

## Thermal Behavior of 2-(Dinitromethylene)-1,3-diazacyclopentane

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A new compound, 2-(dinitromethylene)-1,3-diazacyclopentane (DNDZ), was prepared by the reaction of 1,1-diamino-2,2-dinitroethylene (FOX-7) with 1,2-diaminoethane in *N*-methylpyrrolidone (NMP). Thermal decomposition of DNDZ was studied under non-isothermal conditions by DSC, TG/DTG methods, and the enthalpy, apparent activation energy and pre-exponential factor of the exothermic decomposition reaction were obtained as 317.13 kJ·mol<sup>-1</sup>, 269.7 kJ·mol<sup>-1</sup> and 10<sup>24.51</sup> s<sup>-1</sup>, respectively. The critical temperature of thermal explosion was 261.04 °C. Specific heat capacity of DNDZ was determined with a micro-DSC method and a theoretical calculation method, and the molar heat capacity was 205.41 J·mol<sup>-1</sup>·K<sup>-1</sup> at 298.15 K. Adiabatic time-to-explosion was calculated to be a certain value between 263—289 s. DNDZ has higher thermal stability than FOX-7.

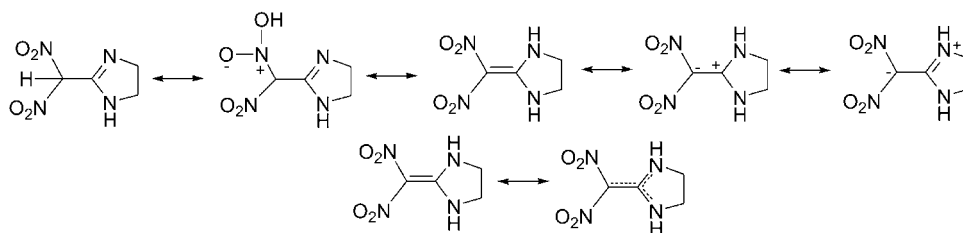
**Keywords** 2-(dinitromethylene)-1,3-diazacyclopentane, 1,1-diamino-2,2-dinitroethylene, thermal behavior, specific heat capacity, adiabatic time-to-explosion

### Introduction

1,1-Diamino-2,2-dinitroethylene (FOX-7) is a novel high energy material with high thermal stability and low sensitivity to impact and friction. When first synthesized in 1998,<sup>1</sup> FOX-7 received much attention. Many researches have been carried out on the synthesis, mechanism, molecule structure, thermal behavior, explosive performance and application of FOX-7.<sup>2-12</sup> According to the molecular structure features, FOX-7 is a special “push-pull” nitro-enamine<sup>13</sup> and possesses a highly polarized carbon-carbon double bond with positive and negative charges being stabilized by the two amino groups and two nitro groups, respectively. So, FOX-7 exists in manifold tautomers and resonances and can react with some nucleophiles to synthesize new high

energy derivatives.<sup>3-5</sup> Our interest mainly consisted in modifying molecular structure of FOX-7 in order to obtain some new high energetic compounds and researching their relationship of structure-property.<sup>14-16</sup> We prepared a new derivative of FOX-7—2-(dinitromethylene)-1,3-diazacyclopentane (DNDZ),<sup>14</sup> and found it had the same structure features as FOX-7 and existed in many manifold tautomers and resonances (Scheme 1). It also could react with strong alkali (KOH), and we have used it to prepare a new high-energy organic potassium salt, which will be used as flame suppressor in propellant to substitute inorganic potassium salt (KCl, K<sub>2</sub>SO<sub>4</sub>, KNO<sub>3</sub> and K<sub>3</sub>AlF<sub>6</sub>) to generate much more energy and clean gas.

Scheme 1



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In this paper, we studied the thermal behavior of DNDZ under non-isothermal conditions by DSC, TG/DTG methods, determined its specific heat capacity with a micro-DSC method and a theoretical calculation method, and calculated its adiabatic time-to-explosion.

