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Bis (1, 5-diamino-4-methyl-tetrazolium) hydrazinetetrazolate: synthesis, structure and energetic properties

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Abstract Bis (1, 5-diamino-4-methyl-tetrazolium) hydrazinetetrazolate (BMDATHBT) was first synthesized with 1, 5-diamino-4-methyl-tetrazolium sulfate (MDATS) and hydrazino bitetrazole barium ($HBTBa•5H_2O$) as raw materials. The structure was characterized by elemental analysis, IR, 1HNMR and MS. The single crystal of BMDATHBT was first cultivated. Its crystalline density is 1.660 g/cm^3. BMDATHBT has high detonation pressure and detonation velocity (P =25.93 GPa, D =7.839 km s^{-1}), which are higher than those of TNT. Its thermal and mechanical sensitivities are moderate. The thermal decomposition products are almost all gases. Therefore, it has potential application prospect in gas generating agent, explosive and solid propellant.

Keywords nitrogen-rich compound; energetic ionic salt; BMDATHBT; synthetic; calculation

1 Introduction

Nitrogen-rich compound is a kind of new type energetic material which has a good potential application prospect in military chemistry field [1-4]. Energetic ionic salt, compared with energetic molecular compound, usually has the advantages of high density, good stability and low vapor pressure etc [5-7]. The nitrogen content of energetic ionic salt with tetrazole ring both in anion and cation is high. Thermal decomposition products of these energetic ionic salts are most nitrogen with low vapor pressure and high density, so they are friendly to the environment [8]. Therefore, energetic ionic salt with tetrazole ring both in anion and cation can be another important research direction in the energetic material field.

The molecular formula of BMDATHBT is $C_6H_{16}N_{22}$. There are tetrazole rings

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both in anion and cation. Its nitrogen content is 77.8%, which is higher than that of the compounds reported in Ref. [5, 6]. There are some hydrogen atoms in the molecule, which can form hydrogen bonds between the molecules. This increase the stability of the compound. Therefore, it has a good application prospect in explosion field. However, there is no report about BMDATHBT.

In this study, BMDATHBT was first synthesized. The structure was characterized by elemental analysis, IR, 1HNMR and MS. The single crystal of BMDATHBT was cultivated, and the single crystal structure was analyzed. The density, heat of formation, detonation pressure and detonation velocity of BMDATHBT were calculated. The thermal analysis and sensitivity of BMDATHBT were first studied in this work.

2. Experimental

2.1 Synthetic of 1, 5-diamino–4–methyl-tetrazolium sulfate (MDATS)

MDATI was prepared according to Ref. [9]. MDATS was synthesized though the reaction of MDATI and silver sulfate. The synthetic route is shown in Fig 1.

Deionized water (300 mL) and Ag_2SO_4 (3.0995 g, 0.01 mol) were added into a three-necked flask equipped with a stirrer and a reflux apparatus. After stirring gently at 80 ℃ to fully dissolve, MDATI (4.8434 g, 0.02 mol) was added into the solution to react for 30 min in the dark condition. The filtrate was evaporated after filtration. The white MDATS was obtained after washing by anhydrous ethanol.

--------------------------------- Fig 1---------------------------------

2.2 Synthetic of hydrazino bitetrazole barium (HBTBa•5H_2O)

5, 5 '-azotetrazolium barium (BAZ•5H_2O) was prepared according to Ref. [10]. BAZ•5H_2O were dissolved in deionized water. The magnesium powders were added into the flask under N_2 atmosphere. And then the solution was heated to 100 ℃ to boil for 30 min with refluxing. The excess magnesium and magnesium hydroxide precipitation were removed by hot filtration under N_2 protection. The filtrate was evaporated to dry and the white HBTBa•5H_2O was gained.

2.3 Synthetic of BMDATHBT

Deionized water (30 mL) and HBTBa•5H_2O (0.7849 g, 2 mmol) prepared in part

2.2 were added into a three-necked flask equipped with a stirrer and a reflux apparatus under N_2 atmosphere. After stirring gently at 50 ℃ to fully dissolve, MDATS (0.6565 g, 2 mmol) prepared in part 2.1 was added into the solution to react. A large amount of white solids precipitated after 5 min. Barium sulfate precipitation was removed by filtration. The filtrate was evaporated to dry. The white BMDATHBT•$2H_2O$ (0.7122 g) was obtained. The yield is 89.92%. The synthetic route is shown in Fig 2. Crystals suitable for X-ray structure determination were obtained by cooling in the fridge for five days.

