

Synthesis, X-Ray Characterization, IR Vibrational Frequencies, NMR Chemical Shifts And DFT Properties Of 2,7-Dimethyl-2,7-Dicyanide-3,6-Diazaoctane



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Abstract: In our research work, we have synthesized 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane and confirmed its structure by using X-ray diffraction and spectrometric experiments. The experimentally obtained results were compared with theoretically results. The electronic properties of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane have been analyzed by DFT. The energy band gap is computed at -1.800349 eV for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane shows that this molecular structure is lower kinetic stability and more reactivity. Molecular electrostatic potential map of electron density on an isosurface of electrostatic potential for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane indicates electron rich reactive sites were located over nitrogen (N≡C) atoms belong cyanide groups. Our research results will be important for syntheses new α-aminonitriles organic compounds and calculate theoretical properties of them.

Keywords: α-amino nitriles, Density Functional Theory, frequency, molecular orbitals, electrostatic potential

I. INTRODUCTION

Different types of α-aminonitriles are important part of organic syntheses chemistry. They are influence on the synthesis of α-aminonitriles derivate like pharmacological chemicals, amino acids, agrochemical agents, plant protectors and pesticides [1].

The using α-amino nitriles in agriculture give many opportunities: they can protect plants from some diseases and aggressive environment impact; they are one of the most important agro-industrial methods for increasing the yield of agricultural crops; these chemicals contribute to increase plant resistance ability to disease and unfavorable conditions,

early ripening of the crop; they increase yield and the production of a higher-grade product [2-3]. Our synthesized α-amino nitrile [2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane] has several reaction centers in their molecule [nitrile, amino and activated methylene groups, as well as (3-carbon atoms (CN), which can gives good positions for various chemical transformations; aldehydes, ketones, nitrocompounds and ethers can react with 3-carbon atoms (CN) through aldol-croton condensation reaction; amino groups (NH) in these molecules are reaction center for nucleophile change, N-alkalization and -acylation reactions; they can easily hydrolysis to carbon acids. They are good biological active because they have hydrophilic (NH, CN, CH₃) and hydrophobic (CH₃) functional groups (Fig.1) [4-6].

II. EXPERIMENTAL SECTION

A. Materials and Methods

Nuclear magnetic resonance spectral results were calculated in internal standard of deuterated methanol (CD₃OD) and hexamethyldisilane (HMDS), and on a δ scale. Nuclear magnetic resonance spectral results were calculated on a JNM-4H-100 Varian Unity 400 (+). Infra-red (IR) spectra are recorded in Fourier spectrometer 2000 spectrometer (Perkin Elmer) using KBr pressed disks. The Optical Excalibur bench contains a interferometer (it is piezoelectric aligned dynamically), far-, mid- and near-infrared ranges, dual internal detector and sources, four Raman ports, emission and external beams, and a host of accessories. Mass spectra are recorded in MX-1303 [7-8].

B. Syntheses of 2,7-dimethyl-2,7-dicyanide-3,6-diaza-octane

To the flat-bottomed flask fitted with magnetic stirrer, poured the solution of 0.058 mmol ethylene diamine in 30 ml benzene, and at stirring 5.5 ml (0.058 mol, 5.0 g) acetone cyanohydrin dropwise mixed at room temperature for 2-2.5 hour. In further first solvent, then the product o the reaction of distilled under vacuum.

6.6 g (89%) product of the reaction was obtained, mp = 53-55°C, R_f=0.50 (benzene (2): acetone(1) IR- spectra: ν_{CN} 2220 cm⁻¹, ν_{NH} 2988 cm⁻¹, ¹H NMR-spectrum (8, m.d.) 1.40 (s, 6H, -(CH₃)₂), 2.74 (m, 4H, N-CH₂ CH₂ -N).

Revised Manuscript Received on January 30, 2020.

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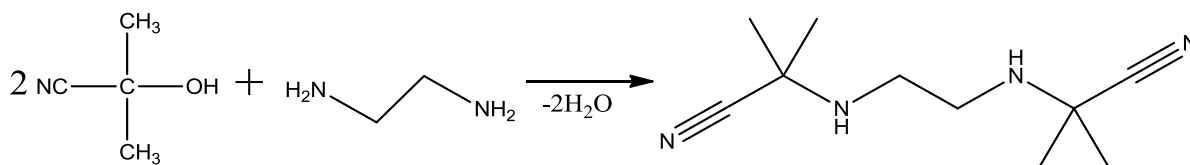


Fig.1. 2,7-Dimethyl-2,7-dicyanide-3,6-diazaoctane

C. X-ray Apparatus Properties

0.60 × 0.50 × 0.05 mm of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane single crystal dimension was selected for X-ray analysis (Oxford Diffraction). X-ray results dates were computed at 300 K. We used Xcalibur Ruby (CCD) diffractometer. CrystalClear was used in order to obtain complete date. The structure of single crystal of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane was solved with theoretical methods and cleared on SHELXS (XL)-97 software. On the beginning, whole non-hydrogen atoms were appeared. Whole hydrogen atoms are geometrical positioned and refined through a riding model. The lastly distinction Fourier map revealed the peaks of no chemical significance after ten cycles of refinement [9].

