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Thermal decomposition and safety assessment of 3,3′-dinitrimino-5,5′-bis(1*H*-1,2,4-triazole) by DTA and ARC

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Abstract

Thermal decomposition and safety assessment of 3,3′-dinitrimino-5,5′-bis(1*H*-1,2,4-triazole) (DNABT) were investigated by thermogravimetry–derivative thermogravimetry–differential scanning calorimetry (TG-DTG-DSC), differential thermal analysis (DTA), and accelerating rate calorimetry (ARC). The result of TG-DTG-DSC at a heating rate of 10 °C min^{-1} indicated that an endothermic decomposition and an exothermic decomposition occurred at 133.98 and 210.86 °C, respectively. The apparent activation energy (E_a) and pre-exponential factor (A) of the exothermic decomposition, and the free energy of activation, activation enthalpy, and activation entropy at initial decomposition temperature (T_{p0}) were calculated from the DTA curves recorded at the heating rates of 1, 2, 4, 8 °C min^{-1}. The critical temperature of thermal explosion (T_{bp0}) obtained by Ozawa's and Kissinger's methods were calculated as 205.01 and 205.14 °C, respectively. The result of ARC indicated that the self-heating decomposition started at 200.22 °C and ended at 232.66 °C. The self-heating decomposition parameters, including the onset temperature, final temperature, temperature at maximum rate, maximum temperature rate, adiabatic temperature rise, and time to maximum rate were obtained, and these parameters were corrected by thermal inertia factor. The E_a and A under adiabatic condition were also calculated. In addition, the self-accelerating decomposition temperature ($T_{\mathrm{SADT,\ 50kg}}$) was calculated as 175.37 °C. These results could contribute to improve the safety in the reaction, transportation, and storage processes of DNABT.

Keywords 3,3′-Dinitrimino-5,5′-bis(1*H*-1,2,4-triazole) · Thermal decomposition · Non-isothermal kinetics · Safety assessment · DNABT · ARC

Introduction

During the last decade, considerable efforts have been focused on the development of nitrogen-rich heterocyclic compounds [1–5]. Nitrogen-rich heterocyclic compounds have played and will continue to play an important role in the field of energetic materials owing to their good thermal stability, low impact sensitivity, and high detonation properties.

3,3′-Dinitrimino-5,5′-bis(1*H*-1,2,4-triazole) (DNABT) is an important nitrogen-rich heterocyclic compound. Its calculated detonation velocity (8355 m s^{-1}) is higher than that of 2,4,6-triamino-1,3,5-trinitrobenzene (TATB) (8114 m s^{-1}), and its impact sensitivity (3 J) is higher than that of 2,4,6-trinitrotolune (TNT) (15 J) [6, 7]. Its high-nitrogen energetic salts were first synthesized by Wang et al. [7], and some of them can be considered as the potential substituted candidates of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), such as diammonium bis[3-(5-nitroimino-1,2,4-triazolate)] and carbonic dihydrazidinium bis[3-(5-nitroimino-1,2,4-triazolate)] (CBNT).

However, before DNABT obtains practical application, much work should be done in order to get a more comprehensive understanding of it. The thermogravimetry–derivative thermogravimetry–differential scanning calorimetry (TG-DTG-DSC), differential thermal analysis (DTA) and accelerating rate calorimetry (ARC) were carried out. The thermokinetic parameters of the exothermic decomposition and thermodynamic parameters at initial

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decomposition temperature (T_{p0}) were obtained from DTA. The self-heating decomposition parameters, adiabatic decomposition kinetic parameters, time to maximum rate (TMR), and self-accelerating decomposition temperature (T_{SADT}) were obtained from ARC. To the best of our knowledge, up to now, there are no report regarding the thermal decomposition and safety assessment of DNABT under non-isothermal and adiabatic conditions.