--------------------------------- Fig 2---------------------------------

2.4 Measurements

U.S. companies Nicolet FT-IR4700 infrared spectroscopy, Switzerland ARX400 Bruker NMR spectrometer, AZB-HS mass spectrograph, Rigaku 742 + single crystals diffractometer.

3. Results and discussion

3.1 Structure characterization

BMDATHBT: $C_6H_{16}N_{22}$, 396.1928 g·mol^{-1}.

IR（cm^{-1}，KBr）：3307, 3174 and 1657 cm^{-1} (N5H2), 3244, 3030 and 1616 cm^{-1} (N6H2), 2843 cm^{-1} (4-CH_3), 1709 cm^{-1} (C1—N5 in cation).

^{1}H NMR（DMSO- d_6，δ）: 8.37 ppm (-NH-NH-), 6.57 ppm (1, 5-NH_2), 3.66 ppm (4- CH_3).

MS (EI，70eV): $[M+H]^+$ 397.34411 is the molecular ion peak of BMDATHBT. It is consistent with the theoretical value of molecular weight 397.2006 [396.1928+1.0078].

3.2 Crystal structure

The molecular structure of BMDATHBT is shown in Fig 3. The cell accumulation of BMDATHBT is shown in Fig 4. The crystal data of BMDATHBT are listed in Table 1. The bond length, bond angle and dihedral angle of BMDATHBT are listed in Table 2. Hydrogen bonding data of BMDATHBT are listed in Table 3.

--------------------------------- Fig 3---------------------------------

--------------------------------- Fig 4---------------------------------

-------------------------------- Table 1--------------------------------

-------------------------------- Table 2--------------------------------

-------------------------------- Table 3--------------------------------

Seen from Fig 3, the two tetrazole rings connected by hydrazino are not in the same plane and the angle between the two planes of the tetrazole ring is 89.72°. Seen from Fig 4, the angle between the tetrazole ring of HBT^{2-} and the adjacent tetrazole ring of $BMDAT^{+}$ is 10.43°. The plane distance between the tetrazole ring of $BMDAT^{+}$ and the adjacent tetrazole ring of HBT^{2-} is 3.107 Å. There is offset face-to-face π-π interaction. Seen from Table 3, there are two kinds of hydrogen bonds N—H…N and C—H…N in the molecule. Except for C1 and C2, other atoms are involved in formation of hydrogen bond in HBT^{2-}. N5 and N6 are donors of hydrogen bond, and other N atoms are acceptors of hydrogen bond. The atoms involved in the formation of hydrogen bond in cationic are outside of the ring, and they are donors of hydrogen bond. Many atoms in HBT^{2-} are involved in formation of hydrogen bond, so BMDATHBT has good stability. However, the hydrogen bonds of HBT^{2-} are disconnected and BMDATHBT exists in the form of HBT^{2-} and $MDAT^{+}$ in aqueous solution, thus BMDATHBT is very easy to be oxidized in aqueous solution.

3.3 Theoretical calculation

3.3.1 Density

In 2007, the density prediction method of energetic ionic salts and compounds at room temperature was reported by Shreeve [11, 12]. The molecular volume can be estimated through this method, and then the density of compounds can be rapidly estimated. The molecular volumes of tetrazolate, tetrazolium, H bonded to C, H bonded to N, NH, NH_2 and CH_3 are 80, 66, 5, 7, 15, 20 and 30 respectively [11, 12]. Isodesmic reactions were designed to obtain the density of $MDAT^{+}$ and HBT^{2-} as follow in Fig 5.

-------------------------------- Fig 5--------------------------------

$V(MDAT^{+}) = V(\text{tetrazolium}) - V(\text{H bonded to C}) - 2V(\text{H bonded to N}) + 2V(NH_2) + V(CH_3) = 66-5-2*7+2*20+30 = 117\ (Å^3)$. $V(HBT^{2-}) = 2V(\text{tetrazolate}) - 2V(\text{H bonded to C}) + 2V(NH) = 2*80-2*5+2*15 = 180\ (Å^3)$. It is assumed that the molecular volume of ionic salt V (BMDATHBT) =V (+) +V (-) =2V ($MDAT^+$) +V (HBT^{2-}) =2*117+180=414 $Å^3$. The density of BMDATHBT can be calculated according to the molecular molar mass as follow: ρ=M/0.6022V=396.19/ (0.6022*414) =1.589 g/cm^3, which is close to the crystalline density 1.660 g/cm^3.