## Experimental

### Sample

DNDZ was prepared according to the following method:<sup>14</sup> FOX-7 (0.02 mol, 2.96 g) was dissolved in 12 mL of *N*-methylpyrrolidone (NMP) and to it 1,2-diaminoethane (0.024 mol, 1.44 g) was added dropwise. After reaction at 110 °C for 48 h, the resulting solution was slowly cooled to ambient temperature and diluted with proper amount of water. A lot of flaxen crystals were formed, which were filtered, washed with water, recrystallized with DMF-water and dried under vacuum, in yield of 2.33 g (67%) and purity >99%. IR (KBr)  $\nu$ : 3354, 2899, 1569, 1507, 1175, 1117, 1038, 990  $\text{cm}^{-1}$ . Anal. calcd for  $\text{C}_4\text{H}_6\text{N}_4\text{O}_4$  (%): C 27.59, H 3.47, N 32.18; found C 27.46, H 3.03, N 32.32. The crystal data of DNDZ have been deposited with Cambridge Crystallographic Data Center with the CCDC number of 669664.

### Experimental equipments and conditions

The DSC and TG-DTG experiments for DNDZ were performed using a SDT-Q600 apparatus (TA, USA) under a nitrogen atmosphere at a flow rate of 100  $\text{mL}\cdot\text{min}^{-1}$  and the amount of sample was about 1 mg. The heating rates used were 2.5, 5.0, 10.0 and 15.0  $^\circ\text{C}\cdot\text{min}^{-1}$  from ambient temperature to 400.0 °C.

The measurement of specific heat capacity ( $C_p$ ) of DNDZ was performed using a Micro-DSC III apparatus (Setaram, France). The amount of sample was 411.68 mg. The heating rate was 0.15  $^\circ\text{C}\cdot\text{min}^{-1}$  from 10.0 to 80.0 °C.

### Theoretical calculation of specific heat capacity

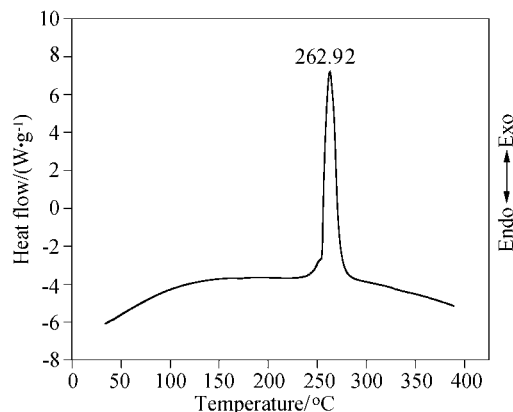
According to the crystal structure of DNDZ,<sup>14</sup> a molecular unit was selected as the initial structure, while HF/6-311++G\*\* and B3LYP/6-311++G\*\* methods in Gaussian 03 package were used to optimize the structure and compute frequencies at different temperatures.<sup>17</sup> We could get a series of thermodynamic data of DNDZ based on the statistic thermodynamic theory. All the convergent precisions were the system default values, and all the calculations were carried out on the personal *Lenovo* computer.

## Results and discussion

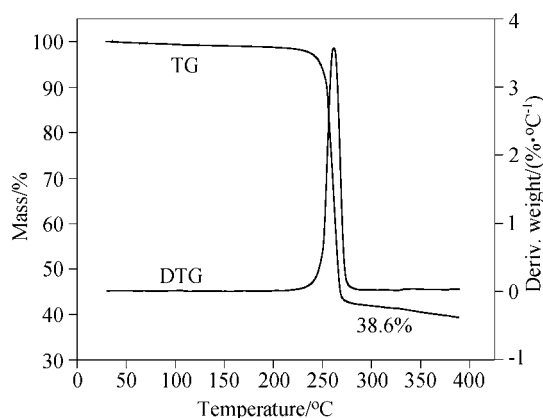
### Thermal behavior of DNDZ

From the typical DSC and TG/DTG curves (Figures 1 and 2), it can be seen that DNDZ has no melting point, and its thermal behavior has only one intense exothermic decomposition process with a mass loss of about

56.2%. The peak temperature and decomposition enthalpy are 262.92 °C and 1821.2  $\text{J}\cdot\text{g}^{-1}$  at the heating rate 5.0  $^\circ\text{C}\cdot\text{min}^{-1}$ , respectively. Comparing the above results with those of FOX-7,<sup>10</sup> DNDZ is much more stable and has higher decomposition enthalpy than FOX-7.



