J Therm Anal Calorim (2011) 104:999–1004
DOI 10.1007/s10973-010-1231-9

Thermal behavior of 1,2,3-triazole nitrate

**Liang Xue · Feng-Qi Zhao · Xiao-Ling Xing ·
Zhi-Ming Zhou · Kai Wang · Hong-Xu Gao ·
Jian-Hua Yi · Si-Yu Xu · Rong-Zu Hu**

Received: 14 August 2010 / Accepted: 30 November 2010 / Published online: 19 December 2010

Abstract The thermal decomposition behaviors of 1,2,3-triazole nitrate were studied using a Calvet Microcalorimeter at four different heating rates. Its apparent activation energy and pre-exponential factor of exothermic decomposition reaction are 133.77 kJ $\mathrm{mol^{-1}}$ and $10^{14.58}$ $\mathrm{s^{-1}}$, respectively. The critical temperature of thermal explosion is 374.97 K. The entropy of activation ($\Delta S^{\neq}$), the enthalpy of activation ($\Delta H^{\neq}$), and the free energy of activation ($\Delta G^{\neq}$) of the decomposition reaction are 23.88 J $\mathrm{mol^{-1}\ K^{-1}}$, 130.62 kJ $\mathrm{mol^{-1}}$, and 121.55 kJ $\mathrm{mol^{-1}}$, respectively. The self-accelerating decomposition temperature (T_{SADT}) is 368.65 K. The specific heat capacity was determined by a Micro-DSC method and a theoretical calculation method. Specific heat capacity equation is $C_{\mathrm{p}}\left(\mathrm{J\ mol^{-1}\ K^{-1}}\right) = -42.6218 + 0.6807T$ ($283.1\ \mathrm{K} < T < 353.2\ \mathrm{K}$). The adiabatic time-to-explosion is calculated to be a certain value between 98.82 and 100.00 s. The critical temperature of hot-spot initiation is 637.14 K, and the characteristic drop height of impact sensitivity (H_{50}) is 9.16 cm.

Keywords 1,2,3-Triazole nitrate · Thermal behavior · Specific heat capacity · Adiabatic time-to-explosion · Critical temperature of hot-spot initiation

Introduction

Triazole is a five-membered heterocyclic compound, which contains three nitrogen atoms. The three nitrogen atoms are on position 1,2,4 or 1,2,3 of a five-membered heterocycle. Triazole derivative has proven to be a novel energetic compound with high nitrogen content. Its high energy comes from its very high positive enthalpy of formation [1–4]. In comparison with TNT with a negative enthalpy of formation (−62.73 kJ $\mathrm{mol^{-1}}$), this difference of enthalpy of formation gives energetic triazole ionic salts an advantage in the explosive performance. Changing cations, anions, and groups can make their performances, including sensitivity, energy, density, and melting point be easy to adjust for achieving the purpose of decreasing the sensitivity, enhancing energy and density, and controlling melting point, and synthesized energetic triazole ionic salts have the advantages of high thermal stability, low volatility, and higher density [4, 5]. Energetic triazole ionic salts in the liquid state are non-toxic, and these can reduce the cost and danger. Because the strong interaction exists between ions, triazole ionic salts as a continuous phase in B explosives can inhibit the migration effect, resolve the permeability problems of explosives, and improve the safety performance of explosives [1–3]. Rich nitrogen ionic salts have a strong solubility and high density, and good or fair compatibility with solid propellant components [6–9]. The polarity of ionic salts can be used for propellant combustion performance adjustment, and, therefore, energetic triazole ionic

---

L. Xue · F.-Q. Zhao (✉) · X.-L. Xing · H.-X. Gao · J.-H. Yi ·
S.-Y. Xu · R.-Z. Hu
National Key Lab of Science and Technology on Combustion
and Explosion, Xi'an Modern Chemistry Research Institute,
Xi'an 710065, China
e-mail: npecc@163.com

L. Xue
School of Chemistry and Materials Science,
Shaanxi Normal University, Xi'an 710062, China

Z.-M. Zhou · K. Wang
School of Chemical Engineering and Environment,
Beijing Institute of Technology, Beijing 100081, China

salts are a kind of energetic materials with good application prospect [10–13].