3.3.2 Heat of formation

The heat of formation is one of the important characteristics for the energetic salts [13]. All ab initio calculations were carried out by using the program package Gaussian 98 [14]. The single-point energies were calculated at the MP2 (full)/6-311++G** level. Heats of formation of the simple cations or anions were determined using atomization energies at G2 level. Isodesmic reactions were designed to obtain the heats of formation of cations and anions [15]. The enthalpy of isodesmic reaction (ΔH°_{r298}) was obtained by combining the MP2/6-311++G** energy difference for the reaction, the scaled zero-point energies (B3LYP/6-31+G**), and other thermal factors.

The heat of formation for BMDATHBT was calculated by Born-Haber energy cycles through the formula:

$$\Delta H_f^0 \text{ (inoic salt, 298K)} = \Delta H_f^0 \text{ (cation, 298K)} + \Delta H_f^0 \text{ (anion, 298K)} - \Delta H_L \quad (1)$$

The lattice energy of ionic salt ΔH_L could be predicted by Jenkins' method [formula (2)] [16]. Where U_{POT} is the lattice potential energy, n_M and n_X depend on the nature of the ions M_p^+ and X_q^-, respectively, and are equal to 3 for monatomic ions, 5 for linear polyatomic ions, and 6 for nonlinear polyatomic ions.

$$\Delta H_L = U_{POT} + [p(n_M/2-2) + q(n_X/2-2)]RT \qquad (2)$$

The lattice potential energy, U_{POT}, can be calculated using equation:

$$U_{POT}\ (\text{KJ mol}^{-1}) = \gamma(\rho_m/M_m)^{1/3} + \delta \qquad (3)$$

In which ρ is the density (g cm^{-3}), M is the chemical formula mass of the ionic material (g), and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) were assigned literature values [16]. The calculated thermochemical values of BMDATHBT were presented in Table 4.

-------------------------------- Table 4--------------------------------

3.3.3 Detonation pressure and detonation velocity

In order to assess the expected detonation properties of BMDATHBT, the expected detonation pressure and detonation velocity were calculated using the semi-empirical equations (eq.4, 5 and 6) according to Ref. [17].

$$P = K\rho^2\varphi \qquad (4)$$

$$D = A\varphi^{1/2}(1+B\rho) \qquad (5)$$

$$\varphi = N\sqrt{M(-\Delta_E H)} \qquad (6)$$

With: *P*=detonation pressure（GPa）；

D=detonation velocity（km/s）；

K=1.558；

ρ =density (g/cm^3) ；

N=moles of gas per g of explosive；

M=average molar mass of formed gases（g/mol）；

$\Delta_E H$ =estimated or guessed heat of detonation (kal/g) ；

A=1.01；

B=1.30.

According to the Le-Chatelier and Brinkley-Wilson method, the explosion and reaction equation of BMDATHBT is:

$$C_6N_{22}H_{16}\,(s) \longrightarrow 8H_2\,(g) + 6/xC_x + 11N_2\,(g)$$

The calculated detonation pressure and detonation velocity of BMDATHBT are shown in Table 5. BMDATHBT: P =25.93 GPa, D =7.839 km s^{-1}. They are both higher than those of TNT (P =19.5 GPa, D =6.881 km s^{-1}) [18].

--------------------------------- Table 5---------------------------------

3.4 Thermal analysis

Thermal decomposition process of the compound is the study foundation of the stability.

------------------------------ Fig 6---------------------------------

The TGA-DTA-DSC curves of BMDATHBT are shown in Fig 6. There was only one exothermic peak during the whole thermal decomposition process. The exothermic peak appeared within 180 to 200 ℃, and the peak temperature was 192.26 ℃. The thermal decomposition enthalpy was 865.3 J·g^{-1}. The mass loss was fast in this stage, accounting for 90.53% of the total mass loss. The mass loss reached the maximum at 190.11 ℃. The residue was 4.707%. Therefore, the thermal decomposition products were almost all gases. There was a short mass increase in the vicinity of 190 ℃. The reason may be that there were a lot of gases generated at the decomposition instant, and the recoil of the gases led to the brief rise of TG curve.