Experimental

Materials

DNABT was prepared [6] (as shown in Scheme 1): Oxalic acid (20.0 g, 159 mmol) was added to a stirred mixture of hydrochloric acid (37.5%, 60 mL) and aminoguanidinium bicarbonate (45.4 g, 332 mmol). The reaction was stirred at 70 °C for 1 h, and the precipitate was collected by filtration. The white solid was dissolved in water (240 mL) and alkalized with sodium hydroxide to pH 14. The reaction mixture was heated to reflux for 1 h and subsequently acidified with acetic acid to pH 4. The white precipitate was collected by filtration and dried to yield 3,3′-diamino-5,5′-bis(1*H*-1,2,4-triazole) (DABT). Nitric acid (65%, 9 mL) was added slowly to a mixture of DABT (3.0 g, 18 mmol) and concentrated sulfuric acid (98.0%, 27 mL) at 0 °C. The reaction mixture was warm to room temperature and stirred for 1 h. The yellow transparent solution was poured on ice, and the white precipitate was collected by filtration and recrystallized from boiling water to yield DNABT (3.7 g, 13 mmol, 70.0%) as colorless crystalline solid. IR (KBr pellet): 3183, 1697, 1575, 1508, 1448, 1383, 1332, 1306, 1237, 1173, 1057, 994, 948, 782, 714 cm^{-1}; ^{1}H NMR (400 MHz, d6-DMSO): 8.46, 6.58 ppm; ^{13}C NMR (100 MHz, d6-DMSO): 153.35, 142.23 ppm.

The compound of DNABT was additionally characterized by single-crystal X-ray spectroscopy. The result of single-crystal X-ray spectroscopy indicated that one molecule of DNABT was associated with two molecules of H_2O. Crystallographic data and parameters as well as the morphology are compiled in Table 1.

Experimental equipments and conditions

The TG-DTG-DSC measurement was performed with a PerkinElmer STA6000 simultaneous thermal analyzer at a heating rate of 10 °C min^{-1} under a nitrogen flow of 50 mL min^{-1}. The non-isothermal DTA measurements were performed with a Shimadzu DTG-60H simultaneous thermal analyzer at the heating rates of 1, 2, 4, 8 °C min^{-1} under a nitrogen flow of 50 mL min^{-1}. All samples were 2.0 mg and placed in open alumina crucibles, and they were heated from 50 to 400 °C.

The ARC measurement was performed with a Thermal Hazard Technology accelerating rate calorimeter in the Heat–Wait–Search mode. The experiment conditions of DNABT by accelerating rate calorimeter are compiled in Table 2.

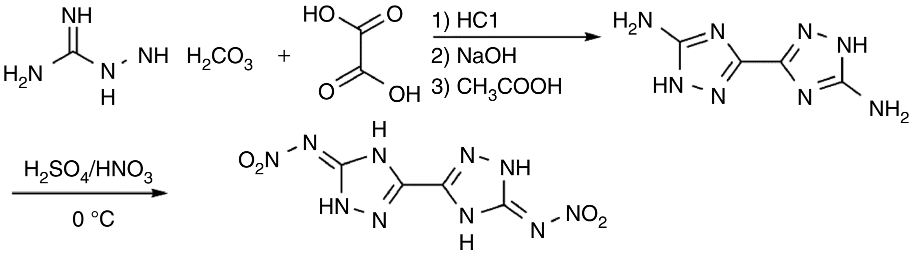
Results and discussion

Thermal decomposition processes

The TG-DTG-DSC curve at a heating rate of 10 °C min^{-1} is given in Fig. 1. From the TG and DTG curves, two mass loss processes were observed. The first process was a slow decomposition in the range between 133.98 and 157.98 °C, and the mass loss was 12.40%. This was a dehydration process, and the theoretically calculated value of the dehydration process was in exact accordance with the experimental value. The second process was an exothermic decomposition in the range between 210.86 and 263.22 °C, and the mass loss was 50.40%. From the DSC curve, the peak temperatures of the two mass loss processes were determined as 142.01 and 237.11 °C, respectively.

Non-isothermal decomposition kinetic parameters

The DTA curves of DNABT are shown in Fig. 2, indicated that there were two exothermic decomposition during the decomposition of DNABT. The onset temperatures (159.03, 164.90, 172.70, 183.21 °C), peak temperatures (193.20, 203.36, 212.60, 221.80 °C), and final



Scheme 1 The synthesis route of DNABT

Table 1 X-ray data and parameters of DNABT·$2H_2O$

Parameters	Values	Parameters	Values
Formula	$C_4H_4N_{10}O_4 \cdot 2H_2O$	F(000)	300.0
Formula mass/g mol^{-1}	292.20	$\lambda_{Mo-K\alpha}$/Å	0.71073
Crystal system	Monoclinic	T/K	296
Space group	P21/n	Theta max/°	25.090
Color, habit	Colorless, needle	Dataset h max	6
a/Å	5.2417	Dataset k max	21
b/Å	17.8787	Dataset l max	7
c/Å	6.3099	Reflections	847
α/°	90	No. of parameters	97
β/°	112.431	R_1, wR_2	0.0370, 0.1059
γ/°	90	S	1.067
Volume/Å^3	546.59	Device type	Oxford Xcalibur3 CCD
Z	2	Solution	SHELXS-97
Calculated density/g cm^{-3}	1.775	Refinement	SHELXL-97
μ/mm^{-1}	0.162	Absorption correction	Multi-scan