However, a great deal of research has focused on the synthesis and application of energetic triazole ionic salts while there have been few studies on the fundamental thermodynamic [1–13]. As far as we know, the thermodynamic properties of energetic triazole ionic salts, such as heat capacity (C_p), apparent activation energy (E), and pre-exponential factor (A) of exothermic decomposition reaction, critical temperature of thermal explosion (T_b), entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), free energy of activation ($\Delta G^{\neq}$), self-accelerating decomposition temperature (T_{SADT}), adiabatic time-to-explosion (t), critical temperature of hot-spot initiation ($T_{cr,\ hot\text{-}spot}$), and characteristic drop height of impact sensitivity (H_{50}) are important properties that reflect the structures and stabilities of compounds but were rarely reported.

In this study, Calvet Microcalorimeter and Micro-DSC methods were applied for researching the thermodynamic properties of 1,2,3-triazole nitrate, and the data were analyzed to obtain the self-acceleration decomposition temperature; the critical temperature of thermal explosion, the adiabatic time-to-explosion, and the critical temperature of hot-spot initiation were obtained at the same time.

Experimental

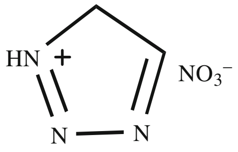
Materials

1,2,3-Triazole nitrate in this research was prepared by Beijing Institute of Technology and Xi'an Modern Chemistry Research Institute, China. The structure was characterized by means of organic elemental analysis, ^{15}N NMR, ^{13}C NMR, and LC–MS. The sample's purity was more than the mass fraction, 0.995. The structure for 1,2,3-triazole nitrate is shown in Scheme 1. The 1,2,3-triazole nitrate was further purified by evacuating the sample to a very low pressure of about 5×10^{-3} Pa at temperature about 70 °C for approximately 5 h. This procedure removed any volatile chemicals and water from the triazole ionic salts.

Equipment and conditions

The heat flow curves of the exothermic decomposition process of 1,2,3-triazole nitrate was measured using a C-500 type Calvet Microcalorimeter, which had a sensitivity of 0.10 μV mW^{-1} and was equipped with two 10-mL vessels. The precision of enthalpy measurement was less than fraction 0.005 after adjusting. The four different heating rates used were 12 K h^{-1} (0.20 K min^{-1}), 18 K h^{-1} (0.30 K min^{-1}), 24 K h^{-1} (0.40 K min^{-1}), and 30 K h^{-1} (0.50 K min^{-1}). The sample used was about 10 mg, and the reference sample was α-Al_2O_3. Each process was repeated three times, and the heat flow curves under the same conditions overlap with each other, indicating that the reproducibility of test is satisfactory.

Scheme 1 The structure of 1,2,3-triazole nitrate



The measurement of specific heat capacity (C_p) was performed using a Micro-DSCIII apparatus. The amount of used sample was 410.98 mg. The heating rate was maintained at 0.15 K min^{-1}for the temperatures ranging from 283.1 to 353.2 K.

Results and discussion

Thermal decomposition behavior

The heat flow curves for 1,2,3-triazole nitrate are show in Fig. 1, which shows that the thermal behavior of 1,2,3-triazole nitrate can be divided into two stages. The first stage is a melting process. The second stage is an intense exothermic decomposition process. The characteristic temperatures of exothermic decomposition process obtained by heat flow curves at different heating rates are listed in Table 1. In Table 1, β is the heating rate, T_p the peak temperature, T_e the onset temperature, and ΔH the enthalpy of decomposition reaction.

In order to obtain the kinetic parameters [the apparent activation energy (E) and the pre-exponential constant (A)] of the decomposition reaction for 1,2,3-triazole nitrate, multiple heating methods (Kissinger method [14] and

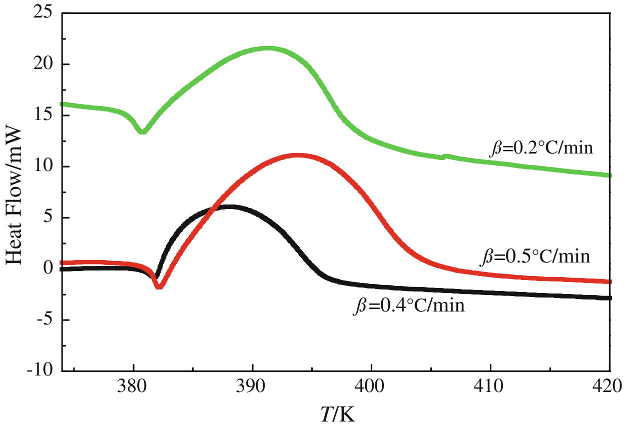


Fig. 1 Heat flow curves of 1,2,3-triazole nitrate at different heating rates

Table 1 Original data of the thermal decomposition reaction of 1,2,3-triazole nitrate at different heating rates