**Figure 1** DSC curve of DNDZ at a heating rate of 5  $^\circ\text{C}\cdot\text{min}^{-1}$ .



**Figure 2** TG-DTG curves of DNDZ at a heating rate of 5  $^\circ\text{C}\cdot\text{min}^{-1}$ .

In order to obtain the kinetic parameters [the apparent activation energy ( $E$ ) and pre-exponential factor ( $A$ )] of the exothermic decomposition reaction for DNDZ, a multiple heating method (Kissinger's method<sup>18</sup> and Ozawa's method<sup>19</sup>) was employed. The Kissinger and Ozawa equations are as follows:

$$\ln\left(\frac{\beta}{T_p^2}\right) = \ln\frac{A_k R}{E_k} - \frac{E_k}{R T_p} \quad (1)$$

$$\lg\beta + \frac{0.4567E_0}{RT_p} = C \quad (2)$$

where  $T_p$  is the peak temperature,  $R$  is the gas constant,  $E$  is the apparent activation energy,  $\beta$  is the linear heating rate and  $C$  is a constant.

The measured values of the beginning temperature ( $T_0$ ), extrapolated onset temperature ( $T_e$ ), peak tempera-

ture ( $T_p$ ) and enthalpy of the exothermic decomposition reaction ( $\Delta H_d$ ) are listed in Table 1. The values of  $T_{00}$ ,  $T_{e0}$  and  $T_{p0}$  corresponding to  $\beta \rightarrow 0$  obtained by Eq. (3) are also listed in Table 1.<sup>20,21</sup>

$$T_{(0, e \text{ or } p)i} = T_{(00, e0 \text{ or } p0)} + n\beta_i + m\beta_i^2 \quad i=1-4 \quad (3)$$

where  $n$  and  $m$  are coefficients.

The above-mentioned values ( $E$  and  $A$ ) determined by Kissinger's method and Ozawa's method and linear correlation coefficients ( $r$ ) are given in Table 2. The result indicates that the apparent activation energy obtained by Kissinger's method agrees well with that obtained by Ozawa's method. The linear correlation coefficients ( $r$ ) are all very close to 1. So, the results are credible. Moreover, the apparent activation energy ( $E$ ) of the exothermic decomposition reaction was quite high, indicating that DNDZ is very stable.

The critical temperature of thermal explosion ( $T_b$ ) obtained by Eq. (4) is 261.04 °C,<sup>20,21</sup> which is much higher than that of FOX-7 as 207.08 °C.<sup>10</sup>

$$T_b = \frac{E_0 - \sqrt{E_0^2 - 4E_0RT_{e0}}}{2R} \quad (4)$$

where  $E_0$  is the value of  $E$  by Ozawa's method.

The entropy of activation ( $\Delta S^\ddagger$ ), enthalpy of activation ( $\Delta H^\ddagger$ ) and free energy of activation ( $\Delta G^\ddagger$ ) corresponding to  $T=T_{p0}$ ,  $E=E_k$  and  $A=A_k$  obtained by Eqs. (5)–(7) taken from Ref. 21 are 219.59 J·mol<sup>-1</sup>·K<sup>-1</sup>, 272.1 kJ·mol<sup>-1</sup> and 156.68 kJ·mol<sup>-1</sup>, respectively.

$$A = \frac{k_B T}{h} \exp\left(\frac{\Delta S^\ddagger}{R}\right) \quad (5)$$

$$A \exp\left(-\frac{E}{RT}\right) = \frac{k_B T}{h} \exp\left(\frac{\Delta S^\ddagger}{R}\right) \exp\left(-\frac{\Delta H^\ddagger}{RT}\right) \quad (6)$$

$$\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger \quad (7)$$

where  $k_B$  is the Boltzman constant and  $h$  is the Plank constant.

Thermal decomposition data of DNDZ by TG-DTG curves at different heating rates are listed in Table 3.  $T$  versus  $\alpha$  (the conversion degree) curves at different heating rates are shown in Figure 3.

By substituting the original data,  $\beta_i$ ,  $T_i$  and  $\alpha_i$ ,  $i=1$ ,

2, 3, ..., tabulated in Table 3 from TG-DTG curves into Eq. (2), the values of  $E_a$  for any given value of  $\alpha$  were obtained and also shown in Figure 4. We can see that  $E_a$  rose with the increment of the conversion degree ( $\alpha$ ), reached the maximum value at  $\alpha$  of about 0.225, and then gradually decreased with the increment of  $\alpha$ , which did not present any visible linear relationship. So, we believed the exothermic decomposition reaction for DNDZ was very complicated, and it is impossible to use a known most probable kinetic model function [ $f(\alpha)$ ] to describe the decomposition process.<sup>24</sup> But, the average value of  $E_a$  of the whole decomposition process is in good agreement with that obtained by Kissinger's method and Ozawa's method from only peak temperature values.