SADABS program was used for absorption correction. In same diffractometer it was obtained three-dimensional datasets for reflections.

D. Computational Methods

The synthesized 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane is theoretically investigated in the details for contrasting investigation to experimentally measured results of X-ray analysis, NMR (^{13}C , ^1H), FT-IR analyses. NMR ^{15}N chemical shifts were theoretically computed. In this research work the contemporary DFT calculations was used. During DFT calculation analysis we have used B3LYP method that it was used in many research works because our synthesized organic compound is large molecule and has many different heterogenic atoms like nitrogen atoms. Before calculation the synthesized 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane is optimized. It was used 6-311G (d, p) for calculation theoretically properties of synthesized 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. In some compute results we have used large 6-311+G(2d,p) because especially NMR theoretically calculation require large basis sets. In IR spectroscopic calculation the vibrational frequencies were scaled on 0.9587. 2,7-Dimethyl-2,7-dicyanide-3,6-diazaoctane was optimized with tetramethylsilane in NMR calculation. In this theoretically calculation we have computed Frontier molecular orbital and Molecular electrostatic potential properties of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. During this calculation it was used large 6-311G (d, p) basis sets [10].

III. RESULTS AND DISCUSSION

A. X-ray Analysis

In our experiments, it was studied the stereochemical properties of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane by X-rays diffraction analysis. Although, according to the schematic representation of the molecule, symmetric geometry is expected, the geometry of the molecule in the

current crystal structure is not symmetric. Nitrogen atoms of the amino group in the molecule are sp^3 hybrid mode; their configurations are mutually mirror-like to each other (Fig. 2). C-N type bonds of N3-C5 (1.141) Å and N4-C6 (1.135) Å are shorter than other C-N type bonds because C5 and C6 atoms are sp hybrid mode so they are stronger than others. Next relatively shorter C-N bonds are N1-C3 (1.456) Å and N2-C4 (1.455) Å. According to C-C type bonds C3-C9 (1.536) Å and C3-C7 (1.26) Å, thus they lower bond broken energy.

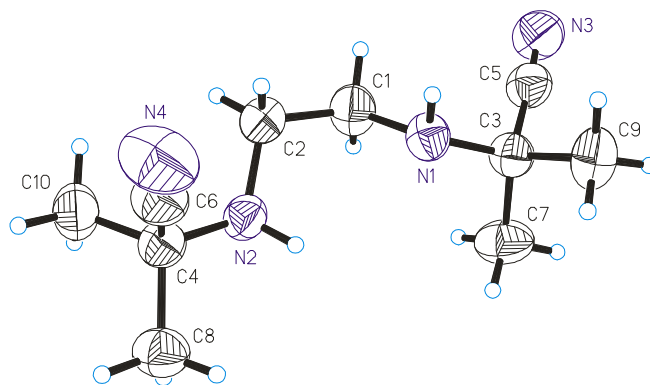


Fig. 1. X-ray molecular structure of
2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

Analysis of intermolecular interactions shows that in the crystal by means of NH...NC-type hydrogen bonds symmetric dimers are formed (Fig. 3).

Table I show that X-ray parameters for crystal of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. The crystals of compound (2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane) is triclinic. At 291 K $a=6.2967$ (14) Å, $b=9.8331$ (16) Å, $c=10.328$ (3) Å, $\alpha=92.539$ (16)°, $\beta=104.90$ (2)°, $\gamma=93.824$ (15)°, $V=615.3$ (3) Å³, $M_r=194.28$, $Z=2$, space group P-1, $T_{\min}=0.576$, $T_{\max}=1.000$, $\mu=0.52$ (mm⁻¹) Intensities of reflections were calculated on the "Xcalibur, Ruby" diffractometer (CuK α Radiation).

The structure of single crystal of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane was solved with theoretical methods and cleared on SHELXS (XL)-97 software. In X-ray analysis it was found that the positions of H atoms which are bonded with carbon atoms in 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. Next these positions of H atoms were refined through $U_{\text{iso}} = nU_{\text{eq}}$. In these parameterizes, U_{iso} is isotropic segment, $n=1.5$ (methyl bounded hydrogen) and $n=1.2$ (nitrogen bounded hydrogen) are coefficient for different type hydrogen atoms. U_{eq} is equivalent isotropic segment, meaning that it can characterize carbon atoms. Full-matrix least-squares refinement of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane structure for non-hydrogen atoms using 2450 reflection was changed to: $R[F^2 > 2\sigma(F^2)] = 0.056$,

$wR(F^2)=0.150$, $S=0.96$. $\Delta\rho_{\max}$ ($e \text{ \AA}^{-3}$) = 0.12 and $\Delta\rho_{\min}$ ($e \text{ \AA}^{-3}$) = -0.14 measured (Tab.1).