β/K min^{-1}	T_e/K	T_p/K	$Q = -\Delta H$/kJ mol^{-1}
0.20	378.62	387.80	217.95
0.30	381.90	391.01	225.79
0.40	383.44	393.96	224.96
0.50	384.17	396.06	221.99

Ozawa method [15]) were employed. Kissinger and Ozawa equations [14–20] are as follows:

$$\ln\left(\frac{\beta_i}{T_{pi}^2}\right) = \ln\frac{AR}{E} - \frac{E}{R}\frac{1}{T_{pi}} \quad [i = 1, 2, \ldots, 4] \tag{1}$$

$$\log\beta_i = \log\left(\frac{AE}{RG(\alpha)}\right) - 2.315 - 0.4567\frac{E}{RT_i} \quad [i = 1, 2, \ldots, 4] \tag{2}$$

where β_i is the linear heating rate, T_{pi} represents the peak temperature of the decomposition process, and R is the gas constant.

From the original data shown in Table 1, the values of E and A obtained by Kissinger method (with a subscript of k) and Ozawa method (with a subscript of o) are listed in Table 2.

With the data listed in Table 2, the entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), and free energy of activation ($\Delta G^{\neq}$) of the decomposition reaction corresponding to $T = T_p$, $E = E_k$, and $A = A_k$ obtained by Eqs. 3–5 [16–19] are 23.88 J mol^{-1} K^{-1}, 130.62 kJ mol^{-1}, and 121.55 kJ mol^{-1}, respectively.

$$A_k = \left(k_B T_{p0}/h\right)e^{\Delta S^{\neq}/R} \tag{3}$$

$$\Delta H^{\neq} = E_k - RT_{p0} \tag{4}$$

$$\Delta G^{\neq} = \Delta H^{\neq} - T_{p0}\Delta S^{\neq} \tag{5}$$

where k_B is the Boltzmann constant (1.3807×10^{-23} J K^{-1}), and h is the Plank constant (6.626×10^{-34} J s^{-1}).

The positive value of $\Delta G^{\neq}$ indicates that the exothermic decomposition reaction for 1,2,3-triazole nitrate must proceed under the heating condition.

Self-accelerating decomposition temperature (T_{SADT}) and critical temperature of thermal explosion (T_b)

The self-accelerating decomposition temperature (T_{SADT}) is defined in the United Nation's recommendation as the lowest temperature at which self-accelerating decomposition may occur in an organic peroxide or self-reactive material in the packaging for transportation purposes. The value T_{SADT} (T_{e0}) of T_e corresponding to $\beta \to 0$ can be obtained by substituting the T_e and β from Table 1 into the Eq. 6 [16, 21–23]. The value of T_{SADT} (T_{e0}) is obtained as 368.65 K.

Table 2 Kinetic parameters obtained from the data in Table 1

Kissinger method			Ozawa method		T_{p0}/K
E_k/kJ mol^{-1}	Log(A_k)/s^{-1}	r_k	E_{op}/kJ mol^{-1}	r_{op}	
133.77	14.58	0.9984	133.41	0.9986	379.45

$$T_{(e,p)i} = T_{(e,p)0} + d\beta_i + e\beta_i^2 \quad [i = 1, 2, \ldots, 4] \tag{6}$$

where d and e are coefficients.

The critical temperature of thermal explosion T_b obtained from Eqs. 7–8 taken from Reference [16, 21] is 374.97 K.

$$\ln\beta_i = \ln\left[\frac{A_0}{bG(\alpha)}\right] + b_B T_i, \quad \mathrm{i} = 1, 2, \cdots, L \tag{7}$$

$$T_b = T_{e0} + \frac{1}{b_B} \tag{8}$$

Specific heat capacity (C_p)

Figure 2 shows the determination results of 1,2,3-triazole nitrate using a continuous specific heat capacity mode [19, 22]. In determining temperature range, specific heat capacity of 1,2,3-triazole nitrate presents a good linear relationship with temperature. Specific heat capacity equation is shown as

$$C_p\left(\mathrm{J\ mol^{-1}\ K^{-1}}\right) = -42.6218 + 0.6807T \quad (283.1\ \mathrm{K} < T < 353.2\mathrm{K})$$

The molar heat capacity of 1,2,3-triazole nitrate is 158.98 J mol^{-1} K^{-1} at 298.15 K. Although only a 70.0 K range was taken in the determination process, the specific heat capacity equation obtained was a stable and continuous equation, which can provide a reference and some help for wide temperature applications [24].

