Structural, Vibrational, Quantum Chemical Calculations, Thermal and Antimicrobial Studies On Nitrate Salt Of 3-Nitroaniline

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Abstract

In this work, 3-nitroanilinium nitrate (3NAN) has been synthesized and crystallized successfully by solution growth combined with solvent evaporation technique. 3NAN molecular structure has been optimized with Density Functional Theory (DFT) using B3LYP function and Hartree-Fock method with a 6-311++G(d,p) basis set. The geometrical parameters of the title molecules have been analyzed. The computed vibrational spectra were compared with experimental result which show appreciable agreement. Thermal stability of the crystal was analyzed with TGA/DTA and the melting points of the salt identified at 209 °C. HOMO-LUMO energy calculations have shown the charge transfer within the molecule. The possible pharmaceutical/biological activity of the salts confirmed by the Frontier Molecular Orbital (FMO) analysis have lower band gap value. The antimicrobial activity of grown crystals were tested against certain potentially threatening microbes.

Introduction

Generally nitroaniline is called as push-pull molecule. Because of the intramolecular charge transfer (ICT) from the $-NH_2$ (electron-donor group) to $-NO_2$ (electron-acceptor group) through the phenyl ring. 3-Nitroaniline and 4-nitroaniline are used as reference compounds for optical nonlinearity [1–3] calculated by computational and experimental method. 3-Nitroaniline and its derivatives are biologically important compounds, such compounds are produced significant antihyperglycemic as well as hypoglycemic effects in alloxan-induced and normal diabetic rabbits [4]. Also m-Nitroaniline plays an essential role in several biological processes and has considerable chemical and pharmacological importance. Since a long time, schiff based compounds are generally considered due to their importance in several electro-optical and other biological applications [5]

In this context, a new family of organic-inorganic crystals with the biological importance, with chemical, physical and thermal properties through inorganic sub networks is proposed. Based on the above specifics, 3-nitroaniline was reacted with nitric acid and the crystals of 3-nitroanilinium nitrate were grown. In this paper, the synthesis, crystal growth, structural, spectroscopic, thermal analyses and biological activity of 3NAN is reported.

Experimental

2.1 Material Preparation

3-nitroanilinium nitrate (3NAN) is synthesized from the AR grade 3-nitroaniline and nitric acid obtained from Himedia fine chemicals taken in 1:1 ratio using acetone, as solvent. This solution was stirred well for about 1 hour to get clear solution filtered and kept in a clean beaker for evaporation. The title crystal was synthesized according to the scheme as shown in Fig. 1. The reaction was allowed in room temperature. After many attempts, the compound 3-nitroaniline nitrate has not yielded good quality single crystal; which is not suitable for single crystal X-ray diffraction. Hence, the powder XRD analysis of 3NAN was taken to prove the new phase of the complex.

2.2 Characterization techniques

Powder XRD studies of grown crystal of 3NAN was carried out by Bruker X-ray diffractometer of D8 advanced ECO XRD system with SSD160 1D Detector. The diffraction was collected in the range of 2θ , 0° to 50° . The preliminary data of the polycrystalline sample were calculated by indexing in the first 2θ strong intensity peaks using DASH

3.3.2 program [6]. FT-IR spectrum of grown crystal was recorded using Nexus 670 FTIR spectrometer and FT-Raman spectrum were recorded using BRUKER RFS 27 FT-Raman Spectrometer. Both the spectra were recorded in the range of 400 to 4000 cm^{-1} with Nd:YAG laser at 1064 nm as source. DTA/TGA of grown crystals were carried out by SII (SEIKO), Japan Analytical Instrument, and Model No: TG/DTA-6200 with N_2 atmosphere with heating rate $20^\circ\text{C}/\text{Min}$.

2.3 Computational Profile

The 3NAN molecular parameters in the ground state were computed by performing both HF and B3LYP with basis set 6-311 + G(d,p). Computational calculations were performed using GAUSSIAN 09W [7] program package on i5 processor/3.20 GHz personal computer without any constraint on the geometry [8]. The geometry of the title compound was optimized by the computational method. The HF and B3LYP method [9] acknowledged as a practical approach for the computation of molecular structure and vibrational frequencies with the Becke’s three parameter exact exchange-functional (B3)[10] combined with gradient-corrected correlational functional of Lee, Yang and Parr (LYP) [11]. Using principle of statistical mechanics, thermodynamic properties of 3NAN have been calculated from normal mode of vibrational frequencies which provide the details about title compound in gas phase. GAUSSVIEW program [12] with symmetry considerations were used to assign vibrational frequencies. The electronic properties, such as HOMO–LUMO energies were calculated and computed by the HF and B3LYP method.

