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Synthesis, Crystal Structure, Thermal Analysis and Sensitivity of Mono-Ammonium Trinitrophloroglucinolate

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Abstract: A new compound of mono-ammonium trinitrophloroglucinolate [$NH_4(H_2TNPG)$, TNPG = Trinitrophloroglucinol] was synthesized and characterized by elemental analysis and Fourier transform infrared (FT-IR) spectrum. Its crystal structure was determined by single crystal X-ray diffraction analysis. The crystal belongs to monoclinic, $C2/c$ space group, $a = 9.307(2)$ Å, $b = 21.144(6)$ Å, $c = 9.797(2)$ Å, $\beta = 99.56(3)°$, $V = 1901.0(8)$ $Å^3$ and $Z = 8$. The compound is an ionic compound consisting of a cation NH_4^+ and an anion $C_6H_2N_3O_9^-$, and it is the mono-substituted salt of TNPG. Since the existence of complicated hydrogen bond networks and electrostatic attraction between NH_4^+ cation and $C_6H_2N_3O_9^-$ anion, the compound possesses better stability and low sensitivity. The thermal analysis of the compound was studied by using differential scanning calorimetry (DSC), and thermogravimetry thermogravimetry-derivative analysis (TG-DTG). Under nitrogen atmosphere with the heating rate of 10 ℃ · min^{-1}, the thermal decomposition of the compound show only one intense exothermic decomposition process at 219.2 – 234.3 ℃ on the DSC curve, and the decomposition products are nearly all gaseous products. Sensitivity Test revealed that the title compound is very insensitive to external stimuli.

Key words: physical chemistry; momo-ammonium trinitrophloroglucinlate; sensitivity; crystal structure; thermal analysis

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1 Introduction

Primary explosives are used in small quantities to generate a detonation wave when subjected to weak stimulations, such as a flame, heat, impact, electric spark or friction. Long term use of lead azide and lead styphnate as primary explosives has resulted in lead contamination at artillery and firing ranges and become a major health hazard and environmental problem for both military and civilian personnel[1]. There is a great demand for energetic materials chemists to find suitable nontoxic, heavy metal free substitutes which can be used as primary detonators[2]. The synthesis of low-toxic energetic materials has been a long term goal in our research group[3-8]. 2,4,6-trinitro-1,3,5-trihydroxybenzene (trinitrophloroglucinol, TNPG) has been used in chemical industry as an ingredient for making dyes and explosive industry as an ingredient for priming composition, percussion caps and detonator formulations[9-10]. As an acidic material, TNPG can form a large number of salts with alkaline and alkali-earth metals which may be of specific interest as potential components of initiating compositions free of toxic heavy metals[10].

Unlike many salts of nitro derivatives of mono- and dihydroxybenzenes, which the structure, thermal decomposition and explosive properties are fairly known[11-12], the crystal structures of salts of TNPG are seldom reported. Wolff[13-14] et al has reported the crystal structures of mono-, di- and tri-substituted potassium salts of trinitrophloroglucinol. Recently, our research group has reported synthesis, crystal structure and thermal decomposition of salts of trinitrophloroglucinol, including a number of salts based on alkali metals, alkaline earth metals and some nitrogen-rich compounds[4-8]. In continuation of our work on the relationship between the structure and properties of salts of TNPG, the title compound ammonium trinitrophlo-

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Corresponding author: ZHANG Tong-lai, male, Research fields: energetic materials. e-mail: ztlbit@bit.edu.cn roglucinolate [$NH_4(H_2TNPG)$] was synthesized, and its crystal structure and thermal analys were also reported.

2 Experimental

2.1 Materials

The starting material, trinitrophloroglucinol, was prepared according to a published procedure[14] and recrystallized before using in the synthesis. All other chemicals were of A. R. grade chemicals and used without further purification as commercially obtained.