Adiabatic time-to-explosion (t)

Energetic materials need a process time from the beginning of thermal decomposition to that of thermal explosion in the adiabatic conditions. The time is named the adiabatic time-to-explosion [16, 22, 23]. Usually, the heating (dT/dt) and critical heating rates ($dT/dt)_{T_b}$ in a thermal decomposition reaction were used to estimate the thermostability of energetic materials. However, the adiabatic time-to-explosion (t) can be calculated by the following Eqs. 10–13 [16, 22, 23] if a series of experimental data were obtained. Thereby, as an important parameter, it is easier to estimate the thermostability of energetic materials according to the length of the adiabatic time-to-explosion.

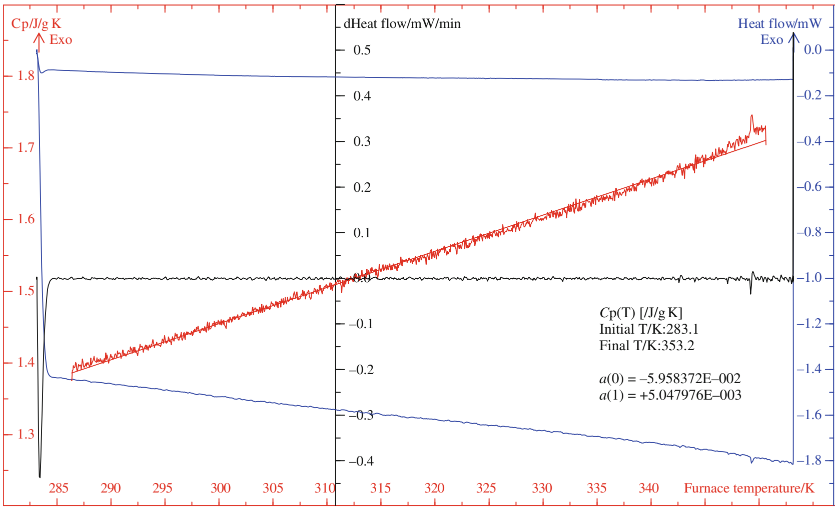


Fig. 2 Determination results of the continuous specific heat capacity of 1,2,3-triazole nitrate

$$C_{\mathrm{p}}\frac{\mathrm{d}T}{\mathrm{d}t}=QA\exp(-E/RT)f(\alpha) \tag{10}$$

$$f(\alpha)=(1-\alpha)^n \tag{11}$$

$$\alpha=\int\frac{C_{\mathrm{p}}}{Q}\mathrm{d}T \tag{12}$$

$$C_{\mathrm{p}}=a+bT \tag{13}$$

where C_{p} is the specific heat capacity (J mol^{-1} K^{-1}), T is the absolute temperature (K), t is the adiabatic decomposition time (s), Q is the exothermic energy (J mol^{-1}), A is the pre-exponential factor (s^{-1}), E is the apparent activation energy of the thermal decomposition reaction (J mol^{-1}), R is the gas constant (J mol^{-1} K^{-1}), $f(\alpha)$ is the most probable kinetic model function, and α is the conversion degree, a and b are coefficients.

The combination of Eqs. 10–13 can give the following equation:

$$\begin{aligned} t&=\int_0^t\mathrm{d}t=\int_{T_{\mathrm{e0}}}^{T}\frac{C_{\mathrm{p}}\exp(E/RT)}{QAf(\alpha)}\mathrm{d}T\\ &=\frac{1}{QA}\int_{T_{\mathrm{e0}}}^{T}\frac{(a+bT)\exp(E/RT)}{(1-\alpha)^n}\mathrm{d}T\\ &=\frac{1}{QA}\int_{T_{\mathrm{e0}}}^{T}\frac{(a+bT)\exp(E/RT)}{\left[1-\frac{1}{Q}\int_{T_0}^{T}(a+bT)\mathrm{d}T\right]^n}\mathrm{d}T \end{aligned} \tag{14}$$

The limit of the temperature integral in Eq. 14 is from T_{e0} to T_{b}.