Table 2 Experimental conditions of DNABT by ARC

Parameters	Values	Parameters	Values
Sample mass/g	0.1017	Start temperature/°C	50
Sample heat capacity default/kJ kg^{-1} K^{-1}	2.00	End temperature/°C	350
Test cell type	Hastelloy	Temperature step/°C	15
Test cell mass/g	14.1784	Temperature rate sensitivity/°C min^{-1}	0.02
Test cell heat capacity/kJ kg^{-1} K^{-1}	0.42	Wait time/min	15
Test mode	Heat-wait-search	Calculation temperature step/°C	0.20

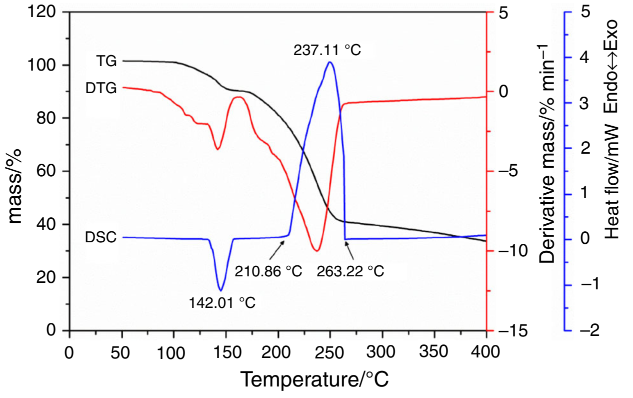


Fig. 1 TG-DTG-DSC curve of DNABT at a heating rate of 10 °C min^{-1}

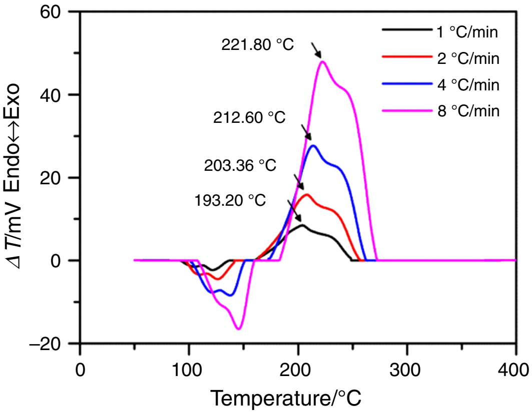


Fig. 2 DTA curves of DNABT at the heating rates of 1, 2, 4, 8 °C min^{-1}

temperatures (211.08, 218.66, 229.01, 239.34 °C) of the first exothermic decomposition were observed at the heating rates of 1, 2, 4, 8 °C min^{-1}, respectively. The onset temperatures (211.08, 218.66, 229.01, 239.34 °C) and final temperatures (248.78, 256.65, 262.66 272.45 °C) of the second exothermic decomposition were observed at the heating rates of 1, 2, 4, 8 °C min^{-1}, respectively. However, it was difficult to identify the peak temperatures of the second exothermic decomposition at the heating rates of 1, 2, 4, 8 °C min^{-1}. There was only a single discernible exothermic peak during the two exothermic decomposition due to the well overlap of the two processes. When the heating rate was high, the final temperature of the first exothermic decomposition and the overlapping of two exothermic decomposition were increased. A complete overlap of the two exothermic decomposition is observed in Fig. 1 at a heating rate of 10 °C min^{-1}.