2.2 Preparation of $NH_4(H_2TNPG)$

A solution containing trinitrophloroglucinol (7.83 g, 0.03 mol) in 40 mL of distilled water was charged into a glass reactor with a water bath. It was kept under mechanical stirring and heated to the temperature of 60 ℃ ammonium hydroxide (0.03 mol, 12 mL, 10% in mass ratio) was added dropwise with continuous stirring over a period of 15 min and the yellow microcrystalline precipitate was formed gradually. The suspension was stirred for an additional 15 min at 60 ℃ and then cooled to room temperature. The precipitate was collected by filtration and dried in an oven. Yield is 86%. Yellow needle shaped single crystals suitable for X-ray measurement were obtained by recrystallization with the distilled water at room temperature for 2 weeks. Elemental analysis for $C_6H_6N_4O_9$ (molar mass: 278.15 g · mol^{-1}) (%): calculated: N 20.14; H 2.17; C 25.91; found: N 20.35; H 2.29; C 25.84. IR (cm^{-1}, KBr pellets): 3637w, 3468w (ν N—H), 3217m (ν O—H), 1645s (ν Ph—OH), 1553s (ν_{as} NO_2), 1347s (ν_s NO_2), 1192s (ν C—O), 938w, 784w, 711w (δ ring bone).

2.3 Physical measurements

Elemental analyses were performed on a Flash EA 1112 full-automatic trace element analyzer. The FT-IR spectra were recorded on a Bruker Equinox 55 infrared spectrometer (KBr pellets) in the range of 4000 - 400 cm^{-1} with the resolution of 4 cm^{-1}.

DSC and TG measurements were carried on a Pyris-1 differential scanning calorimeter and Pyris-1 thermogravimetric analyzer (Perkin Elmer, USA), respectively, using dry nitrogen as atmosphere with flowing rate of 20 mL · min^{-1}. The analysis conditions were as follows: for Pyris-1 DSC, the crystal sample was powdered and sealed in aluminum pans with a linear heating rate of 5, 10, 15, 20 and 25 ℃ · min^{-1} from 50 ℃ to 450 ℃; for Pyris-1 TGA, the crystal sample was powdered and put in the platinum open pans with heating rate of 10 ℃ · min^{-1} from 50 ℃ to 450 ℃.

The sensitivities of the title compound was tested by following standard methods[15]. The impact sensitivity was determined by the drop hammer method using a 0.8 kgdrop weight on the CGY-1 mechanical impact sensitivity instrument. The friction sensitivity was determined on the MGY-1 pendulum friction sensitivity apparatus. After the sample was compressed between two steel poles with mirror surfaces at the pressure of 1.96 MPa firmly, one of the steel pole was horizontally hit with a 1 kg hammer pendulum dropping from 90°. The flame sensitivity was determined on the HGY-1 flame sensitivity apparatus, the pressed sample was ignited by standard black powder pellet on the apparatus.

2.4 Crystal structure determinations and refinements

A yellow needle shaped single crystal with dimensions of 0.14 mm × 0.10 mm × 0.06 mm was selected for X-ray diffraction analysis. The data collection was performed on a Rigaku MicroMax-007 diffractometer equipped with a Saturn 70 CCD by using MoK_α radiation ($\lambda = 0.71073$ Å) at 113(2) K with phi and omega scans mode. A total of 7274 reflections (2265 unique, $R_{int} = 0.0645$) were measured in the range of $2.42° < \theta < 27.85°$, of which 1683 were observed with $I > 2\sigma(I)$. Empirical absorption corrections were applied by using the Crystal Clear program. The structure was solved directly by using SHELXS-97 program and refined by full-matrix least-squares methods on F^2 with SHELXL-97 program. All non-hydrogen atoms were obtained from the difference Fourier map and refined anisotropically. The hydrogen atoms were obtained geometrically and treated as riding on the parent atoms or were constrained in the locations during refinements. A full-matrix least-squares refinement gave the final $R_1 = 0.0394$ and $wR_2 = 0.0981$ ($w = 1/[\sigma^2(F_0{}^2) + (0.0541P)^2 + 0.0000P]$, where $P = (F_0{}^2 + 2F_c{}^2)/3$). The goodness-of-fit on F^2 is 0.986. The largest difference peak and hole were 0.372 e · Å^{-3} and -0.461 e · Å^{-3}. In the final circle of refinement the largest parameter shift (Δ/σ) max is 0.001. The detailed crystallographic data are listed in Table 1.