(1) When $n=0$

$$t_0=\frac{1}{QA}\int_{T_{\mathrm{e0}}}^{T_{\mathrm{b}}}(a+bT)\exp(E/RT)\mathrm{d}T \tag{15}$$

(2) When $n=1$

$$t_1=\frac{1}{QA\left\{1-\frac{1}{Q}\left[a(T_{\mathrm{e0}}-T_{\mathrm{b}})+\frac{b}{2}(T_{\mathrm{e0}}^2-T_{\mathrm{b}}^2)\right]\right\}}\times\int_{T_{\mathrm{e0}}}^{T_{\mathrm{b}}}(a+bT)\exp(E/RT)\mathrm{d}T \tag{16}$$

(3) When $n=2$

$$t_2=\frac{1}{QA\left\{1-\frac{1}{Q}\left[a(T_{\mathrm{e0}}-T_{\mathrm{b}})+\frac{b}{2}(T_{\mathrm{e0}}^2-T_{\mathrm{b}}^2)\right]\right\}^2}\times\int_{T_{\mathrm{e0}}}^{T_{\mathrm{b}}}(a+bT)\exp(E/RT)\mathrm{d}T \tag{17}$$

We can directly get $t_2=100.00$ s, $t_1=99.41$ s, and $t_0=98.82$ s from Eqs. 15–17, so the adiabatic time-to-explosion of 1,2,3-triazole nitrate is a certain value between 98.82 and 100.00 s.

Critical temperature of hot-spot initiation ($\mathrm{T}_{\mathrm{cr,hot\text{-}spot}}$)

In order to obtain the critical temperature of hot-spot initiation($T_{\mathrm{cr,hot\text{-}spot}}$) of 1,2,3-triazole nitrate, assuming that $T_{\mathrm{cr,\ hot\text{-}spot}}$ is a function of the size and duration of hot-spot and of the physical and chemical properties of the explosive, the equation for calculating the value of $T_{\mathrm{cr,hot\text{-}spot}}$ may be expressed as [16, 21–23]

Table 3 Explosive parameters and comparison of experimental and predicted 50% drop heights (H_{50})

Acronym	$10^4\lambda^a$/J cm^{-1} s^{-1} K^{-1}	ρ/g cm^{-3}	Log(A_k)/s^{-1}	Q_d/J g^{-1}	E^b/J mol^{-1}	H_{50}/cm		n	D_2	D_3
						Exp.^{a}	Pre.			
HMX	34.43	1.79	33.80	2764	373700	32	33.4	0.564623	33.8765	−0.347174
RDX	10.58	1.66	12.50	2810	140000	26	20.1			
TNT	21.30	1.57	11.10	1506	155017	59	56.4			
BTF	20.92	22.81	22.81	2949	255000	28	28			
1,2,3-Triazole nitrate	33.06	1.82	11.38	575.32	130800		9.16			

[a] Reference [25]

[b] Reference [26]

$T_{\text{room}} = 300$ K

$$\left(\frac{4}{3}\pi a^3\right)\rho Q_d\left\{1-\exp\left[-(t-t_0)Ae^{\frac{-E}{RT_{\text{cr}}}}\right]\right\}$$
$$=\int_a^\infty 4\pi r^2\rho C_p\left[\frac{a\theta_0}{r}erfc\left[\frac{r-a}{2\sqrt{Bt}}\right]\right]\mathrm{d}r$$
$$=\int_a^\infty 4\pi r^2\rho c_p\left\{\frac{a\left(T_{\text{cr,hot-spot}}-T_{\text{room}}\right)}{r}\text{erfc}\left[\frac{r-a}{2\sqrt{\frac{\lambda t}{\rho c_p}}}\right]\right\}\mathrm{d}r \tag{18}$$

where a is the radius of the hot-spot in cm, ρ is the density in g cm^{-3}, Q_d is the heat of reaction in J g^{-1}, $t-t_0$ is the time interval in s, A is the frequency factor in s^{-1}, E is the activation energy in J mol^{-1}, R is the gas constant in J mol^{-1} K^{-1}, $T_{\text{cr, hot-spot}}$ is the critical temperature of hot-spot initiation in K, C_p is the specific heat in J mol^{-1} K^{-1}, T_{room} is the ambient temperature in K, λ is the thermal conductivity in J cm^{-1} s^{-1} K^{-1}.

