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Molecular structure, vibrational analysis and electronic properties of 5-amino-1, 3, 4-thiadiazol-2(3h)-one using density functional theory

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ABSTRACT

This work is devoted to theoretical study on molecular structure of 5-amino-1, 3, 4-thiadiazol-2(3H)-one. The equilibrium geometry, harmonic vibrational frequencies and infrared intensities were calculated by density functional B3LYP methods with the 6-31 G (d, p) basis set. A detailed interpretation of the infrared spectra of 5-amino-1, 3, 4-thiadiazol-2(3H)-one is reported. The thermodynamic functions of the title compound were also performed at B3LYP/6-31 G (d) level of theory. The molecular HOMO, LUMO composition, energy gap, and MESP contours have also been drawn to explain the activity of 5-amino-1, 3, 4-thiadiazol-2(3H)-one.

Keywords: 5-amino-1, 3, 4-thiadiazol-2(3H)-one, molecular structure, vibrational spectra, Electronic properties.

INTRODUCTION

Five membered heterocyclic compounds show various types of biological activity among them 2,5-disubstituted 1,3,4-thiadiazoles are associated with diverse biological activity probably virtue of –N=C-S- grouping. Therapeutic importance of these rings prompted us to develop selective molecules in which substituent could be arranged in a pharmacophoric pattern to display higher pharmacological activities. Thiadiazoles have occupied an important place in drug industry, 1,3,4-thiadiazoles have wide applications in many fields. Earliest uses were in the pharmaceutical area as an antibacterial with known sulphonamides drugs. Some of other uses are antitumor, antiinflammtory, pesticides, dyes, lubricants, and analytical reagents [3]. 1,3,4 thiadiazole derivatives posses interesting biological activity probably conferred to them due to strong aromaticity of the ring system which leads to great in vivo stability and generally, a lack of toxicity for higher vertebrates, including humans when diverse functional group that interact with biological receptor are attached to aromatic ring [4]. Approach to practice of medicinal chemistry has developed from an empirical one involving synthesis of new organic compounds based on modification of chemical compounds of known biological activities could be better explored. It is well established that slight alteration in the structure of certain compounds are able to bring drastic changes to yield better drug with less toxicity to the host it observed that chemical modification not only alters physiochemical properties but also pharmacological properties [5]. The thiadiazoles have occupied an important place in drug industry. 1,3,4-Thiadiazoles have wide applications in many fields. The earliest uses were in the pharmaceutical area as an antibacterial with known sulphonamides drugs. Some of the later uses are as antitumor and anti-inflammatory agents, pesticides, dyes, lubricants and analytical reagents. 1,3,4-Thiadiazole and its derivatives possess wide range of activities anticonvulsant [6],

herbicidal [7], pesticidal [8], amoebicidal [9], CNS depressant [10] antibacterial [11], antiviral [12]. In continuation of our work on benzo[b]thiophene nucleus [13], it was contemplated to synthesize some new 1,3,4-thiadiazoles derivatives bearing benzo[b]thiophene moiety. In recent years 1, 3, 4-Thiadiazole derivatives have received significant attention and have been increasingly investigated due to their diverse range of biological properties. They exhibit for example, antimicrobial [14, 15], anti-micro bacteria [16], anticancer [17], anti-inflammatory [18,19], carbonic anhydrase inhibiting effect [20], antanxiety, anti-depressant [21], anti-oxidant properties [22],. 1,3,4-Thiadiazole exhibit diverse biological activities, possibly due the present of =N-C-S moiety [23]. 1, 3, 4-Thiadiazole are very interesting compounds due to their important applications in many pharmaceutical biological and analytical fields [24, 25].

As a part of our ongoing research [26-33], the main objective of the present study is to investigate in detail the vibrational spectra of important biological molecule 5-amino-1, 3, 4-thiadiazol-2(3H)-one. To the best of our knowledge no detailed DFT calculations have been performed on 5-amino-1, 3, 4-thiadiazol-2(3H)-one so far in the literature.

