330/1345 and 1247/1254  $\text{cm}^{-1}$  (B3LYP/M062X), respectively. Other related modes in plane bending, in and out of plane modes are reported in Table 2.

### 3.2.2 N-H Vibrations

Generally, amines N-H stretching modes appear within 3500-3300  $\text{cm}^{-1}$  region. Aliphatic primary amines indicate modes appeared within in the 3400-3000  $\text{cm}^{-1}$  region. But, N-H stretching modes in aromatic amines are lightly higher compared to other amines [14] and [20]. N-H stretching modes have been observed at around 3130  $\text{cm}^{-1}$  on the FTIR spectrum, and these modes were calculated at 3523/3513 and

3123/3114  $\text{cm}^{-1}$  (B3LYP/M062X) in this work. The calculated N-H vibration modes are lightly different from the observed experimental values. This result did not surprise us. For similar structure, 3-amino-5-mercapto-1,2,4-triazole [14], the IR band at 3379  $\text{cm}^{-1}$  is assigned to the N-H stretching mode. Other N-H stretching modes of NH could be examined in Table 2.

### 3.2.3 NH<sub>2</sub> Vibrations

Amino group vibrations can be generally seen at 3350  $\text{cm}^{-1}$  (stretching), 1700-1600  $\text{cm}^{-1}$  (scissoring) and 1150  $\text{cm}^{-1}$  (rocking deformations) [14] and [21]. In this study, the asymmetric and symmetric stretching fundamental modes of 3-amino-1,2,4-triazole have been calculated at 3544/3532 and 3443/3428  $\text{cm}^{-1}$  (B3LYP/M062X), respectively. The asymmetric mode was not observed in the experimental FTIR spectrum. The symmetric stretching was appointed to 3420  $\text{cm}^{-1}$ . For 3-amino-5-mercapto-1,2,4-triazole molecule these stretching modes have been observed at 3299  $\text{cm}^{-1}$  for asymmetric mode and 286  $\text{cm}^{-1}$  (IR) for symmetric mode by Xavier et. al. [14]. The scaled asymmetric stretching modes are computed as 3311 for B3LYP and 3306  $\text{cm}^{-1}$  for M062X methods in our study. Other symmetric modes have been computed as 3274 for B3LYP and 3264  $\text{cm}^{-1}$  for M062X. The NH<sub>2</sub> scissoring modes have been observed at 1592 and 1540  $\text{cm}^{-1}$ . These modes have been calculated as 1587/1586  $\text{cm}^{-1}$  and 1526/1536  $\text{cm}^{-1}$  (B3LYP/M062X). The N-H scissoring modes have reported as 1654 and 1640  $\text{cm}^{-1}$  by B3LYP and as 1663 and 159  $\text{cm}^{-1}$  using HF methods by Xavier et. al [14]. They match the IR and FT-Raman values that have been identified at 1645 (very strong) and 1655 (strong).

The rocking modes of the compound under investigation have been observed at 1153, 1047 and 1026  $\text{cm}^{-1}$ . These rocking vibration modes have been computed at 1146/1159, 1066/1072  $\text{cm}^{-1}$  and 1023/1038  $\text{cm}^{-1}$  (B3LYP/M062X), respectively. Table 2 shows other related vibrations. The harmony between the experimental and calculated wavenumbers is shown in Figure 4, which indicates that the experimental frequencies correlate well with the calculated ones, particularly for B3LYP. The correlations between the experimental and computed vibrational wavenumbers are linear and, given with Equations 1 and 2.

$$\text{Cal} = 1.00 \text{ exp} + 14.89 \text{ for B3LYP method} \quad (1)$$

$$\text{Cal} = 1.00 \text{ exp} + 10.013 \text{ for M062X method} \quad (2)$$

The correlation coefficients (R values) between the experimental and calculated wavenumbers were calculated as 0.9997 (regression or harmony value) for B3LYP and 0.9996 (regression or value) for M062X. This indicates that the calculation methods give reasonable agreement with the values measured experimentally, particularly in the case of the B3LYP method.



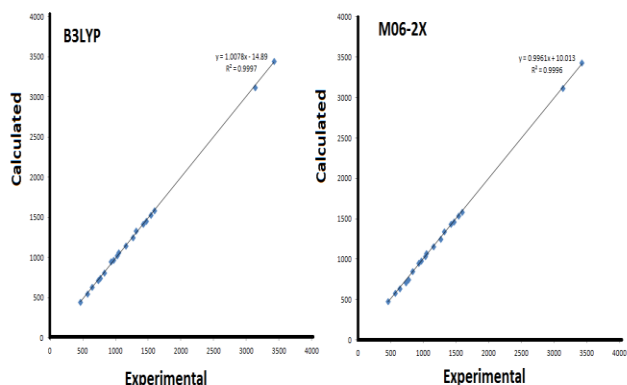


Figure 4: Frequency correlation graphics of amino-1,2,4-triazole.