3.5 The sensitivity tests

3.5.1 The friction sensitivity test

The friction sensitivity tests of BMDATHBT were measured by MGY-1 friction sensitivity instrument with the friction sensitivity explosion probability method in GJB772A-97. The test results are shown in Table 6. The friction sensitivity of BMDATHBT is moderate.

-------------------------------- Table 6--------------------------------

3.5.2 The impact sensitivity test

The impact sensitivity tests of BMDATHBT were measured by WL impact sensitivity instrument with the impact sensitivity explosion probability method in GJB772A-97. The test results are shown in Table 7. The impact sensitivity of BMDATHBT is moderate.

-------------------------------- Table 7--------------------------------

There are many hydrogen bonds in the molecule, so BMDATHBT has good stability.

4. Conclusion

BMDATHBT was first synthesized. The single crystal of BMDATHBT was first cultivated in this work. Its crystalline density is 1.660 g/cm^3. BMDATHBT has high detonation pressure and detonation velocity (P =25.93 GPa, D =7.839 km s^{-1}), which are higher than those of TNT (P =19.5 GPa, D =6.881 km s^{-1}) [18]. Its thermal and mechanical sensitivities are moderate. The thermal decomposition products are almost all gases. Therefore, it has potential application prospect in gas generating agent, explosive and solid propellant.

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Caption of Figures

Fig 1 the synthetic route of MDATS

Fig 2 the synthetic route of BMDATHBT

Fig 3 the molecular structure of BMDATHBT

Fig 4 the cell accumulation of BMDATHBT

Fig 5 the isodesmic reactions of MDAT^{+} and HBT^{2-}

Fig 6 the TGA-DTA-DSC curves of BMDATHBT

Fig 1

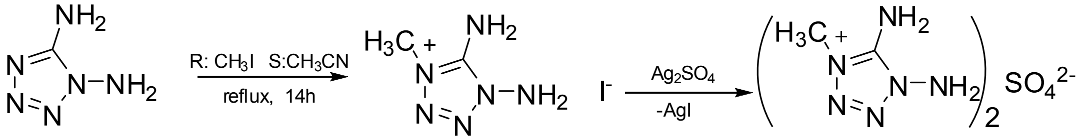

Fig 2

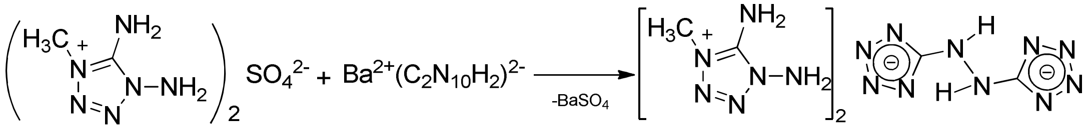

Fig 3

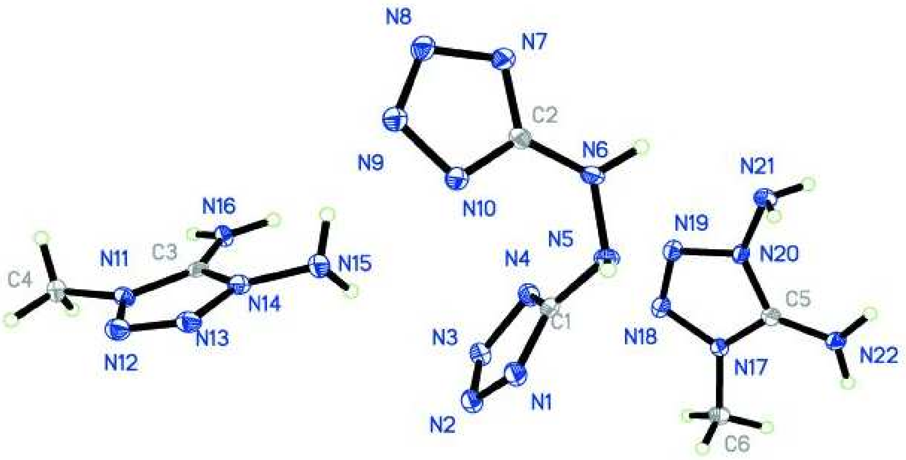
N8
N7
C2
N6
N9
N10
N21
N16
N19
N5
N20
N11
C3
N4
C4
N15
N14
C5
C1
N3
N18
N13
N22
N17
N12
N1
N2
C6