MATERIALS AND METHODS

Computational Methods

Initial geometry was generated from standard geometrical parameters and was minimized without any constraint in the potential energy surface. The gradient corrected Density Functional Theory (DFT) with the three-parameter hybrid functional (B3) [34] for the exchange part and the Lee-Yang-Parr (LYP) correlation function [35] has been employed for the computation of molecular structure, vibrational frequencies, HOMO-LUMO, and energies of the optimized structures, using GAUSSIAN 09 [36]. The calculated vibrational frequencies have also been scaled by a factor of 0.963 [37]. By combining the results of the GAUSSVIEW'S program [38] with symmetry considerations, vibrational frequency assignments were made with a high degree of accuracy. We used this approach for the prediction of IR frequencies of title compound and found it to be very straightforward. Density functional theory calculations are reported to provide excellent vibrational frequencies of organic compound if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation, for basis set deficiencies and for anhormonicity. A number of studies [39, 40] have been carried out regarding calculations of vibrational spectra by using B3LYP methods with 6-311 G (d, p) basis set. The scaling factor (0.963) was applied successfully for B3LYP method and was found to be easily transferable in a number of molecules. Thus vibrational frequencies calculated by using the B3LYP functional with 6-311G (d, p) as basis set, can be utilized to eliminate the uncertainties in the fundamental assignment in the IR spectra.

RESULTS AND DISCUSSION

Optimization

The optimized Structure parameters of monoclinic polymorph of 5-amino-1,3,4-thiadiazol-2(3H)-one calculated by B3LYP method with the 6-31G (d, p) basis set are listed in Table 1 and are in accordance with the atom numbering scheme as shown in Figure 1, respectively. After geometry optimization local minimum energy obtained for structured optimization of monoclinic polymorph of 5-amino-1, 3, 4-thiadiazol-2(3H)-one with 6-31G (d, p) basis set is approximately -715.68034855 (a.u.) for B3LYP method. The optimized bond parameters of molecule calculated by various methods are listed in Table 1.

The (C-N) bond length varies between the values 1.3675Å- 1.2933Å, while (C-S) bond length varies between 1.8429Å- 1.7705Å. (N-H) bond length varies between 1.0135Å- 1.0092Å while (N-N) bond length is at 1.379 Å whereas (C-O) bond length is at 1.2079 Å. The (C-N-N) bond angle varies from 109.7357- 122.8579 while (C-N-H) varies between 112.4368- 121.0234. The (S-C-N) bond angle varies between 104.6991- 116.2412. All the calculated bond lengths and bond angles are in good agreement with experimental data as given in Table 1.

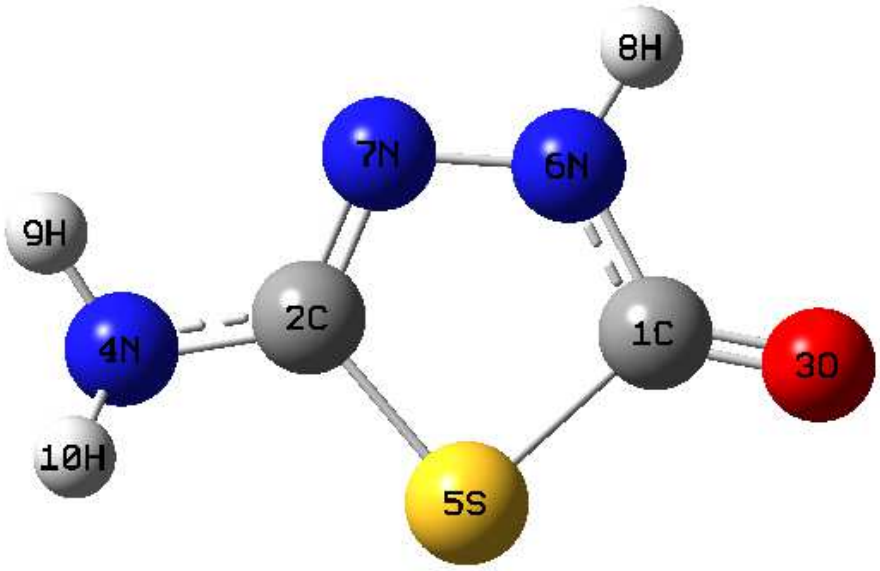

Figure 1:- Model molecular structure of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

TABLE-1 Bond Length (Å) and Bond Angle of monoclinic polymorph of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