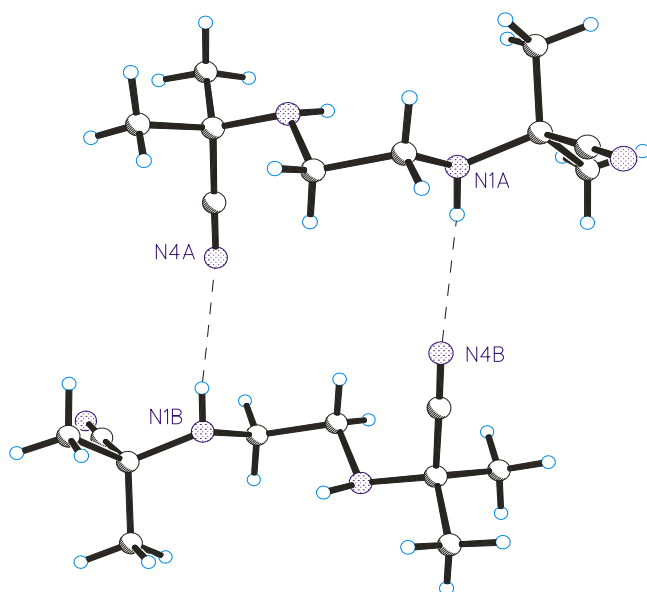


Fig. 2. Inter-molecular hydrogen bonding of molecular structure of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

**Table-I. X-ray analysis properties
2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane**

Chemical formula	C ₁₀ H ₁₈ N ₄
M_r	194.28
Crystal system, space group	Triclinic, <i>P</i> -1
Temperature (K)	291
a, b, c (Å)	6.2967 (14), 9.8331 (16), 10.328 (3)
α, β, γ (°)	92.539 (16), 104.90 (2), 93.824 (15)
V (Å ³)	615.3 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	0.52
Crystal size (mm)	0.60 × 0.50 × 0.05
Data collection	
Diffractometer	Xcalibur, Ruby diffractometer
Absorption correction	Multi-scan, <i>CrysAlis PRO</i> (Oxford Diffraction Ltd., 2009)
T_{\min}, T_{\max}	0.576, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3993, 2450, 1251
R_{int}	0.050
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.150, 0.96
No. of reflections	2450
No. of parameters	140
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($e \text{ \AA}^{-3}$)	0.12, -0.14

B. IR Vibration and NMR Chemical Shifts

The experimentally frequencies of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane (Fig.4) were contrasted theoretically frequencies of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane (Fig.5).

The experimentally and theoretically measured infra-red frequency of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane are listed in Table II. It was shown from this table the

experimentally observed infra-red frequencies were noticeable differ from theoretically calculated infra-red frequencies. There are some factors related to these difference: the initial factor is environment, means that B3LYP/6-311G (d,p) compute methods can calculate vibrational frequencies in gaseous phase with compared to experimental method calculations are carried out in solid phase. Next important factor is that experimental frequency measures were carried out in the limit of the harmonic approximation. However, in theoretically methods the calculated wave number were leveled down by using scaling factor 0.9587 to neglect the anharmonicity present in the real system.

The chemical structure of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane was characterized by IR vibrations: the bands 2220 cm⁻¹ and 2988 cm⁻¹ were reported symmetric stretching for respectively CN and NH functional groups in experimentally way. In contrast to theoretically these values were relatively 2351 cm⁻¹ and 2933 cm⁻¹. The asymmetric stretching frequencies of CH₃ and CH₂ reported in respectively 2942 cm⁻¹ and 2853 cm⁻¹ in experimentally way. The asymmetric stretching frequencies of CH₃ and CH₂ observed experimentally calculated at 2939 cm⁻¹ and 2933 cm⁻¹. The experimentally stretching frequencies of C-C bonds were viewed at 1464-1627 cm⁻¹ spectra ranges, in B3LYP/6-311G(d,p) compute methods these frequencies appear in the region between 1485 cm⁻¹ and 1526 cm⁻¹.

The theoretical ¹H, ¹⁴N and ¹³C NMR (ppm) spectra for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane were calculated by DFT on fully geometry optimization of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane (Fig. 6). These spectra were presented in Fig. 7, 8 and 9. The calculated chemical shifts were presented in Tables III, IV and V. The position and number of H, N and C atoms displayed on Fig.6.

In obtained spectra of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane 16H, 17H, 18H and 19 number protons NMR signals were calculated at 2.44 ppm because neighbor electrodonor 1N and 4N nitrogen atoms share them unpaired electrons to these protons located carbon atoms. At lowest point is 0.44 ppm was computed for 15H and 20 H, the reason that they directly bonded electronegative 1N and 4N atoms which can change shift to downfield area. On the other hand, another CH₃ (sp³) proton atoms located in nearly same positions and directly linked C (sp³) atoms which were not electronic withdraw substituents group and cannot impact on proton shift change.

