

Thermal decomposition behavior and thermal stability of DABT·2DMSO

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Abstract The thermal decomposition behavior and thermal stability of 3,3'-diamino-5,5'-bis(1H-1,2,4-triazole) with 2DMSO (DABT·2DMSO) were investigated by thermo gravimetry-derivative thermo gravimetry-differential scanning calorimetry (TG-DTG-DSC), differential thermal analysis (DTA) and accelerating rate calorimeter (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 388.23 and 468.23 °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 heating rates of 1, 2, 4, 8 °C min⁻¹. The critical temperature of thermal explosion (T_{bp0}) obtained by the Ozawa's and Kissinger's methods were calculated as 470.46 and 470.73 °C, respectively. The result of ARC indicated that the self-heating decomposition started at 443.61 °C and ended at 480.91 °C, within the time span of 1397.50 min. The self-heating decomposition parameters, including the onset temperature, final temperature, temperature at max rate, max 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

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calculated. In addition, the self-accelerating decomposition temperature ($T_{\text{SADT, 50kg}}$) was calculated as 429.54 °C.

Keywords 3,3'-Diamino-5,5'-bis(1H-1,2,4-triazole) \cdot DABT·2DMSO \cdot Thermal decomposition behavior \cdot Thermal stability \cdot Non-isothermal kinetics

Introduction

3,3'-Diamino-5,5'-bis(1H-1,2,4-triazole) (DABT) is an important raw material and widely used in the production of bistriazoles energetic materials, such as 3,3'-dinitro-5,5'-bis(1H-1,2,4-triazole) (DNBT) [1, 2], 3,3'-dinitrimino-5,5'-bis(1H-1,2,4-triazole) (DNABT) [1, 3], 3,3'-diazide-5,5'-bis(1H-1,2,4-triazole)-1,1'-diol (DNBTO) [4] and their derivatives [2–4], carbonic dihydrazidinium bis[3-(5-ni-troimino-1,2,4-triazolate)] (CBNT) [3], dihydroxylammonium 3,3'-dinitro-5,5'-bis-1H-1,2,4-triazole-1,1'-diolate (HBNTO) [3], which were reported as two of most promising ionic salts to possibly replaced 1,3,5-trinitro-1,3,5-trinazole)energetic (RDX).

We investigated the heat of formation and detonation properties of DABT by using density functional theory (DFT-B3LYP) method. Previous studies have shown that the basis set 6-311 + G(2df, 2p) is able to predict the molecular structures and energies of energetic organic compounds [5–7]. The heat of formation of DABT (334.77 kJ mol⁻¹) in the gas phase was determined at the B3LYP/6-311 + G(2df, 2p) theory level through isodesmic reaction. The detonation velocity (5.70 km s⁻¹) and detonation pressure (13.79 GPa) were evaluated by Kamlet– Jacob equations. For the process safety of these bistriazoles energetic materials synthesized with DABT, the

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investigations of thermal decomposition behavior and thermal stability of DABT were very necessary.

In order to acquire the thermal decomposition behavior and thermal stability of DABT under non-isothermal and adiabatic conditions, the thermo gravimetry-derivative thermo gravimetry-differential scanning calorimetry (TG-DTG-DSC), differential thermal analysis (DTA) and accelerating rate calorimetry (ARC) were carried out. The thermo-kinetic parameters of the exothermic decomposition and thermodynamic parameters at the initial decomposition temperature (T_{p0}) under non-isothermal condition were obtained from DTA. The self-heating decomposition parameters, adiabatic decomposition kinetics 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 behavior and thermal stability of DABT under non-isothermal and adiabatic conditions.

Experimental

Materials

DABT was home-made and purified according to the literature [1, 2]. The synthesis route of DABT was shown in Scheme 1.

The compound of DABT was additionally characterized by single-crystal X-ray spectroscopy. The result of singlecrystal X-ray spectroscopy indicated that one molecule of DABT was associated with two molecules of DMSO. Crystallographic data and parameters as well as the morphology have been compiled in Table 1. The crystal structure of DABT was shown in Fig. 1.