### Specific heat capacity

Figure 5 shows the determination results of DNDZ using a continuous specific heat capacity mode of a Micro-DSCIII apparatus. In determining temperature range, specific heat capacity of DNDZ presents a good linear relationship with temperature. Specific heat capacity (J·mol<sup>-1</sup>·K<sup>-1</sup>) equation is shown as:

$$C_p = 47.990 + 0.528T \quad (283.0 \text{ K} < T < 353.0 \text{ K}) \quad (8)$$

The molar heat capacity of DNDZ is 205.41 J·mol<sup>-1</sup>·K<sup>-1</sup> 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.

The vibrational frequency calculations found no imaginary frequencies, showing that our theoretical calculation is reliable. Table 4 shows the results of specific heat capacity obtained by the theoretical calculation and experimental determination and their relative deviation at different temperatures. We can see that the calculated results by B3LYP/6-311++G\*\* method are greater than those by HF/6-311++G\*\* method, but they are all less than the experimental results. The relative deviation between the calculation results by B3LYP/6-311++G\*\* method and the experimental results is comparatively large, from 19.53% to 19.85%, and gradually reduced with the rising of temperature. The reason for the results is that only single gas-phase molecule was used in theoretical calculation process, which is clearly different to the actual solid phase molecule.

In addition, DNDZ exists in a reversible crystal phase transition (Figure 6) in the process of specific heat ca-

**Table 1** Values of  $T_0$ ,  $T_e$ ,  $T_p$ ,  $\Delta H_d$ ,  $T_{00}$ ,  $T_{e0}$  and  $T_{p0}$  of the thermal decomposition for DNDZ determined by DSC curves at various heating rates ( $\beta$ )

$\beta/(\text{°C}\cdot\text{min}^{-1})$	$T_0/\text{°C}$	$T_e/\text{°C}$	$T_p/\text{°C}$	$\Delta H_d/(\text{kJ}\cdot\text{mol}^{-1})$	$T_{00}/\text{°C}$	$T_{e0}/\text{°C}$	$T_{p0}/\text{°C}$
2.5	217.42	253.57	256.82				
5.0	219.79	254.56	262.92				
10.0	220.68	256.64	267.60	317.13	215.86	252.16	252.46
15.0	221.52	257.75	272.57				

**Table 2** Kinetic parameters obtained from the data in Table 1<sup>a</sup>

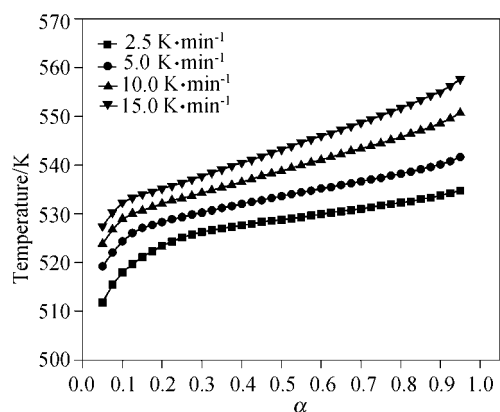
$E_k/$ (kJ·mol <sup>-1</sup> )	$\lg(A_k/s^{-1})$	$r_k$	$E_o/$ (kJ·mol <sup>-1</sup> )	$r_o$	$\bar{E}/$ (kJ·mol <sup>-1</sup> )
272.1	24.51	0.9953	267.3	0.9956	269.7

<sup>a</sup> Subscript k, data obtained by Kissinger's method; subscript O, data obtained by Ozawa's method.

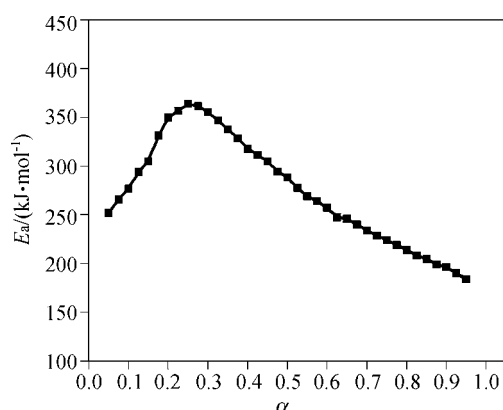
capacity determination. The extrapolated onset temperature, peak temperature and enthalpy of the crystal phase transition are 31.47 °C, 34.21 °C and 13.44 J·mol<sup>-1</sup>, respectively. From the results, we can see that the phase transition is easy to be neglected. However, we did not find any obvious phase transition process in the DSC curve of thermal behavior determination.