By substituting the following data of 1,2,3-triazole nitrate $a = 10^{-3}$ cm, $\rho = 1.822$ g cm^{-3} [25], $Q_d = 1704.26$ J g^{-1}, $t-t_0 = 10^{-4}$ s, $A = A_k = 10^{14.58}$ s^{-1}, $E = E_k = 133.77$ kJ mol^{-1}, $R = 8.3145$ J mol^{-1} K^{-1}, $C_p = 159.023$ J mol^{-1} K^{-1}, $T_{\text{room}} = 300$ K, and $\lambda = 33.04 \times 10^{-4}$ J cm^{-1} s^{-1} K^{-1} into Eq. 18, the value of $T_{\text{cr, hot-spot}}$ of 637.14 K is obtained.

Characteristic drop height of impact sensitivity (H_{50})

The characteristic drop height of impact sensitivity (H_{50}) of 1,2,3-triazole nitrate can be obtained by substituting the values of λ, ρ, A, Q_d, and E of 1,2,3-triazole nitrate from Table 3 and the values of n, D_2, and D_3 into Eq. 19 [16, 21–23]. The corresponding value of H_{50} of 1,2,3-triazole nitrate is 9.16 cm.

$$\frac{1}{2}n\log H_{50}+\log\sqrt{\frac{\lambda}{A\rho Q_d}}+D_3+\frac{0.02612E}{T_1+D_2H_{50}^n}=0 \tag{19}$$

where n, D_2, and D_3 are parameters of the correlation.

Conclusions

The thermal decomposition process of the exothermic decomposition reaction of 1,2,3-triazole nitrate at four different heating rates under atmospheric pressure could be described by Fig. 1 shown in the text. The apparent activation energy and pre-exponential factor of the above mentioned reaction are 133.77 kJ mol^{-1} and $10^{14.58}$ s^{-1}, respectively. The critical temperature of thermal explosion is 374.97 K. The entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), and free energy of activation ($\Delta G^{\neq}$) of the reaction are 23.88 J mol^{-1} K^{-1}, 130.62 kJ mol^{-1}, and 121.55 kJ mol^{-1}, respectively. The self-accelerating decomposition temperature (T_{SADT}) is 368.65 K. The critical temperature of hot-spot initiation ($T_{\text{cr, hot-spot}}$) is 637.14 K, and the characteristic drop height of impact sensitivity (H_{50}) is 9.16 cm. The molar heat capacity of 1,2,3-triazole nitrate is 158.98 J mol^{-1} K^{-1} at 298.15 K. The adiabatic time-to-explosion of 1,2,3-triazole nitrate was calculated to be a certain value between 98.82 and 100.00 s.

Acknowledgements The financial supports received from the National Natural Science Foundation of China (Grant No. 20573098), and the Science and Technology Foundation of the National Key Lab of Science and Technology on Propellant and Explosive Combustion in China (Grant No. 9140C3501020901) are gratefully acknowledged.

References

1. Gao HX, Ye CF, Piekarski CM. Computational characterization of energetic salts. J Phys Chem C. 2007;111:10718–26.
2. Agrawal JP. Recent trends in high-energy materials. Prog Energ Combust Sci. 1998;24:1–13.
3. Huang HF, Meng ZH, Zhou ZM, Gao HX, Zhang J, Wu YK. Energetic salts and energetic ionic liquids. Prog Chem. 2009;21:152–61 (in Chinese).
4. Drake G, Kaplan G, Hall L, Hawkins T, Larue J. A new family of energetic ionic liquids 1-amino-3-alkyl-1,2,3-triazolium nitrates. J Chem Crys. 2007;37:15–22.
5. Ye CF, Shreeve JM. Rapid and accurate estimation of densities of room-temperature ionic liquids and salts. J Phys Chem A. 2007;111:1456–61.