¹³C NMR peaks values depend on carbon atom positions in a different environment. The theoretically chemical shifts of 7C and 8C atoms were

calculated at 124.25 ppm because 7C and 8C carbon atoms linked electronegative nitrogen atoms which can alter ¹³C NMR peaks to upward trend. ¹³C NMR peaks values for 5 and 6 number carbon atoms were measured at 53.06 ppm the reason that they connected with 2CH₃ and CN functional groups which can change NMR shifts to downsides. To contrast 2C and 3C atoms directly connected CH₃ and NH groups, these functional groups also change chemical shifts to 45.25 ppm.

Lastly, 9C, 10C, 11C and 12C atoms were located same position so their chemical shifts were locate at 10-25 ppm.

^{15}N NMR chemical shifts for 1N and 4N atoms were calculated at 71 ppm. These nitrogen atoms with direct linked CH_2 and $\text{CR}_3(\text{R}=\text{CH}_3)$ functional groups which were

electrodonor groups and low electronegative atoms, and change chemical shifts of 1N and 4N atoms to downsides. On the other sides, 13N and 14N atoms with connect sp hybrid C atoms, means that this positions of 13N and 14N atoms are reason for peaks at 288.27 ppm.

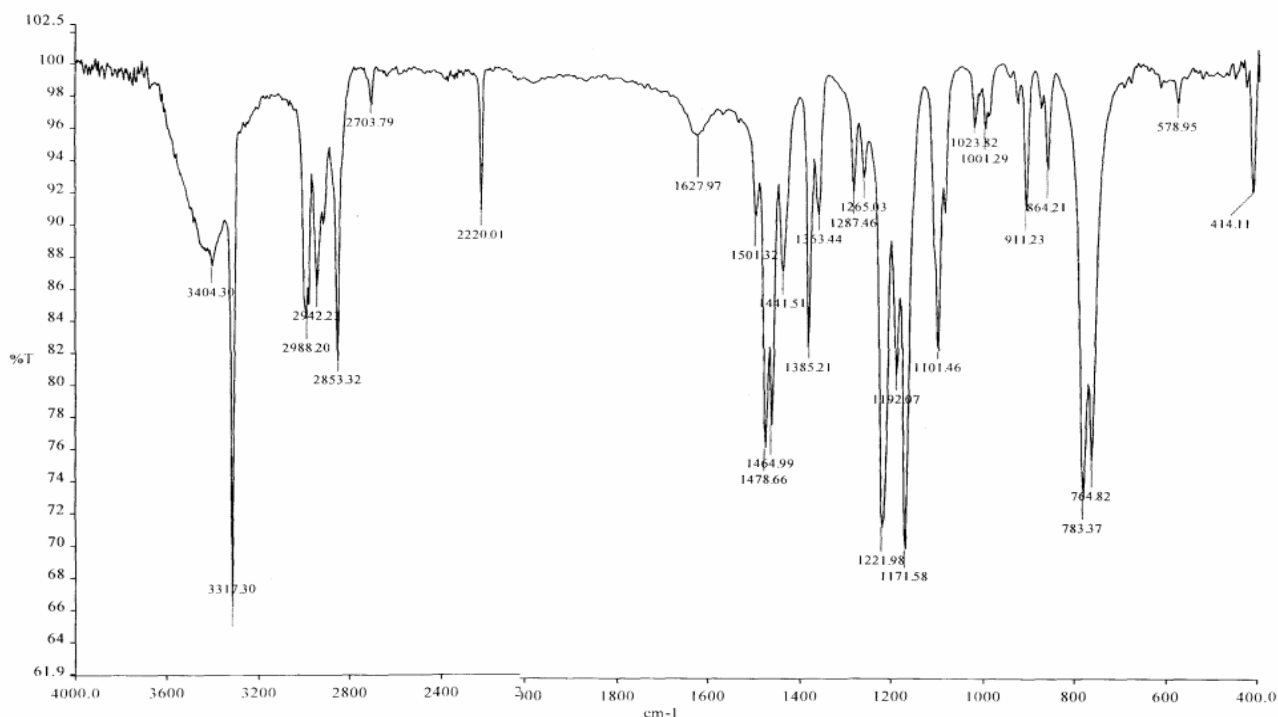


Fig. 4. Experimental vibrational frequencies (cm^{-1}) of 2,2'-(ethane-1,2-diylbis(azanediyl))bis(2-methylpropanenitrile)