Results And Discussion

3.1 Structural and molecular geometry analyses

The possible unit cell parameters for 3NAN given in the Table 1. By comparing the powder XRD pattern of grown crystal 3NAN compared with its pure 3-nitroaniline and shown in Fig. 2. With the help of XRD pattern and the unit cell values are confirmed the 3NAN salt formation. Some of the new intensity peaks are appear in 3NAN crystals and some of the peaks are disappear compared to 3-nitroaniline. The possible unit cell parameters were identified and 3NAN crystal belongs to orthorhombic system was notable using DASH 3.3.2 program.

Table 1 Unit cell parameters of 3NAN	
Unit cell Parameters	Values
a (Å)	21.486 (8)
b (Å)	19.163 (1)
c (Å)	3.884 (1)
α ($^\circ$)	90
β ($^\circ$)	90
γ ($^\circ$)	90
Volume (Å ³)	1599.4

In 3NAN, asymmetric part of unit cell contains 3-nitroaniline (cation) charge is neutralized with nitrate (anion). The optimized molecular structure of 3-nitroanilinium nitrate diagram and atom numbering scheme are shown in the

Fig. 3 and geometrical parameters are given in Table 2. In phenyl ring, optimized C–C bond length is calculated by HF method around 1.381–1.390 Å and by B3LYP method around 1.389–1.400 Å. The N–O bond lengths are calculated around 1.167–1.321 Å by HF method and 1.199–1.382 Å by B3LYP method in nitrate anion.

Table 2
Optimized molecular geometrical parameters of 3NAN

Bond length (Å)	HF/6-311++ (d,p)	B3LYP/6-311++ (d,p)	Bond angle (°)	HF/6-311++ (d,p)	B3LYP/6-311++ (d,p)
N1–C2	1.414	1.422	N1–C2–C3	120.2	120.3
C4–N8	1.470	1.483	N1–C2–C7	120.3	120.1
C2–C3	1.385	1.394	C3–C2–C7	119.4	119.6
C2–C7	1.390	1.400	C2–C3–C4	118.6	118.7
C3–C4	1.381	1.390	C3–C4–C5	123.1	122.8
C4–C5	1.378	1.389	C3–C4–N8	118.2	118.2
C5–C6	1.385	1.392	C5–C4–N8	118.8	119.0
C6–C7	1.382	1.392	C4–C5–C6	117.5	117.7
N8–O9	1.187	1.225	C5–C6–C7	120.8	120.8
N8–O10	1.186	1.223	C2–C7–C6	120.6	120.3
N18–O19	1.167	1.199	C4–N8–O9	117.6	117.6
N18–O20	1.189	1.222	C4–N8–O10	117.5	117.6
N18–O21	1.321	1.382	O9–N8–O10	125.0	124.8
			O19–N18–O20	127.8	128.2
			O19–N18–O21	115.5	115.0
			O20–N18–O21	116.7	116.7

3.2 Mulliken charge analysis

The histogram of atomic charges of 3NAN given in Table 3 and it shown in Fig. 4. By quantum chemical methods, Mulliken atomic charge distribution was calculated, which has a vital role to the molecular system because atomic charges effect dipole moment, polarizability and electronic structure [13]. The hydrogen atom (H11) (0.497e in HF and 0.451e in B3LYP) in HNO₃ group of 3NAN was more electropositive, this hydrogen atom was attached with electronegative atoms (N18, O19, O20, O21). Also, nitrogen atom has more electro negativity (N1) (-0.535e in HF and -0.474e in B3LYP), this nitrogen atom enclosed by H12 and H13 (electropositive atom) and C2 (carbon atom).