Table 1 Crystal data and structure refinement parameters for $NH_4(H_2TNPG)$

CCDC number	670293
empirical formula	$C_6H_6N_4O_9$
molar mass/g · mol^{-1}	278.15
temperature/K	113(2)
crystal system	C2/*c*
space group	monoclinic
crystal size /mm	0.14 × 0.10 × 0.06
a/Å	9.306(2)
b/Å	21.144(6)
c/Å	9.797(2)
β/°	99.563)
V/Å^3	1901.0(8)
Z	8
h	$-12 \leq h \leq 11$
k	$-27 \leq k \leq 23$
l	$-10 \leq l \leq 12$
D_c/g · cm^{-3}	1.944
λ/Å	0.71073
$\mu(MoK_\alpha)$/mm^{-1}	0.187
F(0 0 0)	1136
θ/(°)	2.42 - 27.85
measured reflections	7274
unique data (R_{int})	2265 (0.0645)
R_1, wR_2 [$I > 2\sigma(I)$]	0.0394, 0.0981
R_1, wR_2 (all data)	0.0507, 0.1027
goodness-of-fit	0.986
δp_{max}, δp_{min}/e · Å^{-3}	0.372, -0.461

3 Results and discussion

3.1 The crystal structure description

The molecular structure of the title compound with the atomic numbering scheme is shown in Fig. 1. The atomic coordinates and displacement parameters, selected bond lengths and angles are listed in Table 2 and Table 3. The crystal structure analysis shows that the title compound is an ionic salt consisting of a cation NH_4^+ and an anion $C_6H_2N_3O_9^-$, and it is the mono-substituted salt of H_3TNPG. However, the title compound is novel in that there are two crystallographically independent sets of $C_6H_2N_3O_9^-$ anions which are bonded together with two NH_4^+ by electrostatic attraction and hydrogen bonds to form a stable salt of ammonium trinitrophloroglucinolate. TNPG offers only one hydroxylic proton from C(1) or C(5), which forms TNPG univalent anions. Whereas the two hydroxylic protons of the other hydroxyl groups in the same $C_6H_2N_3O_9^-$ anion are bonded to the oxygen atom (O(5), O(5A) or O(8), O(8B)) of neighboring nitro groups by hydrogen bonds.

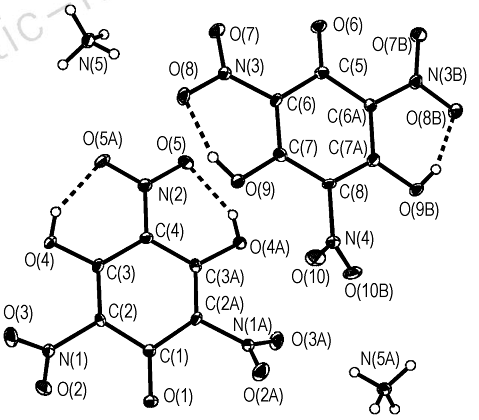

Fig. 1 The molecular structure and atomic numbering scheme for $NH_4(H_2TNPG)$

Table 2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $NH_4(H_2TNPG)$

atom	*x*	*y*	*z*	*U*(eq)
O(1)	0	4574(1)	2500	15(1)
O(2)	436(1)	4324(1)	-249(1)	21(1)
O(3)	2503(1)	3843(1)	280(1)	18(1)
O(4)	1419(1)	2671(1)	640(1)	16(1)
O(5)	-635(1)	1652(1)	3336(1)	17(1)
O(6)	0	319(1)	7500	15(1)
O(7)	1400(1)	401(1)	5428(1)	22(1)
O(8)	2311(1)	1295(1)	4950(1)	16(1)
O(9)	1599(1)	2289(1)	5896(1)	14(1)
O(10)	1172(1)	3232(1)	7539(1)	19(1)
N(1)	1237(1)	3948(1)	451(1)	13(1)
N(2)	0	1953(1)	2500	13(1)
N(3)	1515(1)	968(1)	5644(1)	13(1)
N(4)	0	2959(1)	7500	13(1)
C(1)	0	3981(1)	2500	11(1)
C(2)	660(2)	3608(1)	1543(2)	12(1)
C(3)	725(2)	2957(1)	1547(2)	11(1)
C(4)	0	2614(1)	2500	11(1)
C(5)	0	906(1)	7500	11(1)
C(6)	796(2)	1281(1)	6616(2)	11(1)
C(7)	844(2)	1952(1)	6662(2)	11(1)
C(8)	0	2270(1)	7500	11(1)
N(5)	2611(2)	452(1)	2576(2)	15(1)