Fig 4

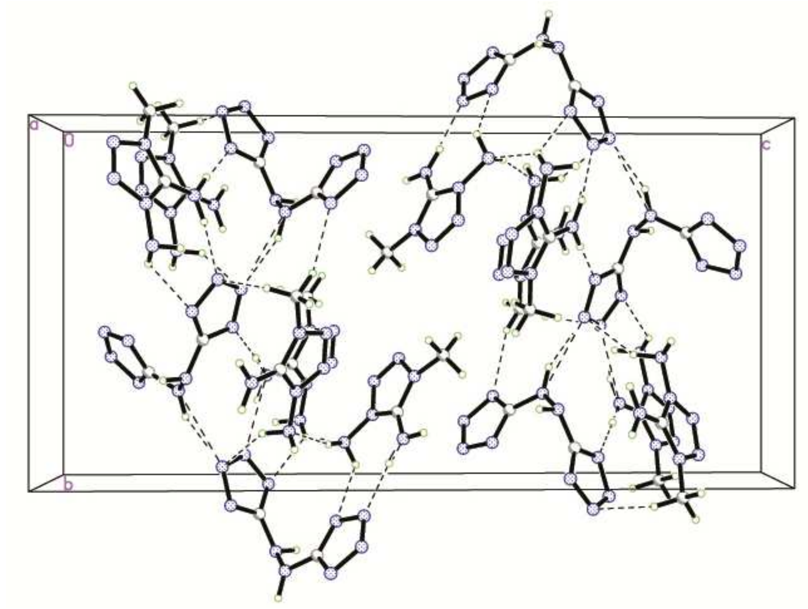
a
0
c
b

Fig 5

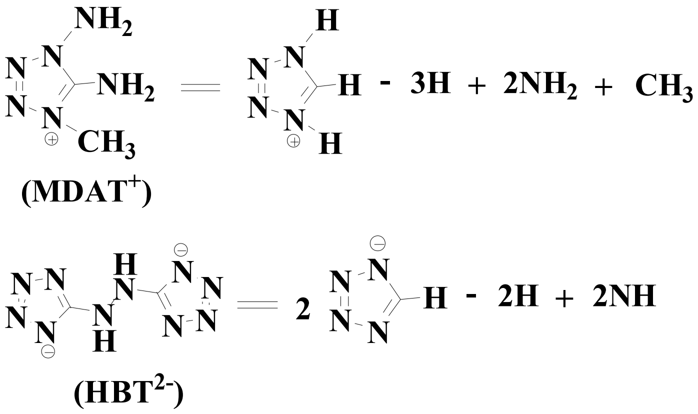
(MDAT$^+$)
- 3H + 2NH$_2$ + CH$_3$
(HBT^{2-})
2
- 2H + 2NH

Fig 6

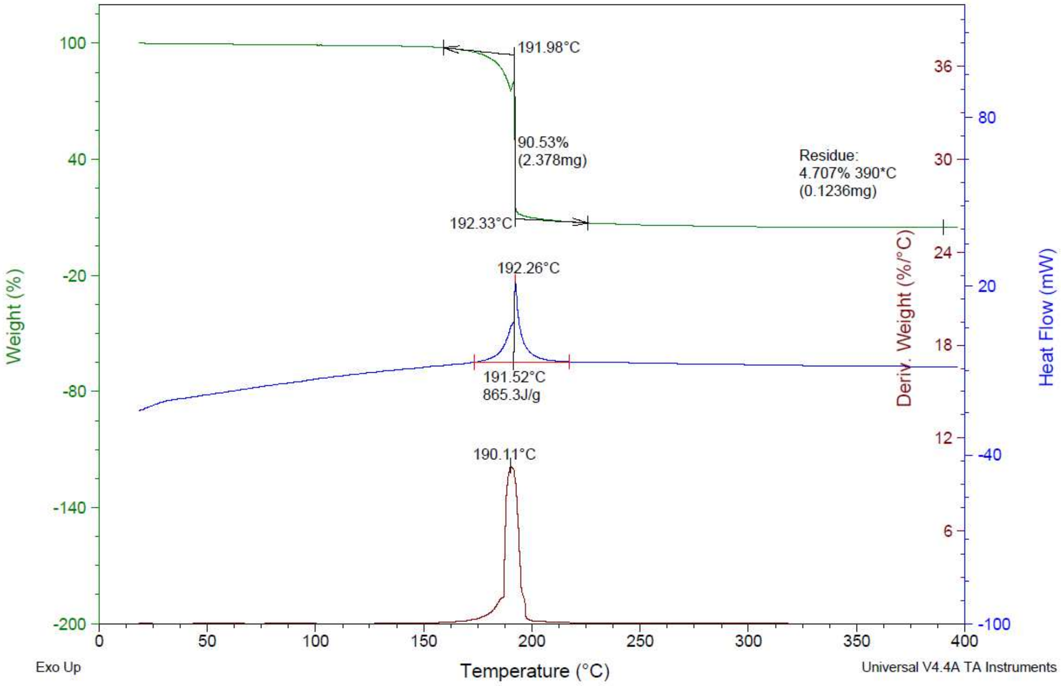
191.98°C
90.53%
(2.378mg)
192.33°C
Residue:
4.707% 390°C
(0.1236mg)
192.26°C
191.52°C
865.3J/g
190.11°C
Weight (%)
Deriv. Weight (%/°C)
Heat Flow (mW)
100
40
-20
-80
-140
-200
36
30
24
18
12
6
80
20
-40
-100
0
50
100
150
200
250
300
350
400
Exo Up
Temperature (°C)
Universal V4.4A TA Instruments