S.NO.	PARAMETER	EXPERIMENTAL VALUE	CALCULATED VALUE
"BOND LENGTH"			
1.	C_1-O_3	1.226	1.2079
2.	C_1-S_5	1.786	1.8429
3.	C_1-N_6	1.328	1.3675
4.	C_2-N_4	1.357	1.3782
5.	C_2-S_5	1.749	1.7705
6.	C_2-N_7	1.289	1.2933
7.	N_4-H_9	0.86	1.0135
8.	N_4-H_{10}	0.85	1.0116
9.	N_6-N_7	1.328	1.379
10.	N_6-H_8	0.77	1.0092
"BOND ANGLE"			
11.	O_3-C_1-S_5	125.5	126.8263
12.	O_3-C_1-N_6	127.9	128.4734
13.	S_5-C_1-N_6	106.5	104.6991
14.	N_4-C_2-S_5	121.2	120.7637
15.	N_4-C_2-N_7	123.6	122.8579
16.	S_5-C_2-N_7	115.1	116.2412
17.	C_2-N_4-H_9	116	112.4368
18.	C_2-N_4-H_{10}	117	115.4455
19.	H_9-N_4-H_{10}	113	112.90662
20.	C_1-S_5-C_2	88.81	88.3673
21.	C_1-N_6-N_7	120.0	120.8964
22.	C_1-N_6-H_8	123	121.0234
23.	N_7-N_6-H_8	115	117.9376
24.	C_2-N_7-N_6	109.5	109.7357

Atomic charge, Polarizability, Hyper polarizability and Thermodynamic Properties:
The Mulliken atomic charges for all the atoms of the 5-amino-1, 3, 4-thiadiazol-2(3H)-one is calculated by B3LYP method with 6-311G (d, p) as basis set in gas phase and are presented in Table 2.

Dipole moment (μ), polarizibility <α> and total first static hyperpolarizlbility β [41, 42] are also calculated (In Tables 2 and 3) by using density functional theory. They can be expressed in terms of *x*, *y*, *z* components and are given by following equations 1, 2 and 3-

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1\backslash 2} \text{---------- (1)}$$

$$<\alpha> = 1\backslash 3\ [\alpha_{xx} + \alpha_{yy} + \alpha_{zz}] \text{ ---------- (2)}$$

$$\beta_{Total} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1\backslash 2}$$

$$= [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1\backslash 2} \text{--- (3)}$$

The β components of Gaussian output are reported in atomic units.
Where (1 a.u. = $8.3693X10^{-33}$ e.s.u.). For 5-amino-1,3,4-thiadiazol-2(3H)-one the calculated dipole moment value is 3.8533Debye. Having higher dipole moment than water (2.16 Debye), 5-amino-1, 3, 4-thiadiazol-2(3H)-one can be used as better solvent. As we see a greater contribution of α_{ZZ} in molecule which shows that molecule is elongated more towards Z direction and more contracted to Y direction. $\beta_{xxx,}$ β_{xxz} contribute larger part of hyperpolarizibity in the molecule. This shows that X-axis and XZ plane are more optical active in these directions.

TABLE-2 Mulliken Atomic Charges of monoclinic polymorph of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

S.NO.	ATOM	ATOMIC CHARGE
1.	C	0.431057
2.	C	0.277697
3.	O	-0.478149
4.	N	-0.051380
5.	S	0.173700
6.	N	-0.049685
7.	N	-0.303240
8.	H	0.000000
9.	H	0.000000
10.	H	0.000000

TABLE-3 Polarizibility and Hyper Polarizibility of monoclinic polymorph of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

S.NO.	PARAMETER	POLARIZIBILITY
1.	α_{XX}	-45.1614
2.	α_{YY}	-43.4805
3.	α_{ZZ}	-47.7019
4.	α_{XY}	5.0227
5.	α_{XZ}	-3.3814
6.	α_{YZ}	-0.6958
α		45.4479
S.NO.	**PARAMETER**	**HYPER POLARIZIBILITY**
1.	β_{XXX}	-51.5364
2.	β_{YYY}	7.7329
3.	β_{ZZZ}	1.0103
4.	β_{XYY}	7.4505
5.	β_{XXY}	7.4223
6.	β_{XXZ}	9.9528
7.	β_{XZZ}	3.1487
8.	β_{YZZ}	0.8944
9.	β_{YYZ}	0.8309
10.	β_{XYZ}	2.4082
β		45.5251