To determine the non-isothermal decomposition kinetic parameters of energetic materials, Ozawa's method [8] and Kissinger's method [9] were employed. The Ozawa's equation (1) and Kissinger's equation (2) are given below:

$$\log \beta = -\frac{0.4567E_\text{a}}{R}\left[\frac{1}{T_\text{p}}\right] + C, \tag{1}$$

$$\ln\left[\frac{\beta}{T_\text{p}^2}\right] = -\frac{E_\text{a}}{R}\left[\frac{1}{T_\text{p}}\right] + \ln\left[\frac{RA}{E_\text{a}}\right], \tag{2}$$

where β is the heating rate, E_a is the apparent activation energy, R is the gas constant, T_p is the peak temperature, C is an arbitrary constant and A is the pre-exponential factor. The logβ against $1/T_\text{p}$ and $\ln(\beta/T_\text{p}^2)$ against $1/T_\text{p}$ were two straight lines. According to Eqs. (1) and (2), the slops of two lines were used to calculate the activation energies. According to Eq. (3), the obtained activation energies were used to calculate the logarithm of pre-exponential factor ($\log A/\text{s}^{-1}$).

$$A = \beta\frac{E_\text{a}}{RT_\text{p}^2}\exp\left(\frac{E_\text{a}}{RT_\text{p}}\right), \tag{3}$$

where E_a is the apparent activation energy which was obtained by Ozawa's or Kissinger's method. The E_a, $\log A/\text{s}^{-1}$ and corresponding regression coefficient (r) are listed in Table 3.

Thermodynamic parameters at initial decomposition temperature (T_{p0})

The initial decomposition temperature (T_{p0}) in the exothermic decomposition process corresponding to $\beta \to 0$ is calculated by Eq. (4) [10, 11]. The free energy of activation ($\Delta G^{\neq}$), activation enthalpy ($\Delta H^{\neq}$), and activation entropy ($\Delta S^{\neq}$) are calculated by Eqs. (5), (6), and (7) [11]:

$$T_{\text{pi}} = T_{\text{p0}} + a\beta_\text{i} + b\beta_\text{i}^2 \quad i = 1, 2, 3, 4, \tag{4}$$

$$\Delta G^{\neq} = E_\text{a} - RT_{\text{P0}}\ln\left[\frac{Ah}{k_\text{B}T_{\text{P0}}}\right], \tag{5}$$

$$\Delta H^{\neq} = E_\text{a} - RT_{\text{p0}}, \tag{6}$$

$$\Delta S^{\neq} = \frac{\Delta H^{\neq} - \Delta G^{\neq}}{T_{\text{p0}}}, \tag{7}$$

where T_{pi} is the peak temperature of a heating rate of β_i, a and b are the coefficients, h is the Planck constant, k_B is the Boltzmann constant. The T_{p0}, $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$ are listed in Table 3.

Critical temperature of thermal explosion (T_{bp0})

The critical temperature of thermal explosion (T_{bp0}) is calculated by Eq. (8) [12, 13]:

$$T_{\text{bp0}} = \frac{E_\text{a} - \sqrt{E_\text{a}^2 - 4E_\text{a}RT_{\text{P0}}}}{2R} \tag{8}$$

where E_a is the apparent activation energy which was obtained by Ozawa's or Kissinger's method.

Self-heating decomposition parameters

Under experiment conditions of ARC, heat from the exothermic reaction of the sample induced the temperature rise of both the sample and the reaction cell. The relationship between the real adiabatic and near-adiabatic conditions was described as follows [14, 15].The corrected and measured self-heating decomposition parameters of DNABT are given in Table 4.

$$\phi = 1 + \frac{M_\text{b}C_{\text{v,b}}}{M_\text{s}C_{\text{v,s}}} \tag{9}$$

$$T_{\text{o,corr}} = \left[\frac{1}{T_\text{o}} + \frac{R}{E_\text{a}}\ln\phi\right]^{-1} \tag{10}$$

$$T_{\text{f,corr}} = \phi\Delta T_{\text{ad}} + T_{\text{o,corr}} \tag{11}$$

$$\Delta T_{\text{ad,corr}} = \phi\Delta T_{\text{ad}} \tag{12}$$

$$m_{\text{o,corr}} = \phi m_\text{o} \tag{13}$$

$$m_{\text{m,corr}} = \phi m_\text{m} \tag{14}$$

$$T_{\text{m,corr}} = T_{\text{o,corr}} + \phi(T_\text{m} - T_\text{o}) \tag{15}$$

Table 3 Non-isothermal kinetic and thermodynamic parameters of DNABT

Method	E_a/kJ mol^{-1}	log A/s^{-1}	r	T_{p0}/°C	$\Delta G^{\neq}$/kJ mol^{-1}	$\Delta H^{\neq}$/kJ mol^{-1}	$\Delta S^{\neq}$/J mol^{-1} K^{-1}	T_{bp0}/°C
Ozawa	132.90	13.73	0.9974	190.71	126.24	129.04	6.04	205.01
Kissinger	131.77	13.61	0.9971	190.71	126.23	127.91	3.64	205.14