Table 3
Computed atomic charges of 3NAN

Atoms connected	HF/ 6-311 ++ G(d,p)	B3LYP/ 6-311 ++ G(d,p)
N1	-0.535	-0.474
C2	0.027	-0.007
C3	-0.152	-0.259
C4	0.036	-0.224
C5	-0.134	0.071
C6	-0.119	-0.222
C7	-0.552	-0.151
N8	-0.120	-0.185
O9	-0.048	-0.002
O10	-0.056	-0.005
H11	0.497	0.451
H12	0.317	0.282
H13	0.294	0.288
H14	0.274	0.229
H15	0.274	0.239
H16	0.241	0.201
H17	0.182	0.166
N18	-0.141	-0.330
O19	-0.052	0.014
O20	-0.125	-0.035
O21	-0.106	-0.048

3.3 Vibrational analysis

The 3NAN consists of 21 atoms, which has 57 modes of vibrations. The comparison of experimental and computed IR and Raman spectra of 3NAN are given in Fig. 5 and frequency values are given in Table 4.

Table 4

The experimental (FT-IR, FT-Raman) and calculated frequencies of 3NAN with their vibrational assignments

Mode Number	Experimental frequency (cm ⁻¹)		Calculated frequency (cm ⁻¹)						Vibrational assignments
			HF/			B3LYP/			
	6-311 ++ G(d,p)			6-311 ++ G(d,p)					
	FT-IR	Raman	V _{cal}	a _I IR	b _I Raman	V _{cal}	a _I IR	b _I Raman	
1			7	1.608	0.677	14	2.508	1.518	Lattice vibration
2			20	0.567	3.971	23	4.937	3.3284	Lattice vibration
3			31	0.519	4.935	38	0.016	5.444	t (NO ₂)
4			41	0.185	0.204	46	0.067	0.4355	t (NO ₂)
5			80	1.181	1.195	83	0.126	1.2479	t (NO ₂ of HNO ₃)
6			93	2.415	0.967	92	1.970	1.1478	ρ (NH ₂)
7			153	11.937	1.431	153	10.453	1.4687	Ring vibration
8			190	5.666	2.227	181	17.463	2.9798	γ (C–H)
9			236	2.515	0.487	217	1.630	0.5016	ρ (NH ₂)
10			279	2.402	0.203	266	12.601	0.1362	ω (NH ₂)
11			383	10.033	0.472	363	4.609	3.1685	ρ (NH ₂)
12			417	1.288	3.882	394	0.685	1.4698	ρ (NH ₂) + ν (C–N)
13			451	1.584	1.411	431	1.455	0.1871	γ (C–H)
14			477	2.143	0.107	465	7.541	1.0761	t (NH ₂)
15	518 m		558	0.207	4.909	518	1.328	4.4912	β (C–C)
16			587	19.027	0.288	537	16.845	0.4917	γ (C–C)
17			605	1.200	1.477	563	1.320	1.1435	β ((C–C) + NH ₂)
18	668 m		724	27.030	1.363	648	5.888	5.2998	β (O–H)
19			730	8.647	1.558	673	27.446	0.2197	γ (C–H)

Mode Number	Experimental frequency (cm ⁻¹)		Calculated frequency (cm ⁻¹)						Vibrational assignments
			HF/ 6-311 ++ G(d,p)			B3LYP/ 6-311 ++ G(d,p)			
	FT-IR	Raman	V _{cal}	a _I IR	b _I Raman	V _{cal}	a _I IR	b _I Raman	
20	736 m		741	9.985	5.824	684	3.007	4.0857	δ (NO ₂ of HNO ₃) + ν (N-O of HNO ₃)
21			798	16.302	2.257	688	2.584	4.3759	β (C-C)
22	829 m	806 w	814	18.377	1.613	727	10.487	1.0618	ω (NH ₂) + γ (C-H + N-O)
23			871	39.206	1.663	784	10.796	0.4096	γ (N-O of HNO ₃) + β (C-H)
24			894	46.143	2.167	800	48.280	1.5888	γ (C-H + O-H + N-H)
25			911	150.048	4.778	818	165.006	5.4327	γ (C-H + O-H + N-H)
26	921 w		919	9.882	2.909	852	74.620	16.878	γ (C-H + O-H + N-H)
27			980	229.064	13.410	910	77.287	1.4858	γ (C-H)
28			1018	105.262	4.118	932	5.485	0.4155	γ (C-H)
29			1031	53.028	2.216	940	63.773	1.8888	ω (NH ₂) + ν (C-N + N-O) + δ (NO ₂)
30		1036 w	1037	26.058	1.744	942	110.273	15.1187	ω (NH ₂) + δ (NO ₂ + NO ₂ of HNO ₃) + ν (O-N)
31		1082 _w	1083	5.662	33.291	993	225.799	29.5752	γ (O-H)
32	1105 m		1110	0.430	0.129	998	1.405	0.5063	γ (C-H)
33			1152	106.961	14.764	1016	7.718	27.1688	β (C-C) + δ (NH ₂)
34	1174 m	1198 w	1155	1.212	1.882	1094	16.099	0.3468	β (C-H) + ρ (NH ₂)
35			1204	38.954	1.737	1105	21.963	17.2829	β (C-H + C-C)