Several calculated thermodynamic properties based on the vibrational analysis at B3LYP and 6-311G (d, p) level, like internal thermal energy (E), constant volume heat capacity (C_v), and entropy (S), have been calculated and listed in Table 4. At the room temperature, conduction band is almost empty so electronic contribution in total energy negligible. Thermodynamic parameters clearly indicate that vibration motion plays a crucial role in assessing

thermodynamical behavior of title compounds. The calculated dipole moments at B3LYP/6-311G (d, p) level are 6.6832 for 5-amino-1, 3, 4-thiadiazol-2(3H)-one.

TABLE-4 Thermodynamic Properties Of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

PARAMETER	E (KCal/Mol)	CV (Cal/Mol-Kelvin)	S (Cal/Mol-Kelvin)
Total	44.954	23.460	79.752
Translational	0.889	2.981	40.186
Rotational	0.889	2.981	27.563
Vibrational	43.176	17.498	12.003

Electronic properties

The interaction with other species in a chemical system is also determined by frontier orbitals, HOMO and LUMO. It can also be determined by experimental data. The frontier orbital gape helps to distinguish the chemical reactivity and kinetic stability of the molecule. A molecule which has a larger orbital gape is more polarized having reactive part as far as reaction is concerted [43]. The frontier orbital gape in case of the given molecule is 4.505 eV for 5-amino-1, 3, 4-thiadiazol-2(3H)-one given in Table 5.