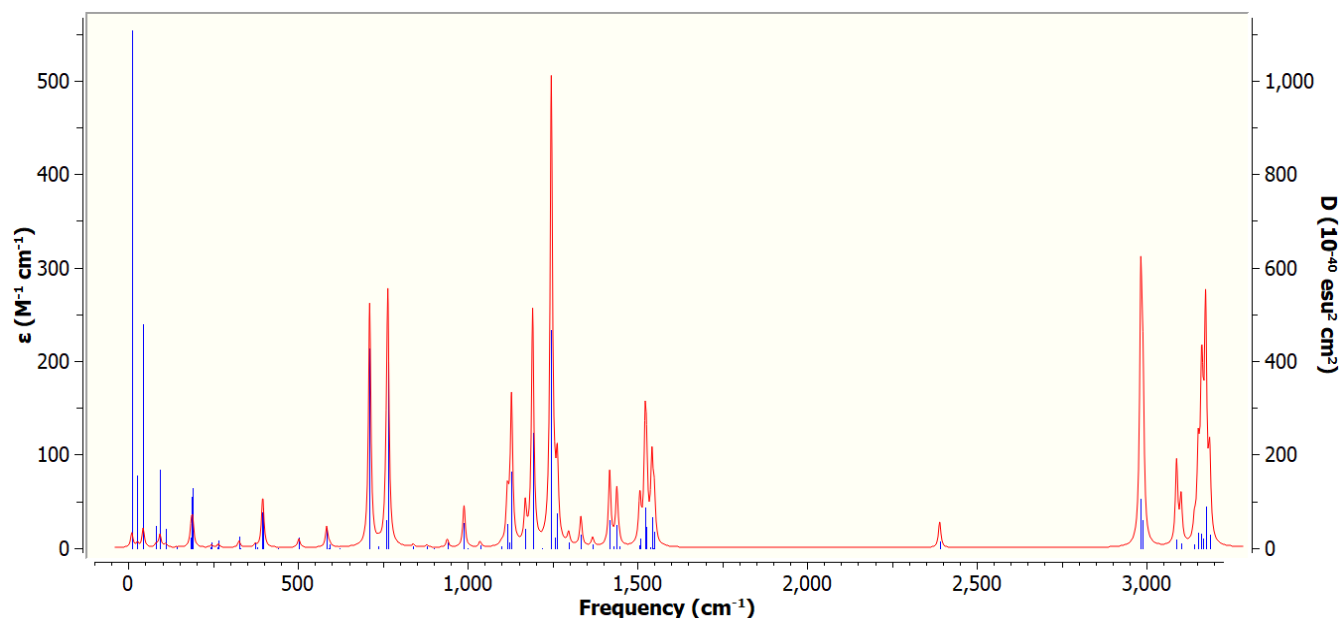


Fig. 5. Theoretical vibrational frequencies (cm^{-1}) of 2,2'-(ethane-1,2-diylbis(azanediyl))bis(2-methylpropanenitrile)

Table-II. IR Frequencies (cm^{-1}) of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

Frequencies of different bond	Experimental	DFT
$\nu_s(\text{CN})$	2220	2351
$\nu_s(\text{NH})$	2988	2933

$\nu_{as}(\text{CH}_3)$	2942	2939
$\nu_{as}(\text{CH}_2)$	2853	2933
$\rho(\text{C-C})$	1464-1627	1485-1526
$\gamma(\text{NH})$	764, 783	751, 756
$\delta(\text{CH}_3)$	1441	1418
$\delta(\text{CH}_2)$	1385	1397

p: stretching, ν_s : symmetric stretching, ν_{as} : asymmetric stretching, δ : bending, γ : out of plane bending.

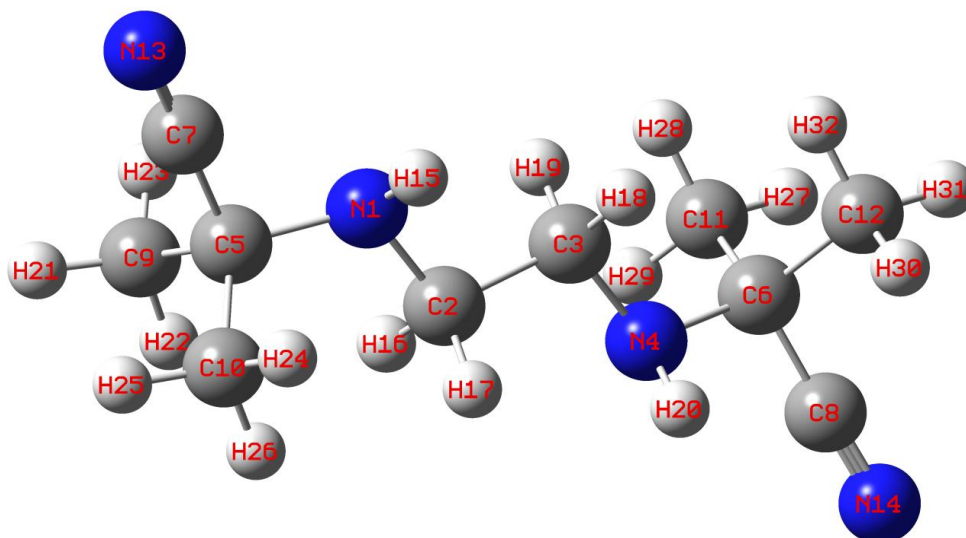


Fig.6. Optimized geometry of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