Mode Number	Experimental frequency (cm ⁻¹)		Calculated frequency (cm ⁻¹)						Vibrational assignments
			HF/ 6-311 ++ G(d,p)			B3LYP/ 6-311 ++ G(d,p)			
	FT-IR	Raman	V _{cal}	a _I IR	b _I Raman	V _{cal}	a _I IR	b _I Raman	
36			1211	5.906	7.893	1148	9.808	3.0772	ρ (NH ₂) + β (C-H)
37			1265	2.534	2.355	1192	0.514	2.704	β (C-H)
38	1324 w	1359 s	1349	24.703	1.378	1263	102.150	43.7652	ν (C-N) + β (C-C)
39			1367	57.057	23.989	1325	214.008	14.5075	ν (C-N) + ν _s (NO ₂)
40			1444	6.034	0.707	1333	47.100	16.056	ν (C-N) + ν _s (NO ₂ HNO ₃) + β (C-H)
41	1531 s		1563	230.085	6.124	1366	43.761	8.9454	ν (C-C + C-N) + ρ (NH ₂)
42			1607	513.942	10.079	1372	268.421	165.089	ν (C-N) + ν _s HNO ₃
43			1611	98.852	7.524	1482	275.940	5.4486	β (O-H of HNO ₃)
44			1628	284.981	69.752	1494	60.513	5.1155	ν (C-C) + t (NH ₂)
45			1647	2.153	7.674	1516	23.302	0.3785	ν (C-C) + β (C-H)
46			1772	285.838	17.106	1591	350.399	24.3597	ν _{as} NO ₂ + ν (C-C + C-N) + β (C-H)
47			1782	125.991	38.190	1632	13.773	55.4454	ν (C-C) + β (C-H + N-H)
48			1808	206.041	10.298	1654	46.729	3.0565	δ (NH ₂)
49			1837	168.388	4.332	1665	40.797	15.5683	δ (NH ₂) + ν (C-C + C-N + N-O)
50	2003 w		1932	618.427	3.249	1735	314.009	3.0517	ν _{as} HNO ₃
51		3073 w	3326	7.812	65.555	3016	2106.123	315.5617	ν (O-H of HNO ₃)
52			3353	7.523	118.434	3176	2.519	60.9266	ν (C-H)

Mode Number	Experimental frequency (cm ⁻¹)		Calculated frequency (cm ⁻¹)						Vibrational assignments
			HF/ 6-311 ++ G(d,p)			B3LYP/ 6-311 ++ G(d,p)			
	FT-IR	Raman	v _{cal}	a _I IR	b _I Raman	v _{cal}	a _I IR	b _I Raman	
53			3380	5.044	43.703	3194	3.565	123.6094	v (C–H)
54			3402	4.013	69.781	3207	4.951	53.6183	v (C–H)
55			3657	1428.708	173.243	3230	4.025	80.2772	v (C–H)
56			3742	60.245	98.258	3510	29.025	153.0756	v _s (NH ₂)
57			3826	31.359	36.003	3596	27.115	40.4919	v _{as} (NH ₂)
w-weak; m- medium; vs - very strong; v-stretching;									
β- in plane bending; γ- out -of- plane bending; v _s , sym.stretching; v _{as} , asym.stretching; ρ -rocking; δ - scissoring; t- twisting; ω-wagging;									