6. Tong B, Liu QS, Tan ZC, Urs WB. Thermochemistry of alkyl pyridinium bromide ionic liquids: calorimetric measurements and calculation. J Phys Chem A. 2010;114:3782–7.
7. Krossing I, Slattery JM, Daguenet C, Dyson PJ, Oleinikova A, Weingärtner H. Why are ionic liquids liquid? A simple explanation based on lattice and salvation energies. J Am Chem Soc. 2006;128:13427–34.
8. Kolaski M, Lee HM, Pak C, Kim KS. Charge-transfer-to-solvent-driven dissolution dynamics of 1-(H_2O)2-5 upon excitation: excited-state ab initio molecular dynamics simulations. J Am Chem Soc. 2008;130:103–12.
9. Mel'yanenko EVN, Verevkin SP, Heintz A. Imidazolium-based ionic liquids. 1-Methyl imidazolium nitrate: thermochemical measurements and Ab initio calculations. J Phys Chem B. 2009;113:9871–81.
10. Urszula D, Andrzej M. Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-ethyl-3-methylimidazolium trifluoroacetate. J Phys Chem B. 2007;111:11984–8.
11. Fischer G, Holl G, Klapötke TM, Weigand JJ. A study on thermal decomposition behavior of derivatives of 1,5-diamino-1H-tetrazole (DAT): a new family of energetic heterocyclic-based salts. Thermochim Acta. 2005;437:168–75.
12. Chowdhury A, Thynell ST. Confined rapid thermolysis/FTIR/ToF studies of triazolium-based energetic ionic liquids. Thermochim Acta. 2007;466:1–11.
13. Chowdhury A, Thynell ST, Lin P. Confined rapid thermolysis/FTIR/ToF studies of triazolium-based energetic ionic liquids. Thermochim Acta. 2009;485:1–12.
14. Kissinger HE. Reaction kinetics in differential thermal analysis. Anal Chem. 1957;29:1702–6.
15. Ozawa T. A new method of analyzing thermogravimetric data. Bull Chem Soc Jpn. 1965;38:1881–6.
16. Hu RZ, Gao SL, Zhao FQ, Shi QZ, Zhang TL, Zhang JG. Thermal analysis kinetics. 2nd ed. Beijing: Science Press; 2008. (in Chinese).
17. Xing XL, Xue L, Zhao FQ, Gao HX, Hu RZ. Thermochemical properties of 1,1-diamino-2,2-dinitroethylene (FOX-7) in dimethyl sulfoxide (DMSO). Thermochim Acta. 2009;35:491–7.
18. Gao HX, Zhao FQ, Hu RZ, Zhao HA, Zhang H. Estimation of the critical temperature of thermal explosion for azido-acetic-acid-2-(2-azido-acetoxy)-ethylester using non-isothermal DSC. J Therm Anal Calorim. 2009;95:477–82.
19. Xu KZ, Song JR, Zhao FQ, Ma HX, Gao HX, Chang CR, Ren YH, Hu RZ. Thermal behavior, specific heat capacity and adiabatic time-to explosion of G(FOX-7). J Hazard Mater. 2008;158:333–9.
20. Xue L, Zhao FQ, Xing XL, Gao HX, Xu SY, Hu RZ. Dissolution properties of 1,3,3-trinitroazetidine (TNAZ) in ethyl acetate and *N*,*N*-dimethylformamide. Acta Phy Chim Sin. 2009;25:2413–21.
21. Xue L, Zhao FQ, Hu RZ, Gao HX. A simple method to estimate the critical temperature of thermal explosion for energetic materials using nonisothermal DSC. J Energ Mater. 2010;28:17–31.
22. Li JZ, Fan XZ, Hu RZ, Zhao FQ, Gao HX. Thermal behavior of copper(II) 4-nitroimidazolate. J Therm Anal Calorim. 2009;96: 01–195.
23. Xu SY, Zhao FQ, Yi JH, Hu RZ, Gao HX, Li SW, Hao HX, Pei Q. Thermal behavior and non-isothermal decomposition reaction kinetics of composite modified double base propellant containing CL-20. Acta Phy Chim Sin. 2008;24:1371–9.
24. Arkady MK, Liubov PS. Molar heat capacities of the (water + acetonitrile) mixtures at T = (283.15, 298.15, 313.15, and 328.15) K. J Chem Thermodyn. 2010;42:1209–12.
25. Dong HS, Zhao FF. Performances of high explosive and its related materials. Beijing: Science Press; 1989.
26. Dong HS, Hu RZ, Yao P, Zhang XX. Thermograms of energetic materials. Beijing: National Defence Industry Press; 2001.