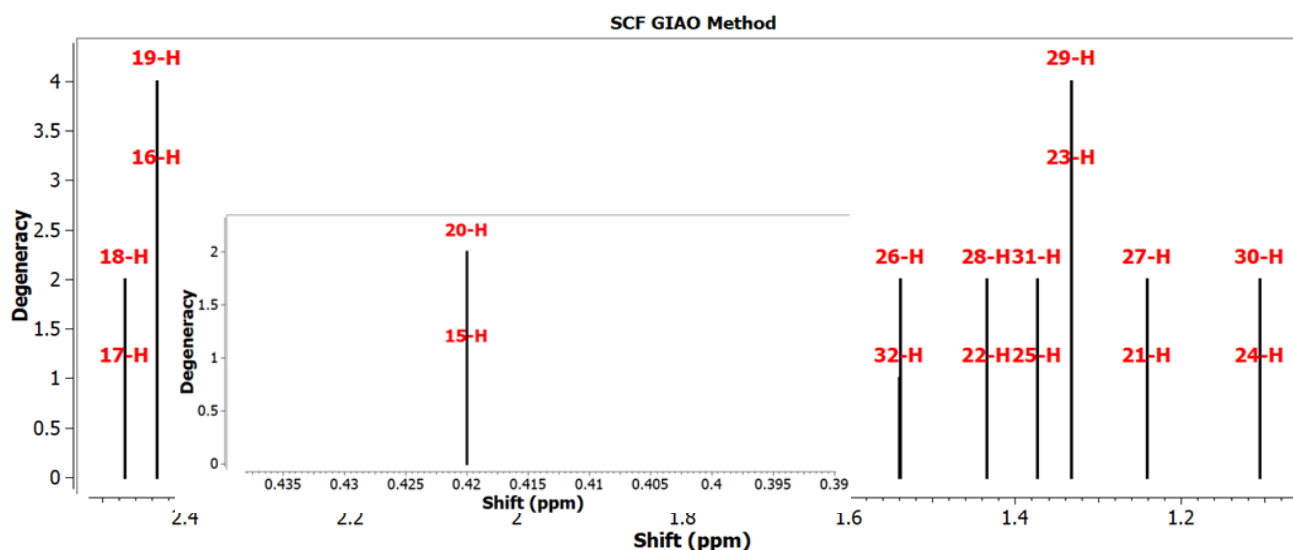


Fig. 7. Theoretical ^1H NMR (ppm) spectra for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

Table-III. Theoretical ^1H NMR (ppm) values for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. Reference: TMS GIAO. Reference shielding: 31.8821 ppm. Degenerate peaks are condensed together (Degeneracy Tolerance 0.05)

Atoms	Shift (ppm)
17,18,16,19-H	2.44
32,26-H	1.54
22,28-H	1.43
25,31,23,29-H	1.35
21,27-H	1.24

24,30-H	1.11
15,20-H	0.41

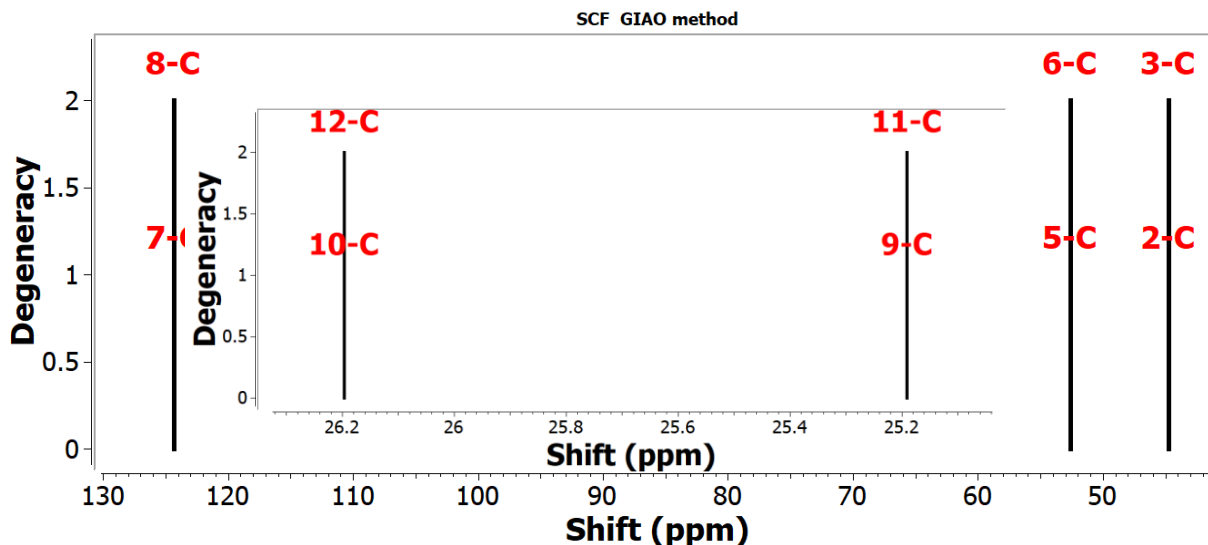


Fig. 8. Theoretical ^{13}C NMR (ppm) spectra for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