**Table 3** Data of DNDZ decomposition determined by TG-DTG curves

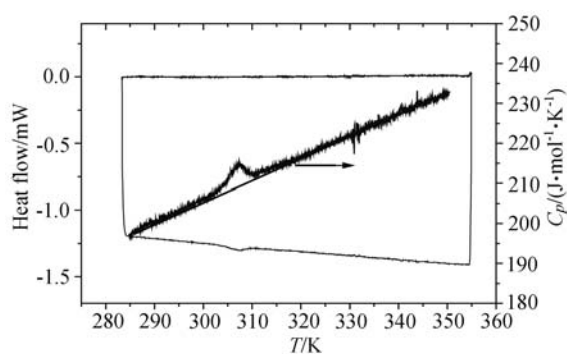
No.	$\alpha$	2.5 K·min <sup>-1</sup>		5.0 K·min <sup>-1</sup>		10.0 K·min <sup>-1</sup>		15.0 K·min <sup>-1</sup>	
		$T/K$	$da/dT$ ×100	$T/K$	$da/dT$ ×100	$T/K$	$da/dT$ ×100	$T/K$	$da/dT$ ×100
1	0.050	511.80	0.550	519.21	0.336	523.83	0.578	527.45	0.449
2	0.075	515.47	0.891	522.08	0.546	526.77	1.413	530.24	1.283
3	0.100	517.99	1.264	524.36	0.943	528.95	2.657	532.28	2.227
4	0.125	519.70	1.585	526.09	1.550	530.01	3.245	533.28	2.573
5	0.150	521.12	1.934	527.11	1.931	530.61	2.502	533.95	2.756
6	0.175	522.32	2.365	527.72	2.168	531.37	3.598	534.49	2.881
7	0.200	523.42	3.117	528.29	2.395	532.01	3.769	535.13	3.018
8	0.225	524.33	3.958	528.91	2.515	532.74	3.928	535.70	3.138
9	0.250	525.14	4.810	529.31	2.635	533.10	4.058	536.28	3.242
10	0.275	525.76	5.479	529.82	2.759	533.68	4.228	536.99	3.305
11	0.300	526.25	5.920	530.22	2.884	534.21	4.321	537.69	3.293
12	0.325	526.64	6.335	530.68	3.014	534.79	4.357	538.38	3.227
13	0.350	527.01	6.644	531.12	3.129	535.36	4.336	539.08	3.131
14	0.375	527.32	6.931	531.57	3.227	535.92	4.301	539.76	3.036
15	0.400	527.64	7.061	531.98	3.309	536.48	4.228	540.44	2.988
16	0.425	527.90	7.275	532.37	3.367	537.10	4.170	541.04	2.962
17	0.450	528.36	7.418	532.76	3.405	537.72	4.155	541.77	2.946
18	0.475	528.56	7.620	533.17	3.431	538.26	4.151	542.5	2.933
19	0.500	528.79	7.721	533.57	3.442	538.74	4.149	543.16	2.923
20	0.525	529.04	7.841	533.97	3.444	539.41	4.149	543.85	2.908
21	0.550	529.30	7.919	534.37	3.443	539.93	4.144	544.63	2.896
22	0.575	529.64	7.955	534.72	3.43	540.53	4.136	545.24	2.883
23	0.600	529.87	7.977	535.14	3.426	541.04	4.123	545.94	2.867
24	0.625	530.21	7.938	535.46	3.407	541.64	4.100	546.51	2.843
25	0.650	530.47	7.877	535.86	3.367	542.22	4.068	547.27	2.814
26	0.675	530.72	7.789	536.22	3.322	542.84	4.024	547.92	2.781
27	0.700	530.96	7.668	536.61	3.258	543.34	3.98	548.67	2.740
28	0.725	531.25	7.437	536.98	3.179	543.93	3.887	549.37	2.686
29	0.750	531.65	7.200	537.37	3.074	544.48	3.795	550.17	2.619
30	0.775	531.94	6.916	537.79	2.975	545.13	3.670	550.89	2.541
31	0.800	532.24	6.634	538.20	2.839	545.71	3.527	551.70	2.431
32	0.825	532.45	6.275	538.62	2.670	546.41	3.339	552.47	2.298
33	0.850	532.97	5.898	539.10	2.495	547.06	3.103	553.33	2.124
34	0.875	533.25	5.511	539.57	2.310	547.76	2.816	554.26	1.896
35	0.900	533.72	5.128	540.10	2.069	548.56	2.472	555.01	1.595
36	0.925	534.16	4.566	540.74	1.802	549.52	1.476	556.23	1.206
37	0.950	534.68	3.952	541.62	1.442	550.69	1.395	557.60	0.594