Instruments

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



Scheme 1 The synthesis route of DABT

Table 1	X-ray data	and parameters	of DABT·2DMSO
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Parameters	Values	Parameters	Values
Formula	C4H6N8·2C2H6OS	F(000)	340.0
Formula mass/ g mol ⁻¹	322.42	$\lambda_{Mo-Ka}/ \mathring{A}$	0.71073
Crystal system	Monoclinic	T/K	296
Space group	P21/c	Theta max/°	28.250
Color, habit	Colorless, needle	Dataset <i>h</i> max	12
a/Å	9.6017	Dataset k max	11
b/Å	8.6632	Dataset <i>l</i> max	13
c/Å	9.9406	Reflections	1564
α/°	90	No. parameters	136
β/°	112.668	R_1, wR_2	0.0433, 0.1188
γ/°	90	S	1.052
Volume/Å ³	763.00	Device type	Oxford Xcalibur3 CCD
Ζ	2	Solution	SHELXS-97
Calculated density/ g cm ⁻³	1.403	Refinement	SHELXL-97
μ/mm^{-1}	0.364	Absorption correction	Multi-scan



Fig. 1 Crystal structure of DABT·2DMSO. Thermal ellipsoids are set to 50% probability. Selected bond lengths/Å: C1–C1' 1.461(2), C1–N1 1.318(15), C1-N3 1.367(15), C2-N2 1.339(16), C2–N3 1.337(2), C2–N4 1.347(17), N1–N2 1.374(15), N4HB…O1 2.058(91). Selected bond angles/°: C1'–C1–N1 121.61(13), C1–N1–N2 102.09(10), C1–N3–C2 102.52(10), N4–C2–N2 122.59(12), N4–C2–N3 127.31(12). Selected torsion angles/°: C2–N3–C1–C1' 178.19(120), N2–N1–C1–C1' – 178.08(116), C1–N3–C2–N4 – 177.36(142), N3–C2–N4–N4HB – 0.028(254), N3–C2–N4–N4HB – 179.97(144), C2–N4–N4HB…O1 167.12(924)

thermal analyzer at 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 650 °C.

The ARC measurement was performed with a Thermal Hazard Technology accelerating rate calorimeter in the Heat-Wait-Search mode. The experiment conditions were listed in Table 2.

Results and discussion

Thermal decomposition processes

The TG–DTG–DSC curve at a heating rate of 10 °C min⁻¹ was given in Fig. 2. From the TG and DTG curves, two stages were obviously seen. The first stage was started at 388.23 °C and ended at 462.73 °C, and the mass loss was 49.00%. This was a process of lost DMSO, and the theoretically calculated value of the process was in exact accordance with the experimental value. The second stage was started at 468.23 °C and ended at 535.73 °C, and the mass loss was 21.20%. From the DSC curve, the first stage was an endothermic decomposition, and the peak temperature was determined as 449.23 °C, and the second stage was an exothermic decomposition, and the peak temperature was determined as 495.23 °C.

Non-isothermal decomposition kinetics

The DTA curves at heating rates of 1, 2, 4, 8 °C min⁻¹ were given in Fig. 3. Both an endothermic decomposition of lost DMSO and an exothermic decomposition were observed. Different onset temperatures (429.62, 446.91, 454.33, 465.45 °C) and peak temperatures (447.59, 466.74, 479.09, 494.09 °C) of the exothermic decomposition processes were observed at heating rates of 1, 2, 4,

Table 2 Experimental conditions of DABT by ARC

Parameters	Values	Parameters	Values
Sample mass/g	0.1008	Start temperature/°C	50
Sample heat capacity/ kJ kg ⁻¹ K ⁻¹	2.00 ^a	End temperature/°C	500
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

^aHeat capacity of organic sample default 2.00, the value is taken from Refs. [17, 18]



Fig. 2 TG–DTG–DSC curve of DABT at a heating rate of 10 $^{\circ}\text{C}\ \text{min}^{-1}$



Fig. 3 DTA curves of DABT at heating rates of 1, 2, 4, 8 °C min⁻¹

8 °C min⁻¹, respectively. When the heating rate was high, the onset temperature of the exothermic decomposition was delayed, and the corresponding peak temperature shifted to a higher temperature.

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

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

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

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 log β against $1/T_p$ and $\ln(\beta/T_p^2)$ against $1/T_p$ 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/s^{-1}).