Note: *U*(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 3 Selected bond lengths and bond angles

bond	bond lengths /Å	bond	bond angles /(°)
O(1)—C(1)	1.254(2)	C(2)—C(1)—C(2)$1^{\#}$	113.6(2)
O(6)—C(5)	1.240(2)	C(3)—C(2)—C(1)	124.6(2)
C(1)—C(2)	1.439(2)	C(2)—C(3)—C(4)	118.8(2)
C(2)—C(3)	1.379(2)	C(3)—C(4)—C(3)$1^{\#}$	119.4(2)
C(3)—C(4)	1.435(2)	C(6)—C(5)—C(6)$2^{\#}$	114.3(2)
C(5)—C(6)	1.463(2)	C(7)—C(6)—C(5)	122.7(2)
C(6)—C(7)	1.420(2)	C(8)—C(7)—C(6)	118.7(2)
C(7)—C(8)	1.399(2)	C(7)—C(8)—C(7)$2^{\#}$	122.5(2)

Note: Symmetry transformations used to generate equivalent atoms: $1^{\#}$ $-x, y, -z+1/2$; $2^{\#}$ $-x, y, -z+3/2$.

For one of the phenyl ring (C(1)—C(2)—C(3)—C(4)—C(3A)—C(2A)), the C—C bond lengths range from 1.379(2) Å (C(2)—C(3)) to 1.439(2) Å (C(1)—C(2)) with average length of 1.4175 Å which is comparable with the C—C bond lengths 1.400 Å of normal benzene ring. The bond angles in phenyl ring range from 113.6(2)° (C(2)—C(1)—C(2A)) to 124.6(2)° (C(1)—C(2)—C(3)) with average angle of 119.96°. Due to strongly electron withdrawing nitro groups on phenyl ring, the C(1)—C(2)—C(3) bond angle (124.6(2)°) is bigger than normal bond angles of benzene ring. Whereas the C(3)—C(4)—C(3A) bond angle (119.4(2)°) is normal, this is because the nitro group bonded with C(4) is coplanar with the phenyl ring and is conjugation with the ring, and there is a special bond in this nitro group, which plays a significant role to the stability of the compound. Moreover, the oxygen atoms of this nitro group are all bonded to the neighboring hydroxylic protons of hydroxyl groups by hydrogen bonds, which decrease the electron withdrawing capacity of the nitro group. But the other two nitro groups are not coplanar with the phenyl ring. Owing to the *p*-*π* conjugation between atoms of phenolic hydroxyl group and phenyl ring, the bond length of C(1)—O(1) is 1.254(2) Å, which is a very close approximation to the value of natural double bond C═O (1.214 Å)[16]. This *p*-*π* conjugation cause to the bond angles of C(2)—C(1)—C(2A) [113.6(2)°] and C(2)—C(3)—C(4) [118.8(2)°] smaller than normal bond angles of benzene ring.