Table 4 Self-heating decomposition parameters of DNABT by ARC

Parameters	Values	Corr.	Parameters	Values	Corr.
Onset temperature/°C	200.22	199.77	Adiabatic temperature rise/°C	32.45	982.34
Onset temperature rate/°C min^{-1}	0.09	3.05	Time to maximum rate/min	31.15	1.03
Temperature at maximum rate/°C	223.66	909.46	Maximum pressure/bar	14.53	–
Maximum self-heating rate/°C min^{-1}	407.84	12,348.08	Thermal inertia factor	30.28	–
Final temperature/°C	232.66	1182.11			

$$\mathrm{TMR}_{\mathrm{corr}} = \frac{\mathrm{TMR}}{\phi} \tag{16}$$

where ϕ is the thermal inertia factor, M_{b} is the test cell mass, $C_{\mathrm{v,b}}$ is the test cell heat capacity, M_{s} is the sample mass, $C_{\mathrm{v,s}}$ is the sample heat capacity. $T_{\mathrm{o,corr}}$ and T_{o} are the corrected and measured onset decomposition temperature, respectively; $T_{\mathrm{f,corr}}$ and T_{f} are the corrected and measured final decomposition temperature, respectively; $\Delta T_{\mathrm{ad,corr}}$ and ΔT_{ad} are the corrected and measured adiabatic temperature rise, respectively; $m_{\mathrm{o,corr}}$ and m_{o} are the corrected and measured onset temperature rate, respectively; $m_{\mathrm{m,corr}}$ and m_{m} are the corrected and measured maximum self-heating rate, respectively; $T_{\mathrm{m,corr}}$ and T_{m} are the corrected and measured temperature at maximum rate, respectively; $\mathrm{TMR}_{\mathrm{corr}}$ and *TMR* are the corrected and measured time to maximum rate, respectively.

The ARC curves of DNABT are given in Fig. 3. As shown in Fig. 3a, both a dehydration process and a self-heating decomposition were observed. The dehydration process started at 109.66 °C and ended at 123.05 °C, and the pressure was increased by 1.30 bar during this period. The self-heating decomposition started at 200.22 °C and ended at 232.66 °C, within the time span of 50.65 min (Fig. 3b). The maximum self-heating rate and maximum temperature rate were 407.84 °C min^{-1} and 20.54 bar min^{-1}, respectively (Fig. 3c, d). It should be noted that the released energy is in excess and therefore would cause damage to the instrument if the decomposition of DNABT was allowed to occur in a closed vessel.

Adiabatic decomposition kinetic parameters

For an *n*th-order single-step reaction with a single reaction, the self-heating rate could be expressed as following [15]:

$$m_{\mathrm{T}} = \frac{\mathrm{d}T}{\mathrm{d}t} = k\left[\frac{T_{\mathrm{f}} - T}{\Delta T_{\mathrm{ad}}}\right]^{\mathrm{n}} \Delta T_{\mathrm{ad}} C_0^{\mathrm{n}-1}, \tag{17}$$

where m_{T} is the temperature rate at the temperature T, k is the rate constant of the reaction at temperature T, T is the temperature at time t, C_0 is the initial concentration of the reactant.

Rearranging Eq. (17), we had [15]:

$$k^{*} = kC_0^{\mathrm{n}-1} = \frac{m_{\mathrm{T}}}{\left[\frac{T_{\mathrm{f}}-T}{\Delta T_{\mathrm{ad}}}\right]^{\mathrm{n}} \Delta T_{\mathrm{ad}}}, \tag{18}$$

where k^{*} is a pseudo-zero-order rate constant at the temperature T. According to the Arrhenius equation, one could obtain [15].

$$\ln k^{*} = \ln C_0^{\mathrm{n}-1} A - \frac{E_{\mathrm{a}}}{R}\left[\frac{1}{T}\right]. \tag{19}$$

The curves of $\ln k^{*}$ versus T^{-1} for the self-heating decomposition of DNABT are illustrated in Fig. 4. The E_{a} and A could be calculated from the plot, and they are listed in Table 5.