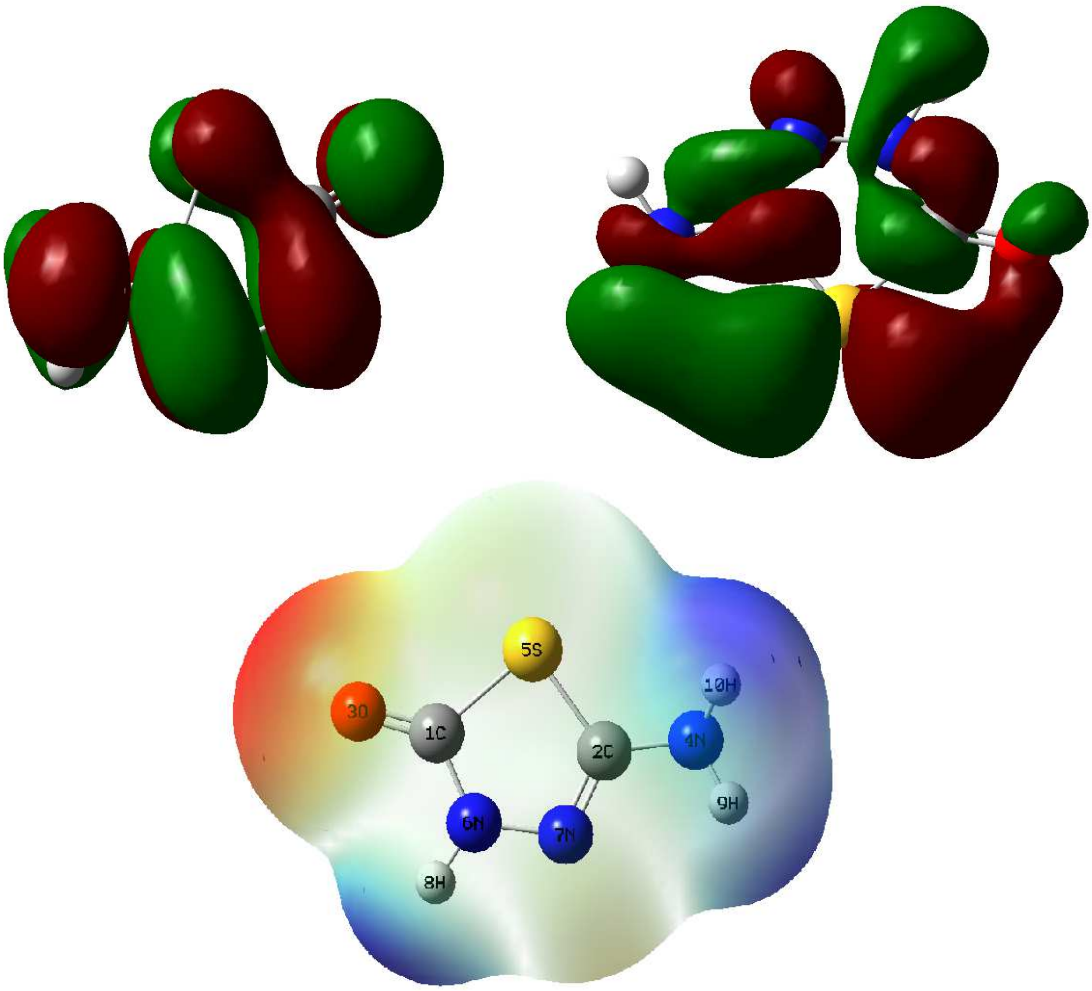

Figure 2. HOMO (Left) - LUMO (Right) and MESP (Below) pictures of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

The contour plots of the HOMO, LUMO and MESP structures of the molecules are shown in Figure 2. The importance of MESP lies in the fact that it simultaneously displays molecular size, shape as well as positive, negative, and neutral electrostatic potential region in terms of grading and is very useful in the investigation of molecular structure with its physiochemical property relationship [44, 45]

TABLE-5 Total Energy, Homo, Lumo, Energy Gap and Dipole Moment Of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

S.NO.	PARAMETER	VALUE
1.	Total Energy E (a.u.)	-715.68034855
2.	Homo	-0.22312
3.	Lumo	-0.05747
4.	Frontier Orbital Energy Gap	-0.16565 (4.50568 ev)
5.	Dipole Moment	3.8533

Assignment of fundamentals

5-amino-1,3,4-thiadiazol-2(3H)-one has 21 atoms 57 normal modes of vibration. We made a reliable one-to-one correspondence between the fundamentals and the frequencies calculated by DFT (B3LYP). The relative band intensities are also very satisfactory along with their positions. Some important modes are discussed hereafter.

Vibrational modes description

Spectral region above 2800 cm^{-1}: N-H stretching vibrations are generally observed in the region 3200-3500 cm^{-1}. Accordingly, in the present study for 5-amino-1,3,4-thiadiazol-2(3H)-one the N-H stretching vibrations are calculated at 1775,3411,3516 and 3520 cm^{-1}, respectively.

TABLE-6 Calculated Wave Numbers and its respective I.R. Intensity of monoclinic polymorph of 5-amino-1, 3, 4-thiadiazol-2(3H)-one

S.NO.	FREQUENCY	I.R. INTENSITY	VIBRATIONAL ASSIGNMENT
1.	117	2.4039	γ (N_4-H_{10})
2.	262	20.868	Twist (NH_2)
3.	300	26.7095	Twist (NH_2)
4.	313	5.1974	Twist(NH_2) + Twist (C_1-O_3)
5.	411	2.2721	Twist in whole ring
6.	446	464.6248	ω(N_6-H_8)
7.	495	5.2282	Deformation of ring
8.	535	48.065	Twist NH_2
9.	592	21.7835	Twist (H_{10}-N_4-H_9)+ τ(O_3-C_1-N_6)
10.	594	46.4155	τ (O_3-C_1-N_6-H_8)
11.	633	181.1654	Twist (H_9-N_4-H_{10})+Slightly breathing of ring
12.	656	80.7017	Breathing of ring
13.	758	9.205	τ Of Whole Ring
14.	1012	56.3443	Twist(H_9-N_4-H_{10})
15.	1128	24.834	β(C_1-N_6-H_8)
16.	1175	17.619	Twist NH_2
17.	1290	135.9362	Twist(N_4-H_9) + ω(N_6-H_8)
18.	1369	3.4956	ω(N_6-H_8)
19.	1562	23.6356	S(H_9-N_4-H_{10})
20.	1612	236.5154	S(H_9-N_4-H_{10}) + υ(N_7-C_2)
21.	1775	517.5488	υ(C_1-O_3)
22.	3411	29.0324	υ(N_9-H_{10})
23.	3516	68.178	υ(N_6-H_8)
24.	3520	33.241	υ(N_9-H_{10})