Interestingly, for the other phenyl ring (C(5)—C(6)—C(7)—C(8)—C(7A)—C(6A)), nitro groups bonded to C(6) and C(6A) are coplanar and conjugation with the phenyl ring, while the other nitro group (bonded to C(8)) not coplanar with the phenyl ring. As a result, the corresponding bond angles [C(5)—C(6)—C(7), C(7)—C(8)—C(7A)] are little bigger than normal bond angles of benzene ring. The bond length of C(5)—O(6) (1.240(2) Å) is very close to the value of natural double bond due to the *p*-*π* conjugation between atoms of phenolic hydroxyl group and phenyl ring. The C—C bond lengths of the phenyl ring ranges from 1.399(2) Å (C(7)—C(8)) to 1.463(2) Å (C(5)—C(6)) with average length of 1.4275 Å. The bond angles range from 114.3(2)° (C(6)—C(5)—C(6A)) to 122.7(2)° (C(5)—C(6)—C(7)) with average angle of 119.94°.

As shown in Fig. 2, there are intramolecular and intermolecular hydrogen bonds in the compound. The hydrogen bond lengths and angles are summarized in Table 4. There are two types of intramolecular hydrogen bonds in the title compound. One is exhibited by oxygen atom (O(4), O(9)) of phenolic hydroxyl group in one anion with other oxygen atom (O(5), O(8)) of nitro group in the same anion [O(4)—H(4A)···O(5)#4, O(9)—H(9)···O(8)], and thus four stable six-membered rings are formed which enhance the robustness of the molecule. The other forms an O—H···N hydrogen bond [O(4)—H(4A)···N(2), O(9)—H(9)···N(3)] which occurs between oxygen atom (O(4), O(9)) of phenolic hydroxyl group in one anion with nitrogen atom (N(2), N(3)) of nitro group in the same anion. There are three types of intermolecular hydrogen bonds among $NH_4(H_2TNPG)$ molecules. The first occurs between nitrogen atom of NH_4^+ and oxygen atom of phenolic hydroxyl group in $C_6H_2N_3O_9^-$: N(5)—H(1)···O(6)#1; the second occurs between nitrogen atom of NH_4^+ and oxygen atom of nitro groups in $C_6H_2N_3O_9^-$: N(5)—H(1)···O(7)#2, N(5)—H(3)···O(3)#3 and N(5)—H(4)···O(8); the third occurs between oxygen atom of phenolic hydroxyl group and oxygen atom of phenolic hydroxyl group of adjacent anion: O(9)—H(9)···O(9)#5. All these intermolecular hydrogen bonds extend the structure into a 3D supramolecular array and make an important contribution to enhance the robustness of the title compound.

Table 4 Hydrogen bond lengths(Å) and angles (°)

D—H···A	d(D—H)	d(H···A)	d(D···A)	D—H···A angle
N(5)—H(1)···O(6)#1	0.88(2)	2.04(2)	2.917(2)	172(2)
N(5)—H(1)···O(7)#2	0.88(2)	2.42(2)	2.857(2)	111(2)
N(5)—H(3)···O(3)#3	0.89(2)	2.27(2)	3.157(2)	173(2)
N(5)—H(4)···O(8)	0.90(2)	2.10(2)	2.980(2)	166(2)
O(4)—H(4A)···N(2)	0.78(2)	2.41(2)	2.858(2)	118(2)
O(4)—H(4A)···O(5)#4	0.78(2)	1.84(2)	2.535(2)	149(2)
O(9)—H(9)···O(8)	0.82(2)	1.67(2)	2.433(2)	154(2)
O(9)—H(9)···N(3)	0.82(2)	2.29(2)	2.805(2)	121(2)
O(9)—H(9)···O(9)#5	0.82(2)	2.49(2)	2.769(2)	101(2)

Note: Symmetry transformations used to generate equivalent atoms: #1 −x, −y, 1−z; #2 −x, −y, −1/2+z; #3 −1/2−x, 1/2−y, −z; #4 −x, y, 1/2−z; #5 −1/2−x, 1/2−y, 1−z.