Table 1 the crystal data of BMDATHBT

Empirical formula	$C_6H_{16}N_{22}$
Formula weight(g/mol)	396.41
Temperature(K)	103(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
Crystal size(mm)	0.37 × 0.20 × 0.10
a(Å)	5.4170(12)
b(Å)	11.956(3)
c(Å)	24.503(6)
β(°)	92.202(3)
V(Å^3)	1585.9(6)
Z	4
ρ_{calcd}(g /cm^3)	1.660
F(000)	824
λ(*Mo Kα*)(Å)	0.71073
θ(°)	3.0-27.5
Reflections collected	4033
Independent reflections	3550
R_{int}	0.047
$h/k/l$	$-5 \le h \le 7$
	$-15 \le k \le 15$
	$-30 \le l \le 31$
Data/ Restraints/ Paramenters	3550/0/295
S	1.0
$\Delta\rho_{max}$, $\Delta\rho_{min}$(e/Å^3)	0.23, -0.21
wR_2	0.099^a

Note: ^{a} $w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.160P]$，$P = (F_o^2+2F_c^2)/3$

Table 2 the geometric parameters of BMDATHBT crystal (Å, °)

bond	bond length /Å	bond	bond length /Å
N1—C1	1.330 (2)	N15—H15B	0.91 (3)
N1—N2	1.356 (2)	N16—C3	1.305 (2)
N2—N3	1.309 (2)	N16—H16A	0.91 (2)
N3—N4	1.355 (2)	N16—H16B	0.93 (3)
N4—C1	1.337 (2)	N17—C5	1.342 (2)
N5—C1	1.397 (2)	N17—N18	1.369 (2)
N5—N6	1.412 (2)	N17—C6	1.456 (2)
N5—H5N	0.88 (2)	N18—N19	1.274 (2)
N6—C2	1.381 (2)	N19—N20	1.363 (2)
N6—H6N	0.92 (2)	N20—C5	1.352 (2)
N7—C2	1.335 (2)	N20—N21	1.387 (2)
N7—N8	1.360 (2)	N21—H21A	0.88 (2)