NH₂ vibrations

The NH₂ group vibrations are expressed as antisymmetric stretching, symmetric stretching, scissoring, wagging, rocking and twisting vibrations are spread over a region in the spectrum [14]. In theoretical spectrum the peak at 3826 cm⁻¹ in HF and 3596 cm⁻¹ in B3LYP method are assigned to NH₂ antisymmetric stretching. NH₂ symmetric stretching wavenumbers are calculated at 3742 and 3510 cm⁻¹ in HF and B3LYP respectively. NH₂ scissoring are calculated at 1808 and 1654 cm⁻¹ in HF and B3LYP respectively. NH₂ twisting is calculated at 1628 and 1494 cm⁻¹ in HF and B3LYP respectively. NH₂ wagging along with scissoring NO₂ vibrations are observed as weak peak at 1036 in Raman and theoretically scaled by HF and B3LYP at 1037 and 942 cm⁻¹ respectively. The rocking NH₂ vibrations are calculated at mode 34 corresponding experimental spectrum identified as a weak peak in Raman at 1198 cm⁻¹ and a medium peak at 1174 cm⁻¹ in IR.

NO₂ vibrations

In nitrobenzene and substituted nitrobenzene, the band around 1500–1570 cm⁻¹ and 1300–1370 cm⁻¹ are represents the asymmetric and symmetric stretching vibrations of NO₂ group, respectively [15]. The NO₂ asymmetric stretching vibrations are theoretically computed by HF and B3LYP at 1772 and 1591 cm⁻¹ respectively. The NO₂ symmetric stretching vibration theoretically scaled by HF and B3LYP method at 1367 and 1325 cm⁻¹, respectively. The scissoring NO₂ vibrations are observed as weak peak at 1036 cm⁻¹ computed at mode 30 and mode 4 represents NO₂ twisting vibrations in theoretical calculation.

C–C and C–N vibrations

The title compounds have C–C and C–N stretching vibrations is usually occur in the region 1300–1600 cm⁻¹. In theoretical spectrum the peak at 1837 cm⁻¹ by HF and 1665 cm⁻¹ in B3LYP method are assigned to C–C stretching vibrations. Similarly, C–N stretching vibrations are assigned to 1444 cm⁻¹ in HF and 1333 cm⁻¹ in B3LYP.

C-H vibrations

In 3NAN, the C–H stretching vibrations confirm aromatic structure. These stretching vibrations are occurs in the characteristic region around 3100 cm^{-1} [16,17]. The C–H stretching vibrations peaks are assigned in the theoretical spectrum in the region $3657 - 3176\text{ cm}^{-1}$. The in-plane bending vibrations are observed with O–H stretching in theoretical spectrum at 1782 cm^{-1} in HF and 1632 cm^{-1} in B3LYP.

Vibrations of nitrate anion

The title compound, NO_3^- asymmetric stretching vibrations are observed as a weak peak at 2003 cm^{-1} in IR and in theoretical spectrum at 1932 and 1735 cm^{-1} in the HF and B3LYP respectively. NO_3^- symmetric stretching vibrations are observed at 1607 and 1372 cm^{-1} in the HF and B3LYP respectively. The O–H stretching is observed as a weak peak in IR at 3073 cm^{-1} , it is scaled at 3326 cm^{-1} in HF and 3016 cm^{-1} in B3LYP. The O–H in-plane bending vibrations are calculated 1611 and 1482 cm^{-1} in the HF and B3LYP respectively. The O–H out-plane bending vibrations observed as a weak peak at 1082 cm^{-1} in IR and it is well matches with experimental spectra.

3.4 Frontier Molecular Orbital Analysis

In the organic molecules, optical and electric properties are proposed by using frontier molecular orbital analysis [18–20]. The molecular orbital have two important interactions; such as HOMO means the ability to donate an electron and LUMO represents accept an electron. Also, these orbitals are named as frontier orbitals. Frontier electron density [21] is used to explain the several types of reaction in conjugated system and most reactive position in π -electron systems. Also, FMO plays an essential part in abiding chemical stability of the compound [22]. The calculated HOMO and LUMO energies and some important parameters of the 3NAN were calculated by HF and DFT/B3LYP method as shown in Table 5. The stimulated energy level diagrams of 3NAN molecule was shown in Fig. 6. A huge amount of charge transfer occurred in 3NAN is indicated by small energy gap, which is connected with a high chemical reactivity. The small value of energy gap and high value of charge transfer leads the molecules to biologically active.

For 3NAN, 356 energy levels are observed in the energy range -20.668 au to 51.757 au and -19.214 au to 49.990 au in HF and B3LYP method respectively. The calculated HOMO and LUMO energy values of 3NAN molecule in HF and B3LYP are $-0.357/0.022\text{ au}$ and $-0.275/-0.116\text{ au}$ repectively. The energy gap value between the frontier orbital was 0.379 a.u in HF and 0.159 a.u in B3LYP.