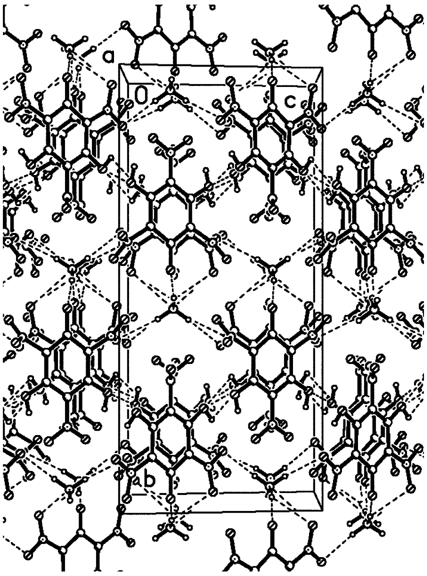

Fig. 2 The packing plot of $NH_4(H_2TNPG)$ along a-axis of unit cell

3.2 Thermal analysis

The DSC and TG-DTG curves of $NH_4(H_2TNPG)$ are shown in Fig. 3 and Fig. 4. There is only one sharp exothermic peak in the DSC curve from 50 to 450 ℃. The exothermic peak starts at 219.2 ℃, ends at 234.3 ℃, and the peak temperature is 223.4 ℃. The enthalpy of this exothermic process is 291.6 kJ · mol^{-1}.

There is one intense mass loss stage from 50 to 450 ℃ in the TG-DTG curves, which corresponds to the exothermic process in the DSC curve. The mass loss stage starts at 210.0 ℃, ends at 220.2 ℃ with mass loss of 86.59%, and the peak temperature is 218.2 ℃. This stage is predicted as the bond cleavages of nitro groups in $C_6H_2N_3O_9^-$ and the breaking-up of the phenyl rings. The weight loss occurs continuously with the heating processes going on, and the final residue of the thermal decomposition at 450 ℃ amounts to 2.54%.

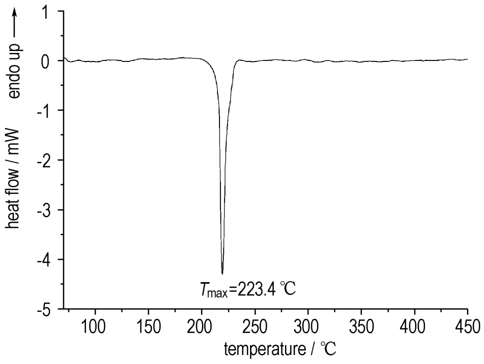

Fig. 3 DSC curve of $NH_4(H_2TNPG)$ under N_2 atmosphere with the heating rate of 10 ℃ · min^{-1}

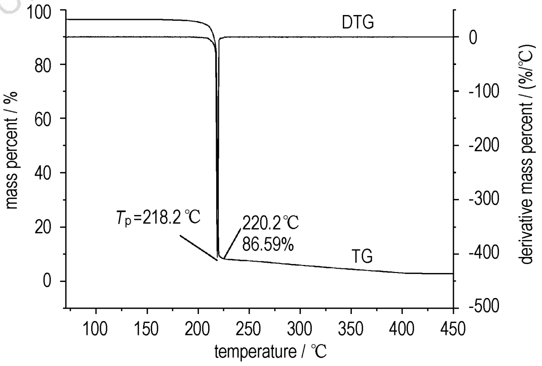

Fig. 4 TG-DTG curve of $NH_4(H_2TNPG)$ under N_2 atmosphere with the heating rate of 10 ℃ · min^{-1}

3.3 Non-isothermal kinetics analysis

In order to obtaining the kinetics parameters of the decomposition process, Kissinger's method[17] and Ozawa-Doyle's[18-19] method are used to determine the apparent activation energy (E) and the pre-exponential factor (A). The Kissinger and Ozawa-Doyle equations are as follows, respectively:

$$\ln\frac{\beta}{T_{\mathrm{p}}^{2}}=\ln\left[\frac{RA}{E}\right]-\frac{E}{R}\cdot\frac{1}{T_{\mathrm{p}}} \qquad (1)$$

$$\log\beta+\frac{0.4567E}{RT_{\mathrm{p}}}=C \qquad (2)$$

Where: T_{p} is the peak temperature, K; A is the pre-exponential factor, s^{-1}; E is the apparent activation energy, $\mathrm{kJ\cdot mol^{-1}}$; R is the gas constant, $\mathrm{kJ\cdot(K\cdot mol)^{-1}}$; β is the linear heating rate, $\mathrm{K\cdot min^{-1}}$, and C is a constant.