Table-IV. Theoretical ^{13}C NMR (ppm) values for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane . Reference: TMS GIAO. Reference shielding: 182.466 ppm. NMR Degeneracy Tolerance: 0.05

Atoms	Shift (ppm)
7-C	124.25
8-C	124.25
5-C	53.06
6-C	53.06
2-C	45.23
3-C	45.23
10-C	26.18
12-C	26.17
9-C	25.20
11-C	25.20

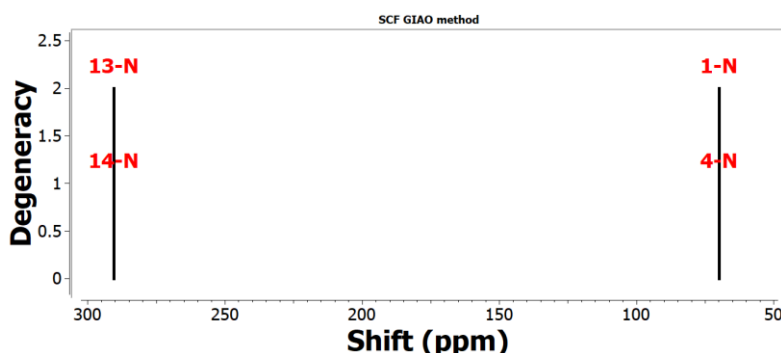


Fig. 9. Theoretical ^{15}N NMR (ppm) spectra for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

Table-V. Theoretical ^{14}N NMR (ppm) values for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane . Reference: NH_3 GIAO. Reference shielding: 258.4 ppm. NMR Degeneracy Tolerance: 0.05

Atoms	Shift (ppm)
14-N	288.27
13-N	288.27
4-N	71.00
1-N	71.00

C. Frontier Molecular Orbital (FMO) Analyses

FMO composition analyses results are very important on measure molecular structural properties. MO energy and occupancy diagrams of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane is presented in Fig.10. The energy of HOMO of the 2,7-dimethyl-2,7- dicyanide-3,6-diazaoctane is equal to the ionization potential of this molecule. Next pattern is that the energy of LUMO of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane is equal to electronic affinity. However, the energy difference between molecular orbitals can calculate stability and reactivity of a molecule, this difference is named energy band gap (E_g) which can also describes molecular structure properties. When E_g is greater this molecular structure can be high stability that this molecule has low reactivity properties. On the other hand, low point energy band gap molecular structure is lower stability, means that this molecule has larger reaction abilities. The HOMO and LUMO energies of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane were calculated at -0.25096 eV and 0.01273 eV. The energy band gap ($E_g = E_{\text{LUMO}} - E_{\text{HOMO}}$) is computed at -1.800349 eV. The lower E_g value of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane shows that this molecular structure is lower stability and more reactivity. Chemical Hardness (η), Electronegativity (χ), Electronic chemical potential (μ), Global electrophilicity Index (ω) and Chemical Softness (s) for 2,7-dimethyl-2,7-dicyanide-3,6- diazaoctane from difference of the HOMO and LUMO energy. The value of calculated the above parameters were presented on Table.VI. The calculation equations were following:

$$\text{Chemical Hardness, } \eta = E_{\text{LUMO}} - E_{\text{HOMO}}/2 \quad (1)$$

$$\text{Electronegativity, } \chi = -(E_{\text{LUMO}} + E_{\text{HOMO}})/2 \quad (2)$$

$$\text{Electronic chemical potential, } \mu = E_{\text{LUMO}} + E_{\text{HOMO}}/2 = -\chi \quad (3)$$

$$\text{Global electrophilicity Index, } \omega = \mu^2/2\eta \quad (4)$$

$$\text{Chemical Softness, } s = 1/2\eta \quad (5)$$

Table-VI. Energy values of global reactivity descriptors for 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane, (E (RB3LYP) = -611.02583 eV, Dipole Moment = 0.3321 Debye)

Parameter	Value (eV)
Chemical Hardness, η	0.13184
Electronegativity, χ	-0.13184
Electronic chemical potential, μ	0.11911
Global electrophilicity Index, ω	0.21522
Chemical Softness, s	3.79247