Abbreviations: ν: Stretching; β: -in plane bending; γ: out of plane bending, τ: torsion, GƆ: wagging, S: scissoring

Spectral region from 1000 cm^{-1} to 2300 cm^{-1}: N-H wagging vibrations are generally observed in the region 1210, 1249, 1259, 1397 cm^{-1}.In plane (β) vibration form in the region 1128 cm^{-1}. In region 495 cm^{-1} the whole ring deformed.

Spectral region below 1000 cm^{-1}: Ring Torsion shown in the region 758 cm^{-1} while Twisting in N-H bond is shown in 262 cm^{-1}, 300 cm^{-1}, 313 cm^{-1}, 592 cm^{-1}, 633 cm^{-1}.

CONCLUSION

Equilibrium geometries and harmonic frequencies of 5-amino-1, 3, 4-thiadiazol-2(3H)-one were determined and analyzed at DFT/B3LYP level of theory using 6-311G (d, p) basis set. The vibrational frequency calculations proved that the structure is stable (no imaginary frequencies). We found the geometry obtained by the B3LYP method to be very accurate. Electronic properties show the reactivity of molecule with the help of HOMO-LUMO gap. Hyperpolarizability is mainly controlled by the planarity of the molecules, the donor and accepter strength, and bond length alteration. The values of hyperpolarizability indicate a possible use of these compounds in electrooptical applications. The present work might encourage the need for an extensive study by the experimentalists interested in the vibrational spectra and the structure of this compound.

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Conflict of interest
The authors declare that there is no conflict of interests regarding the publication of this paper. Also, we declare that this paper or part of it has not been published elsewhere.

Contribution of the authors
Dr. Apoorva Dwivedi and Dr. Anoop Kumar Pandey both designed data collection tools, monitored data collection for the whole trial, wrote the statistical analysis plan, cleaned and analysed the data, and drafted and revised the paper. Mukesh Kumar Niyal drafted and revised the paper. All authors read and approved the final version that is send for publication.

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Appendix

5-amino-1, 3, 4-thiadiazol-2(3H)-one

	x	*y*	*z*
S1	0.5670 (2)	0.33458 (7)	0.36148 (3)
C2	0.4389 (8)	0.4860 (3)	0.33723 (13)
N3	0.5448 (8)	0.5631 (3)	0.38116 (12)
H3	0.487 (9)	0.631 (3)	0.3829 (14)
N4	0.7091 (7)	0.5177 (2)	0.43328 (11)
C5	0.7362 (8)	0.3992 (3)	0.42932 (13)
O6	0.2779 (7)	0.5107 (2)	0.28964 (10)
N7	0.8708 (8)	0.3270 (3)	0.47486 (13)
H7A	0.968 (9)	0.259 (3)	0.4641 (14)
H7B	0.983 (10)	0.364 (3)	0.5033 (17)
S8	0.0629 (2)	1.02405 (7)	0.34352 (4)
C9	0.2461 (8)	1.0171 (3)	0.41853 (13)
N10	0.3361 (7)	0.9003 (2)	0.42943 (12)
H10	0.438 (8)	0.884 (3)	0.4630 (14)
N11	0.2747 (8)	0.8126 (2)	0.38422 (11)
C12	0.1325 (8)	0.8645 (3)	0.33686 (13)
O13	0.2843 (7)	1.1052 (2)	0.45367 (10)
N14	0.0397 (10)	0.8045 (4)	0.28504 (14)
H14A	−0.052 (11)	0.853 (4)	0.2546 (19)
H14B	0.074 (10)	0.738 (4)	0.2852 (17)

$$x = a\,x_{frac} + c\,z_{frac}\,\cos(\beta)$$
$$y = b\,y_{frac}$$
$$z = c\,v\,z_{frac} = c\,z_{frac}\,\sin(\beta)$$

We have directly modeled the molecule with help of Gauss View software. We are providing the fractional coordinates of the title molecule and formula of conversion of fractional coordinates to Cartesian coordinates