Based on the first exothermic peak temperatures measured at five different heating rates as show in Table 5, Kissinger's and Ozawa-Doyle's method were applied to calculate the kinetics parameters of the compound $NH_4(H_2TNPG)$. The results from Kissinger's method are: $E_{\mathrm{k}}=396.4\ \mathrm{kJ\cdot mol^{-1}}$ and $\ln(A_{\mathrm{k}}/\mathrm{s}^{-1})=40.18$ with $R_{\mathrm{k}}=-0.9941$, and the results from Ozawa-Doyle's method are: $E_{\mathrm{o}}=384.8\ \mathrm{kJ\cdot mol^{-1}}$ with $R_{\mathrm{o}}=-0.9943$. The calculated results using both methods are within the normal range of kinetic parameters of the solid materials' thermal decomposition reaction[20], and corresponding with each other.

Table 5 The peak temperatures of the first exotherm at different heating rates and the kinetics parameters

heating rates/K · min^{-1}	peak temperatures/K
5	493.75
10	496.55
15	498.65
20	500.35
25	501.95

3.4 Sensitivity

The explosion probability is zero by a 0.8 kg hammer dropped from the impact sensitivity apparatus highest point of 50 cm.

Friction sensitivity was determined with the standard method, and the firing rate is 11%.

The sample of $NH_4(H_2TNPG)$ couldn't be fired by the black powder flame on the flame sensitivity apparatus.

Compared to sensitivities of potassium and sodium salt of TNPG[6-8] under the same conditions, $NH_4(H_2TNPG)$ is relatively insensitive to the external stimuli.

4 Conclusion

The new compound $NH_4(H_2TNPG)$ was synthesized and characterized. Its crystal structure was analyzed. It is an ionic compound consisting of a cation NH_4^+ and an anion $C_6H_2N_3O_9^-$, and it is the mono-substituted salt of TNPG. The existence of complicated hydrogen bond networks and electrostatic attraction between NH_4^+ cation and $C_6H_2N_3O_9^-$ anion cause to the title compound has better stability and low sensitivity. The thermal decomposition enthalpy is higher and the decomposition products all nearly are gaseous products. It can be further studied as the gas-generating composition and component of primary explosives, emission reagents and propellant components. Sensitivity Test show that the title compound is relatively insensitive to external stimuli.

Supplementary materials

CCDC-670293 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

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三硝基均苯三酚一铵盐的合成、晶体结构、热分析及感度性能研究

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摘要: 合成了三硝基间苯三酚一铵盐 $NH_4(H_2TNPG)$,并对其进行了元素分析及红外表征。利用 X 射线单晶分析测定了其晶体结构,晶体属于单斜晶系,空间群为 $C2/c$,晶体学数据为: $a=9.307(2)$ Å,$b=21.144(6)$ Å,$c=9.797(2)$ Å,$\beta=99.56(3)°$,$V=1901.0(8)$ Å^3,$Z=8$。该化合物是由一个铵根离子与一个一价的三硝基均苯三酚负离子相结合而形成的离子型化合物,分子中存在的大量氢键及铵根离子与三硝基均苯三酚负离子之间的静电引力使得该化合物具有较高的热稳定性和较低的感度。用 DSC、TG-DTG 技术研究了标题化合物的热分解,研究结果表明: 在 10 ℃·min^{-1}的升温速率下,标题化合物只有一个剧烈的放热分解过程,该过程发生在 219.2~234.3 ℃之间,分解产物主要是气体产物。感度测试结果表明,该化合物对外部刺激钝感。

关键词: 物理化学; 三硝基间苯三酚一铵; 感度性能; 晶体结构; 热分析

中图分类号: TJ55; O741$^+$.6; O625.32$^+$1 **文献标识码:** A

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更 正

2008 年第 2 期 188 页右栏倒数第 4 行“图 3 为 250 MPa 条件下观察到的 HMX 颗粒形貌”应为“图 3 为 100 MPa 条件下观察到的 HMX 颗粒形貌”。特此更正。