N8—N9	1.307 (2)	N21—H21B	0.87 (3)
N9—N10	1.353 (2)	N22—C5	1.306 (2)
N10—C2	1.332 (2)	N22—H22A	0.94 (3)
N11—C3	1.341 (2)	N22—H22B	0.90 (3)
N11—N12	1.366 (2)	C4—H4A	0.9800
N11—C4	1.455 (2)	C4—H4B	0.9800
N12—N13	1.270 (2)	C4—H4C	0.9800
N13—N14	1.361 (2)	C6—H6A	0.9800
N14—C3	1.350 (2)	C6—H6B	0.9800
N14—N15	1.387 (2)	C6—H6C	0.9800
N15—H15A	0.89 (2)		
bond	bond angle /°	bond	bond angle /°
C1—N1—N2	103.17 (13)	C5—N20—N19	110.25 (14)
N3—N2—N1	110.55 (14)	C5—N20—N21	130.61 (15)
N2—N3—N4	109.10 (14)	N19—N20—N21	118.44 (14)
C1—N4—N3	103.85 (14)	N20—N21—H21A	106.3 (14)
C1—N5—N6	112.97 (14)	N20—N21—H21B	108.7 (15)
C1—N5—H5N	110.9 (13)	H21A—N21—H21B	107 (2)
N6—N5—H5N	112.0 (13)	C5—N22—H22A	120.7 (15)
C2—N6—N5	118.58 (15)	C5—N22—H22B	116.2 (15)
C2—N6—H6N	121.5 (13)	H22A—N22—H22B	123 (2)
N5—N6—H6N	113.7 (13)	N1—C1—N4	113.32 (16)
C2—N7—N8	103.44 (14)	N1—C1—N5	123.13 (16)
N9—N8—N7	109.58 (14)	N4—C1—N5	123.45 (16)
N8—N9—N10	110.10 (14)	N10—C2—N7	113.29 (15)
C2—N10—N9	103.59 (14)	N10—C2—N6	123.15 (16)
C3—N11—N12	109.96 (14)	N7—C2—N6	123.50 (16)
C3—N11—C4	127.67 (14)	N16—C3—N11	128.53 (16)
N12—N11—C4	122.11 (14)	N16—C3—N14	127.72 (16)
N13—N12—N11	108.24 (14)	N11—C3—N14	103.74 (14)
N12—N13—N14	107.95 (14)	N11—C4—H4A	109.5
C3—N14—N13	110.10 (14)	N11—C4—H4B	109.5
C3—N14—N15	129.86 (15)	H4A—C4—H4B	109.5
N13—N14—N15	119.93 (14)	N11—C4—H4C	109.5
N14—N15—H15A	111.1 (15)	H4A—C4—H4C	109.5
N14—N15—H15B	107.8 (16)	H4B—C4—H4C	109.5
H15A—N15—H15B	110 (2)	N22—C5—N17	128.08 (17)
C3—N16—H16A	117.9 (13)	N22—C5—N20	128.36 (16)
C3—N16—H16B	120.6 (14)	N17—C5—N20	103.55 (15)
H16A—N16—H16B	121.2 (19)	N17—C6—H6A	109.5

C5—N17—N18	110.22 (14)	N17—C6—H6B	109.5
C5—N17—C6	129.08 (15)	H6A—C6—H6B	109.5
N18—N17—C6	120.48 (15)	N17—C6—H6C	109.5
N19—N18—N17	108.01 (14)	H6A—C6—H6C	109.5
N18—N19—N20	107.93 (14)	H6B—C6—H6C	109.5
bond	dihedral angle /°	bond	dihedral angle /°
C1—N1—N2—N3	−0.33 (18)	N9—N10—C2—N7	0.36 (19)
N1—N2—N3—N4	0.65 (19)	N9—N10—C2—N6	−176.98 (16)
N2—N3—N4—C1	−0.68 (18)	N8—N7—C2—N10	−0.07 (19)
C1—N5—N6—C2	69.8 (2)	N8—N7—C2—N6	177.26 (16)
C2—N7—N8—N9	−0.27 (18)	N5—N6—C2—N10	−6.4 (3)
N7—N8—N9—N10	0.51 (19)	N5—N6—C2—N7	176.52 (15)
N8—N9—N10—C2	−0.52 (18)	N12—N11—C3—N16	−179.02 (16)
C3—N11—N12—N13	−0.31 (19)	C4—N11—C3—N16	−4.8 (3)
C4—N11—N12—N13	−174.88 (16)	N12—N11—C3—N14	0.71 (18)
N11—N12—N13—N14	−0.24 (18)	C4—N11—C3—N14	174.90 (16)
N12—N13—N14—C3	0.71 (19)	N13—N14—C3—N16	178.87 (16)
N12—N13—N14—N15	177.22 (15)	N15—N14—C3—N16	2.8 (3)
C5—N17—N18—N19	1.05 (19)	N13—N14—C3—N11	−0.85 (18)
C6—N17—N18—N19	176.10 (15)	N15—N14—C3—N11	−176.91 (17)
N17—N18—N19—N20	0.32 (18)	N18—N17—C5—N22	177.68 (17)
N18—N19—N20—C5	−1.57 (19)	C6—N17—C5—N22	3.2 (3)
N18—N19—N20—N21	−172.93 (15)	N18—N17—C5—N20	−1.91 (18)
N2—N1—C1—N4	−0.12 (19)	C6—N17—C5—N20	−176.43 (16)
N2—N1—C1—N5	−176.65 (16)	N19—N20—C5—N22	−177.48 (16)
N3—N4—C1—N1	0.50 (19)	N21—N20—C5—N22	−7.5 (3)
N3—N4—C1—N5	177.01 (15)	N19—N20—C5—N17	2.11 (18)
N6—N5—C1—N1	−140.30 (17)	N21—N20—C5—N17	172.10 (17)
N6—N5—C1—N4	43.5 (2)		