**Figure 3**  $T$  vs.  $\alpha$  curves for the decomposition reaction of DNDZ at different heat rates.



**Figure 4**  $E_a$  vs.  $\alpha$  curve for the decomposition reaction of DNDZ by Ozawa's method.



**Figure 5** Determination results of the continuous specific heat capacity.

### Thermodynamic properties

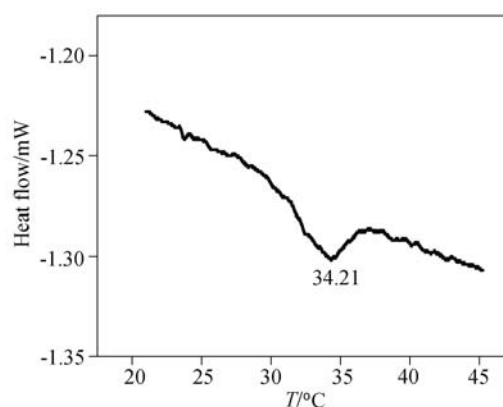
The enthalpy change, entropy change and Gibbs free energy change of DNDZ were calculated by Eqs. (9)–(11) during 288.0–488.0 K from ambient temperature to thermal decomposition temperature, taking 298.15 K as the benchmark. The results are listed in Table 5.

$$H_T - H_{298.15} = \int_{298.15}^T C_p dT \quad (9)$$

$$S_T - S_{298.15} = \int_{298.15}^T C_p \cdot T^{-1} dT \quad (10)$$

**Table 4** Results of specific heat capacity obtained by theoretical calculation and experimental determination and their relative deviation in 283–353 K

$T/K$	$C_p/(J \cdot mol^{-1} \cdot K^{-1})$		Experimental value	RD/%
	Theoretical calculation value			
	HF	B3LYP		
283.0	139.58	158.23	197.41	19.85
288.0	141.55	160.40	200.05	19.82
293.0	143.53	162.57	202.69	19.79
298.0	145.51	164.74	205.33	19.77
303.0	147.48	166.90	207.97	19.75
308.0	149.46	169.07	210.61	19.72
313.0	151.44	171.24	213.25	19.70
318.0	153.42	173.41	215.89	19.68
323.0	155.39	175.58	218.53	19.66
328.0	157.37	177.75	221.17	19.65
333.0	159.35	179.92	223.81	19.63
338.0	161.32	182.09	226.45	19.60
343.0	163.30	184.26	229.09	19.57
348.0	165.28	186.43	231.73	19.55
353.0	167.25	188.60	234.37	19.53



**Figure 6** DSC curve of DNDZ at a heating rate of 0.15 °C·min<sup>-1</sup>.

$$G_T - G_{298.15} = \int_{298.15}^T C_p dT - T \int_{298.15}^T C_p \cdot T^{-1} dT \quad (11)$$

### Adiabatic time-to-explosion

Energetic materials need a time from the beginning thermal decomposition to thermal explosion in the adiabatic conditions. The time is named the adiabatic time-to-explosion.<sup>21–24</sup> Ordinarily, the heating rate ( $dT/dt$ ) and critical heating rate  $(dT/dt)_{T_b}$  in a thermal decomposition reaction were used to estimate the thermal stability of energetic materials. However, the adiabatic time-to-explosion ( $t$ ) can be calculated by the following

**Table 5** Thermodynamic function data of DNDZ

$T/K$	$(H_T - H_{298.15})/$ (kJ·mol <sup>-1</sup> )	$(S_T - S_{298.15})/$ (J·mol <sup>-1</sup> ·K <sup>-1</sup> )	$(G_T - G_{298.15})/$ (kJ·mol <sup>-1</sup> )
288.0	-2.06	-7.02	-0.04
308.0	2.05	6.76	-0.03
328.0	6.37	20.34	-0.30
348.0	10.90	33.74	-0.85
368.0	15.64	46.98	-1.65
388.0	20.59	60.08	-2.72
408.0	25.75	73.05	-4.06
428.0	31.12	85.91	-5.64
448.0	36.71	98.66	-7.49
468.0	42.51	111.32	-9.59
488.0	48.51	123.89	-11.94