### 3.3 Homo-Lumo Analysis

Chemical stability is mainly influenced by the frontier orbitals (HOMO and LUMO). The HOMO represents electron donating capability, while the LUMO represents electron accepting capability [22]. The HOMO and LUMO energies of amino-1,2,4-triazole have been computed by the methods of B3LYP/6-311++G(d,p) and M06-2X/6-311++G(d,p) (Figure 5 and Figure 6; positive phase represented in red and negative phase represented in green). A big HOMO width value means that the compound is a stiff molecule while a minor HOMO LUMO with value means that the compound is a smooth or so molecule. The chemical reactivity of a molecule is also related to the HOMO-LUMO gaps.

being more reactive [23]. The frontier molecular orbital energy gap therefore helps in understanding the kinetic stability and reactivity of molecules [24][25]. For our molecule the HOMO lies at 8.834/8.880 eV (B3LYP/M062X) whereas the LUMO is located at 3.936/3.911 eV (B3LYP/M062X). As is evident from Figure 5, for B3LYP method the HOMO is located on the entire molecule and the LUMO is concentrated on the triazole ring and over the C8 atom. But from Figure 6 for M06-2X we see that the HOMO clouds are concentrated on the whole molecule and LUMO clouds are more focused upon the C7 bond and over the H3 atom. Between HOMO and LUMO energy width of our compound is calculated as 4.898 eV at B3LYP/6-311++G(d,p) and, 4.969 eV at M06-2X/6-311++G(d,p) level.

This width shows the chemical activity of the molecule and influences its biological activity. We can find other important parameters (the ionization energy (I) and electron affinity (A)) by using HOMO and LUMO orbital energy values as  $I = -E_{HOMO}$  and  $A = E_{LUMO}$ . Similarly, related theoretical chemical factors related to HOMO-LUMO gap value have been figured out. For the calculation of these parameters, the formula have been given first line in Table 3. Total dipole moment is an important indicator in reaction mechanism and express the ability of the studied molecule to interact with the other related surroundings. According to this comment, calculated results have showed that the investigated compound possess a dipole moment of 2.060 debye for B3LYP and 2.2863 debye for M062X which indicates high reactivity to interact with surrounding media. Dipole moment values have been given in Table 3.

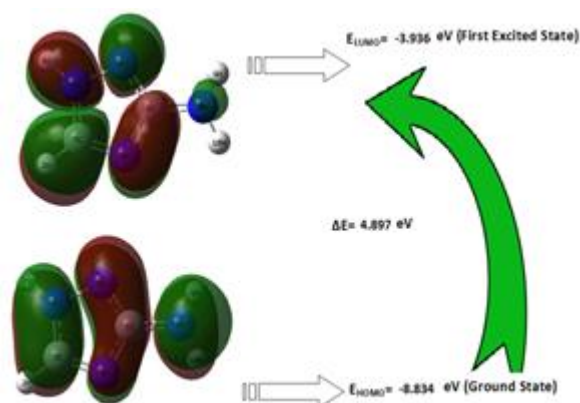


Figure 5: Calculated HOMO and LUMO plots of amino-1,2,4-triazole with B3LYP.

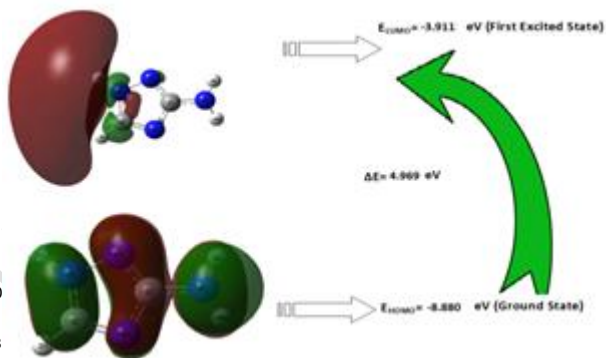


Figure 6: Calculated HOMO and LUMO plots of amino-1,2,4-triazole with M06-2X.