Table 3 Hydrogen bonding data of BMDATHBT

D—H···*A*	*D*—H(Å)	H···*A*(Å)	*D*···*A*(Å)	*D*—H···*A*(°)
N5—H5N···N7^{i}	0.88 (2)	2.26 (2)	3.134 (2)	169.2 (19)
N6—H6N···N3^{ii}	0.92 (2)	2.10 (2)	2.966 (2)	157.4 (18)
N15—H15A···N1^{iii}	0.89 (2)	2.48 (2)	3.190 (2)	136.9 (18)
N15—H15A···N21^{iv}	0.89 (2)	2.56 (2)	3.300 (2)	140.6 (18)
N15—H15B···N3	0.91 (2)	2.43 (3)	3.180 (2)	140 (2)
N16—H16A···N2^{iii}	0.92 (2)	1.94 (2)	2.837 (2)	166.1 (19)

N16—H16B···N4^{iv}	0.93 (2)	1.89 (2)	2.817 (2)	172 (2)
N21—H21A···N15^{ii}	0.88 (2)	2.34 (2)	3.197 (2)	164.4 (19)
N21—H21B···N10^{ii}	0.86 (2)	2.54 (2)	3.040 (2)	117.5 (17)
N22—H22A···N9^{ii}	0.94 (2)	1.91 (2)	2.843 (2)	173 (2)
N22—H22B···N8^{v}	0.90 (2)	1.99 (2)	2.878 (2)	167 (2)
C4—H4B···N7^{vi}	0.98	2.50	3.446 (2)	162
C4—H4C···N2^{vii}	0.98	2.56	3.209 (2)	124

Symmetry codes: (i) x−1, y, z; (ii) −x+1, y−1/2, −z+3/2; (iii) x+1, y, z; (iv) −x+2, y+1/2, −z+3/2; (v) x−1, −y−3/2, z−5/2; (vi) x, y+1, z; (vii) −x+1, y+1/2, −z+3/2.

Table 4 the calculated thermochemical values of BMDATHBT

cation	anion	γ	δ	U_{POT}	p	q	n_M	n_X	$\Delta_f H_{cation}$ [a]	$\Delta_f H_{anion}$ [b]	$\Delta_f H_L$ [c]	$\Delta_f H(298K)$ [d]
$MDAT^+$	HBT^{2-}	8375.6	-178.8	1171.21	2	1	6	6	+998.74	+721.32	1178.65	+1540.15

Note: [a] calculated molar enthalpy of formation of cation [kJ mol^{-1}]. [b] Calculated molar enthalpy of formation of anion [kJ mol^{-1}]. [c] Calculated molar lattice energy [kJ mol^{-1}]. [d] Calculated molar enthalpy of formation of salts [kJ mol^{-1}].

Table 5 the detonation pressure and detonation velocity of BMDATHBT

Compound	ρ（g/cm^3）	$\Delta_E H^0$ (cal/g)	N	M	φ	P（GPa）	D（km/s）
BMDATHBT	1.660	-927.93	0.0480	17.05	6.04	25.93	7.839

Table 6 friction sensitivity test results of BMDATHBT

compound	group	number	sparking rate /%	average sparking rate /%	test condition
BMDATHBT	1	25	60	64	tilt angle: 66° pressure: 2.45MPa
	2	25	68		

Table 7 impact sensitivity test results of BMDATHBT

compound	group	number	sparking rate /%	average sparking rate /%	test condition
BMDATHBT	1	25	68	70	hammer quality: 10 kg hammer height: 250 mm
	2	25	72		

BMDATHBT

- **BMDATHBT was first synthesized**
- **The structure was characterized**
- **The single crystal was cultivated**
- **The detonation pressure and detonation velocity were calculated**
- **The thermal analysis was first studied**
- **The sensitivity was first studied**