Eqs. (12) and (13)<sup>21,23,24</sup> if a series of experimental data were obtained. Thereby, as an important parameter, it is easier and intuitionistic to estimate the thermal stability of energetic materials according to the length of the adiabatic time-to-explosion.

$$C_p \frac{dT}{dt} = QA \exp(-E/RT) f(\alpha) \quad (12)$$

$$\alpha = \int_{T_0}^{T_b} \frac{C_p}{Q} dT \quad (13)$$

where  $C_p$  is the specific heat capacity (J·mol<sup>-1</sup>·K<sup>-1</sup>),  $T$  is the absolute temperature (K),  $t$  is the adiabatic decomposition time (s),  $Q$  is the exothermic energy (J·mol<sup>-1</sup>),  $A$  is the pre-exponential factor (s<sup>-1</sup>),  $E$  is the apparent activation energy of the thermal decomposition reaction (J·mol<sup>-1</sup>),  $R$  is the gas constant (J·mol<sup>-1</sup>·K<sup>-1</sup>),  $f(\alpha)$  is the most probable kinetic model function and  $\alpha$  is the conversion degree.

According to the above experimental results, we use:

$$C_p = a + bT \quad (14)$$

where  $a$  and  $b$  are coefficients.

In fact, the conversion degree ( $\alpha$ ) of energetic materials from the beginning thermal decomposition to thermal explosion in the adiabatic conditions is very small, the most probable kinetic model function [ $f(\alpha)$ ] at this beginning decomposition process is unimportant and almost has no influence on the result of the adiabatic time-to-explosion. So, we used Eq. (15) and supposed that the rate order of the mechanism function ( $n$ ) of DNDZ in the process equaled 0—2.

$$f(\alpha) = (1 - \alpha)^n \quad (15)$$

The combination of Eqs. (12)—(15) can give the following equation:

$$\begin{aligned} t &= \int_0^t dt = \int_{T_0}^{T_b} \frac{C_p \exp(E/RT)}{QA f(\alpha)} dT \\ &= \frac{1}{QA} \int_{T_0}^{T_b} \frac{(a+bT) \exp(E/RT)}{(1-\alpha)^n} dT \\ &= \frac{1}{QA \left\{ 1 - \frac{1}{Q} \left[ a(T_b - T_0) + \frac{b}{2}(T_b^2 - T_0^2) \right] \right\}^n} \times \\ &\quad \int_{T_0}^{T_b} (a+bT) \exp(E/RT) dT \end{aligned} \quad (16)$$

The limit of the temperature integral in Eq. (16) is from  $T_0$  to  $T_b$ . We can directly get  $t_0=263.94$  s,  $t_1=276.46$  s and  $t_2=289.58$  s from Eq. (16), according to the above-obtained data. As a rule, the rate order ( $n$ ) of energetic materials ranges from 0 to 2, so the adiabatic time-to-explosion of DNDZ is a certain value between 263—290 s, which is much longer than that of FOX-7 as 78.94—88.93 s.<sup>23</sup> In another aspect, it further proves the higher thermal stability of DNDZ than that of FOX-7.

## Conclusion

The thermal behavior of DNDZ under non-isothermal conditions by DSC, TG/DTG methods was studied. The enthalpy, apparent activation energy and pre-exponential factor of the exothermic decomposition reaction are 317.13 kJ·mol<sup>-1</sup>, 269.7 kJ·mol<sup>-1</sup> and 10<sup>24.51</sup> s<sup>-1</sup>, respectively. The critical temperature of thermal explosion is 208.6 °C.

The specific heat capacity of DNDZ was determined with a micro-DSC method and a theoretical calculation method. Specific heat capacity (J·mol<sup>-1</sup>·K<sup>-1</sup>) equation is  $C_p = 47.990 + 0.528T$  (283.0 K <  $T$  < 353.0 K). The molar heat capacity of DNDZ is 205.41 J·mol<sup>-1</sup>·K<sup>-1</sup> at 298.15 K. The adiabatic time-to-explosion of DNDZ was calculated to be a certain value between 263—290 s. DNDZ has higher thermal stability than FOX-7.

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