Table 3. Zero point energies, homo and lumo energies in the amino-1,2,4-triazole, gap values and other related calculations	B3LYP	M062X
Zero Point Energies (a.u.)	-297.627	-297.506
$E_{HOMO}$ (eV)	-8.834	-8.880
$E_{LUMO}$ (eV)	-3.936	-3.911
Energy Gap (eV)	4.897	4.969
Ionization potential (I)	8.834	8.880
Electron affinity (A)	3.936	3.911
$\mu$	2.449	2.485
$\alpha$	-6.385	-6.396
$\beta$	8.325	8.232
$\gamma$	0.408	0.403
Dipol moment (debye)	2.060	2.286

### 3.4 Molecular Electrostatic Potential (MEP) Analysis

Molecular electrostatic potential (MEP) gives information about the net electrostatic effect of the molecule. The electrophilic and nucleophilic attacks for the investigated molecule were predicted by the help of MEP. The MEP was computed by the above mentioned two methods and same levels and demonstrated in Figure 7 and 8. Figure 7 shows that the negative charge covers over the N4 atom within the triazole group, and the positive plot is over the H2, H3 atoms and partially over the N group in B3LYP method. In MO62X method the negative region (yellow color) is over the N6, N4 atoms and partially over the N group whereas the positive region (blue color) has been distributed over the H3, H2 atoms. The negative regions are responsible for electrophilic attack while, the positive regions are responsible for nucleophilic attack.

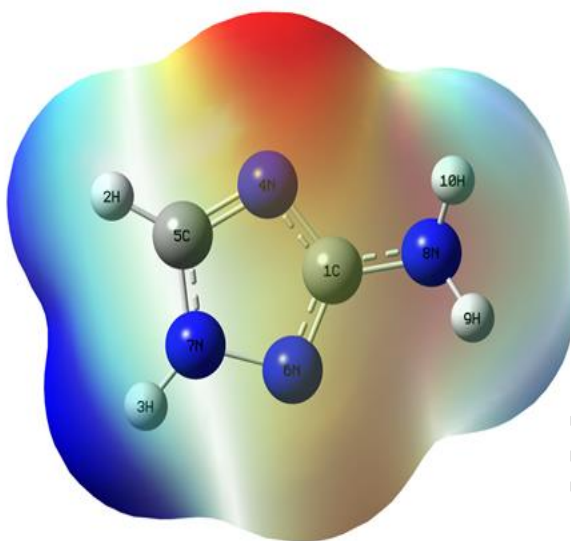


Figure 7: MEP plot of amino-1,2,4-triazole with B3LYP.

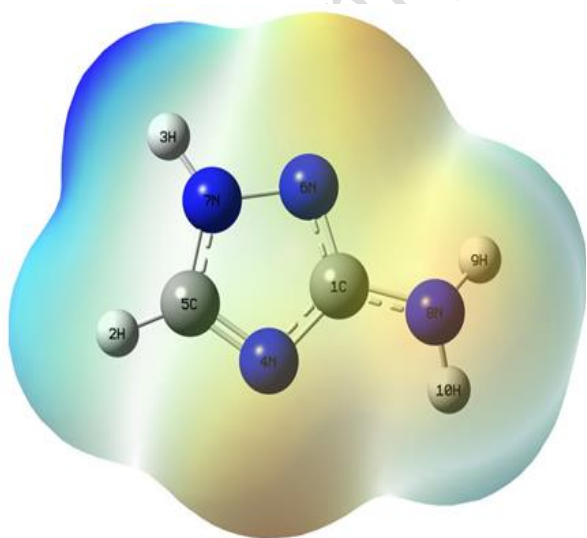


Figure 8: MEP plot of amino-1,2,4-triazole with MO62X.

### 4 Conclusion

The optimized structure, vibrational analyses, HOMO orbitals, dipole moment values and MEP analysis of our title compound have been computed and examined with the B3LYP and MO62X methods and 3-11++G(d,p) basis set. We have used Gaussian 09W program for all the calculations. For the theoretical frequencies, exact vibration movements have been done by using PED% analysis. It has also been seen that B3LYP method is superior to MO62X method for the both frequency analysis and bond lengths, but for the angles MO62X method is marginally seen to be closer to the data obtained experimentally. The HOMO graphics and gap values explain the eventual charge transfer interaction taking place within the molecule. Also, MEP analysis has been done in order to clarify studied molecule. When these obtained theoretical and experimental results are taken into account; we can say that the investigated compound is very inviting matter for both next medicinal and pharmacological applications.

### 5 Acknowledgment

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