Time to maximum rate (TMR)

According to the literature, the TMR and T have the following relationship [15].

$$\ln \mathrm{TMR} = \frac{E_{\mathrm{a}}}{R}\left[\frac{1}{T}\right] - \ln A + \ln \frac{RT^{2}}{C_0^{\mathrm{n}-1}\left[\frac{T_{\mathrm{f}}-T}{\Delta T_{\mathrm{ad}}}\right]^{\mathrm{n}} \Delta T_{\mathrm{ad}} E_{\mathrm{a}}}. \tag{20}$$

From Table 5, $n = 4$, E_{a} was 659.59 kJ mol^{-1}, log A/s^{-1} was 66.01. Then, the plot of *TMR* versus T is given in Fig. 5.

Self-accelerating decomposition temperature (T_{SADT})

The T_{SADT} is defined as the lowest ambient temperature in air at which self-accelerating decomposition may occur within a substance in the packaging as used in transport and storage. The adiabatic decomposition kinetic parameters were used for the estimation of the T_{SADT} for DNABT in a 50 kg package. Firstly, Eq. (21) is used to get the time constant (τ), and then, the temperature of no return (T_{NR}) would be obtained from the curve of TMR versus T. Lastly, the T_{SADT} was calculated based on Eq. (22) [16, 17].

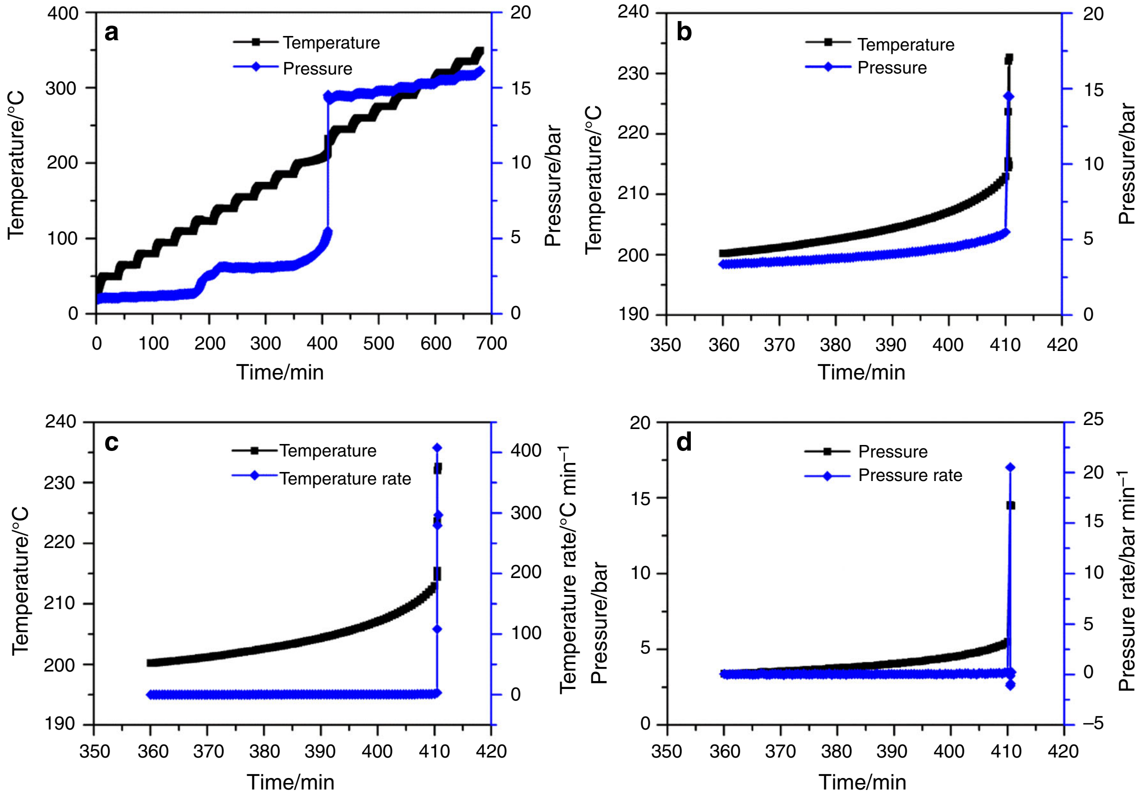


Fig. 3 ARC curves of DNABT. **a** Temperature and pressure versus time, **b** decomposition temperature and pressure versus time, **c** decomposition temperature and temperature rate versus time, **d** decomposition pressure and pressure rate versus time