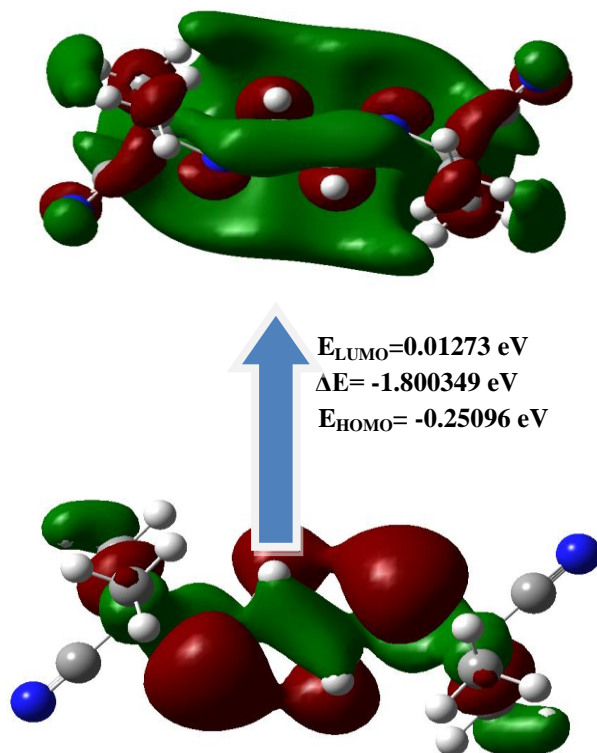


Fig.10. HOMO and LUMO difference of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

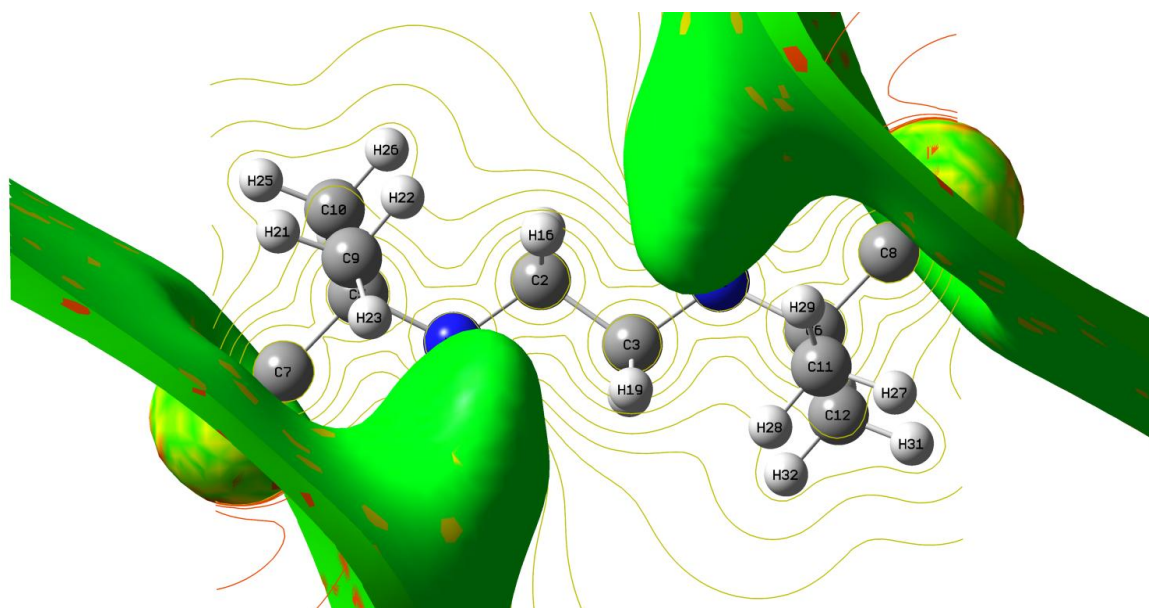


Fig. 11. MEP surface of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane

D. Molecular Electrostatic Potential (MEP) Analysis

MEP calculation is one of quantum-molecular descriptor methods, it gives the description of that one properties of some molecule how can sited in another properties of this molecule. In our experiment, we have examined that the map of electron density on an isosurface of electrostatic potential for the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. This method results presented perhaps significant reactive sites of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. In Fig.11 rainbow color scheme is electrostatic potential in the range from -1.004 eV to +1.004 eV for 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane.

In the MEP of the 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane the brightest green and red color site is electron rich areas, means that this sites are convenient for electrophilic reaction attack. With regard to this MEP these electron rich sites were located over nitrogen ($N\equiv C$) atoms belong cyanide groups. Furthermore, dark sites show the location of low electron density areas which are convenient for nucleophilic attacks. These electron poor regions were located over hydrogen of CH, CH_2 , CH_3 and NH groups.

IV. CONCLUSIONS

In conclusion, we have syntheses new α -amino nitrile namely 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. We have proven that molecular structure of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane by X-ray, IR and NMR results. X-ray analysis results clarified that crystallographic parameters, bond types, angles, length, intermolecular interaction for 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. These X-ray date have proven molecular structure of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. IR and NMR spectra of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane were theoretically calculated by DFT, resulting that experimentally

and DFT spectra were nearly similarly. DFT methods results can also prove molecular structure of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane. FMO results indicate the lower E_g value of 2,7-dimethyl-2,7-dicyanide-3,6-diazaoctane shows that this molecular structure is lower stability and more reactivity. It was found that electron rich sites were located over nitrogen ($N\equiv C$) atoms belong cyanide groups; electron poor regions were located over hydrogen of CH, CH_2 , CH_3 and NH groups.

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