Table 5
Calculated energy values of 3NAN

Parameters (a.u.)	HF	B3LYP
	6-311 ++ G(d,p)	
HOMO	0.022	-0.116
LUMO	-0.357	-0.275
$\Delta(E_{\text{LUMO}} - E_{\text{HOMO}})$	0.379	0.159
Electron affinity (A)	-0.022	0.116
Ionization potential (I)	0.357	0.275
Chemical hardness (η)	0.190	0.080
Chemical potential (μ)	-0.168	-0.196
Electronegativity (χ)	0.168	0.196
Electrophilicity Index	0.074	0.240

3.5 Thermal analysis

3NAN thermal behaviour was analyzed by using simultaneous DTA/TGA analysis in the temperature range 30-650°C in air atmosphere. The TGA/DTA curves of 3NAN are given in the Fig. 7. The TGA/DTA curve represent that the decomposition in the range of 190-650°C. The three main stages of decomposition in 3NAN occurred within this temperature range as given Fig. 8. In TGA/DTA curve, weight loss 11% noted in temperature range 150-190°C due to the elimination of water group from 3NAN, it indicates first stage of decomposition. The second stage of major weight loss 41% occurs at 190-220°C temperature range, which is due to the liberation of NO and CO from the earlier intermediate compound. The next decomposition stage is owing to the removal of NO and C₂H₄ in the temperature range 220-420°C with weight loss of 29%. An endothermic peak observed at 209°C is may be the melting point of the compound. The soft exothermic peaks at 485°C are due to the decomposition of the organic compound.

3.6 Antimicrobial activity analysis

To analyze the antimicrobial activity of 3NAN, the crystal was tested against Staphylococcus Aureus (G⁺ve) and Klebsiella Pneumoniae (G⁻ve) by disc diffusion method with 50 and 100 mg mL⁻¹ concentrations. Similarly, the title compound antifungal activity was tested against Candida Albicans (C. albicans). The zone of inhibition were measured in diameter are shown in Table 6. The biological activity of 3-nitroanilinium nitrate complex results indicate, it is a moderately active material against all the organisms [23,24].

Table 6
Antibacterial and Antifungal activity of 3NAN compound against some human pathogens

Sample	Concentration (mg/ml)	Zone Of Inhibition In diameter (mm)		
		Micro organisms used		
		<i>K. Neumoniae</i> (G ⁺ ve)	<i>S. Aureus</i> (G ⁻ ve)	<i>C. Albicans</i>
3NAN	50	12	R	13
	100	12	R	13
SD	50/100	16	18	16

R = Resistant

SD-Standard drug (Antibacterial activity)–Amikacin

SD-Standard drug (Antifungal activity)–Ketokonazole

Conclusion

3-nitroanilinium nitrate has been synthesized and characterized by various methods. The detailed interpretation of the vibrational spectra between calculated (IR, Raman) and computed spectra, experimental results of 3NAN molecule show the good reliability with computed results. The higher stability of the title molecule is confirmed from the computed HOMO-LUMO energy gap. TGA and DTA exposed about the material, thermal analysis confirmed the absence of phase transition before the material reach the melting point. Antimicrobial activity of the title compound has been calculated.

Declarations

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Declarations of interest

None

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Figures

Figure 1

Reaction scheme of 3-Nitroanilinium nitrate

Figure 2

Powder XRD pattern of 3NAN and 3NA

Figure 3

Optimized geometry of 3NAN by (a) HF and (b) B3LYP method

Figure 4

Histogram of atomic charges on 3NAN by HF and B3LYP methods

Figure 5

Experimental and computed IR & Raman spectra of 3NAN

Figure 6

Molecular orbital energy level diagram of 3NAN by (a) HF and (b) B3LYP levels

Figure 7

DTA/TGA curve of 3NAN

Step-I

Step-II

Step-III

Note: The values given in parenthesis stand for the molecular weights of the respective species.

Figure 8

Decomposition steps of 3NAN

Figure 9

The antibacterial activity of 3NAN against Staphylococcus Aureus

Figure 10

The antibacterial activity of 3NAN against *Klebsiella Pneumoniae*

Figure 11

The antifungal activity of 3NAN against Candida Albicans