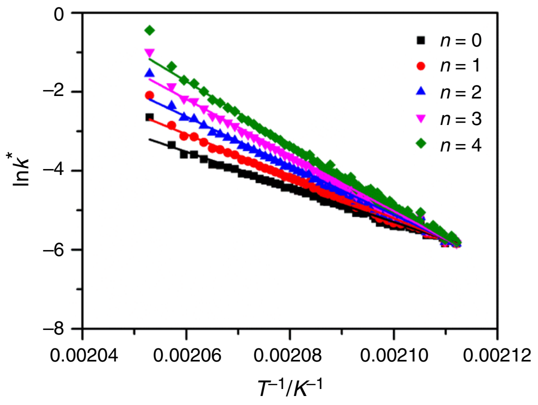


Fig. 4 Curves of ln$k$* versus T^{-1} for the self-heating decomposition of DNABT

Table 5 Thermal decomposition kinetic parameters of DNABT by ARC

n	E_a/ kJ mol^{-1}	log A/s^{-1}	r
0	368.11	37.08	0.9801
1	441.59	44.40	0.9846
2	515.06	51.72	0.9873
3	588.54	59.04	0.9890
4	659.59	66.11	0.9910

$$\tau = \frac{M_s C_{v,s}}{Ua}, \tag{21}$$

$$T_{SADT} = T_{NR} - \frac{RT_{NR}^2}{E_a}, \tag{22}$$

where U is the heat transfer coefficient and a is the contact area of the system and environment. Assuming 50 kg DNABT is loaded in the cylinder with the height of 60 cm and the diameter of 30 cm, so the contact area of the system and environment was 0.5652 m^2. In this study, the heat transfer coefficient U = 5 J m^{-2} K^{-1} s^{-1} had been chosen for prediction of the T_{SADT}. The T_{SADT} of DNABT was calculated as 175.37 °C.

Comparison of onset temperatures of DNABT with other energetic materials

Muravyev et al. [5] obtained the onset temperatures of some widely used energetic materials by ARC, such as 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate (TKX-50), and octogen (HMX). Their onset temperatures are listed in Table 6.

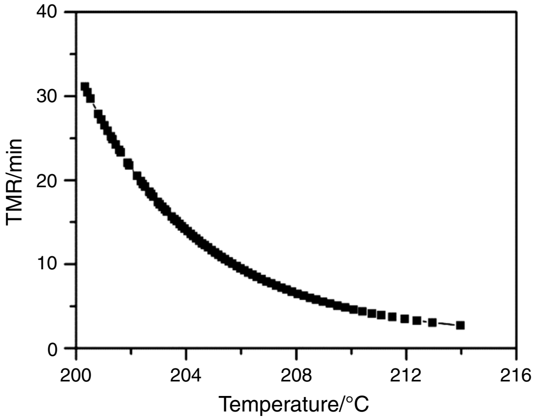


Fig. 5 TMR versus temperature

Table 6 Onset temperatures of DNABT and other energetic materials

Compounds	RDX	TKX-50	DNABT	HMX
T_o/°C	177	192	200.22	217

From Table 6, it could be concluded that the onset temperature of DNABT was determined in the ARC experiments was found to be lower than that of HMX, but higher than that of TKX-50.

Conclusions

In conclusion, the thermal decomposition and safety assessment of DNABT by TG-DTG-DSC, DTA, and ARC were reported in detail.

1. The TG-DTG-DSC measurement showed that the endothermic dehydration process started at 133.98 °C and ended at 157.98 °C, and the exothermic decomposition started at 210.86 °C and ended at 263.22 °C.
2. The non-isothermal decomposition kinetic and thermodynamic parameters that were obtained by the Ozawa's and Kissinger's methods for DNABT showed good correlation, but the values obtained by Ozawa's method were slightly higher than those obtained by Kissinger's method.
3. The critical temperature of thermal explosion (T_{bp0}) obtained by Ozawa's and Kissinger's methods were calculated as 205.01 and 205.14 °C, respectively.
4. The adiabatic experiment by ARC revealed that the self-heating decomposition started at 200.22 °C and ended at 232.66 °C, within the time span of 50.65 min. The maximum self-heating rate was calculated as 407.84 °C min^{-1}. The apparent activated energy under adiabatic condition was calculated as 659.59 kJ mol^{-1} ($n = 4$). The self-accelerating decomposition temperature ($T_{\mathrm{SADT,\ 50kg}}$) was calculated as 175.37 °C.

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