 Table 3
 Non-isothermal kinetics and thermodynamics parameters of DABT obtained by Ozawa's and Kissinger's methods

Method	$E_{\rm a}/{\rm kJ}~{\rm mol}^{-1}$	$\log A/s^{-1}$	r	$T_{\rm p0}/^{\circ}{\rm C}$	$\Delta G^{\neq}/\text{kJ mol}^{-1}$	$\Delta H^{\neq}/\text{kJ mol}^{-1}$	$\Delta S^{\neq}/J \text{ mol}^{-1} \text{ K}^{-1}$	T _{bp0} /°C
Ozawa	197.54	12.94	0.9843	447.19	200.77	191.55	-12.80	470.46
Kissinger	195.41	12.79	0.9824	447.19	200.78	189.42	-15.77	470.73

Table 4 Self-heating decomposition parameters of DABT by ARC

Parameters	Values	Corr.	Parameters	Values	Corr.
Onset temperature/°C	443.61	403.72	Adiabatic temperature rise/°C	37.30	1139.06
Onset temperature rate/°C min ⁻¹	0.02	0.55	Time to maximum rate/min	686.30	22.47
Temperature at max rate/°C	463.00	996.00	Max pressure/bar	7.84	_
Max self-heating rate/°C min ⁻¹	0.04	1.34	Thermal inertia factor	30.54	-
Final temperature/°C	480.91	1542.78			

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

The E_a , logA/s⁻¹ and corresponding regression coefficient (*r*) which were obtained by Ozawa's and Kissinger's methods were listed in Table 3.

Thermodynamics at initial decomposition temperature (T_{p0})

The value of initial decomposition temperature $(T_{\rm p0})$ in the exothermic decomposition process corresponding to $\beta \rightarrow 0$ was calculated by Eq. (4) [10, 11]

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

where T_{pi} is the peak temperature of a heating rate of β_i , *a* and *b* are the coefficients.

The free energy of activation (ΔG^{\neq}) , activation enthalpy (ΔH^{\neq}) and activation entropy (ΔS^{\neq}) were calculated by Eqs. (5), (6) and (7) [11]:

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

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

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

where $E_{\rm a}$ is the apparent activation energy, *h* is the Planck constant, $k_{\rm B}$ is the Boltzmann constant. The $T_{\rm p0}$, ΔG^{\neq} , ΔH^{\neq} and ΔS^{\neq} were listed in Table 3.

Critical temperature of thermal explosion (T_{bp0})

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

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

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 [14–16]. The corrected and measured self-heating decomposition parameters of DABT were given in Table 4.

$$\phi = 1 + \frac{M_b C_{\rm v,b}}{M_s C_{\rm v,s}} \tag{9}$$

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

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

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

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

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

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

$$TMR_{corr} = \frac{TMR}{\phi}$$
(16)

where φ is the thermal inertia factor, $M_{\rm b}$ is the test cell mass, $C_{\rm v,b}$ is the test cell heat capacity, $M_{\rm s}$ is the sample mass, $C_{\rm v,s}$ is the sample heat capacity. $T_{\rm o,corr}$ and $T_{\rm o}$ are the corrected and measured onset decomposition temperature, respectively; $T_{\rm f,corr}$ and $T_{\rm f}$ are the corrected and measured final decomposition temperature, respectively; $\Delta T_{\rm ad,corr}$ and $\Delta T_{\rm ad}$ are the corrected and measured adiabatic temperature rise, respectively; $m_{\rm o,corr}$ and $m_{\rm o}$ are the corrected and

measured onset temperature rate, respectively; $m_{m,corr}$ and m_m are the corrected and measured max self-heating rate, respectively; $T_{m,corr}$ and T_m are the corrected and measured temperature at max rate, respectively; TMR_{corr} and TMR are the corrected and measured time to maximum rate, respectively.

The ARC curves of DABT were given in Fig. 4. As seen from Fig. 4a, an endothermic decomposition and an exothermic decomposition were observed. The endothermic decomposition of lost DMSO started at 395.10 °C and ended at 441.09 °C, and the pressure of the period increased 5.80 bar (Fig. 4b). The exothermic decomposition started at 443.61 °C and ended at 480.91 °C, within the time span of 1397.50 min (Fig. 4c). The max selfheating rate was 0.04 °C min⁻¹ at 463.00 °C (Fig. 4d). From Fig. 4, it could be concluded that when the ambient temperature below 395.10 °C, DABT was not decomposition.

Adiabatic decomposition kinetics

For an *n*th-order single step reaction with a single reaction, the self-heating rate could be expressed as following [14, 16]:

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

where $m_{\rm T}$ 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.

Fig. 4 ARC curves of DABT. a Temperature and pressure versus time, b loss of DMSO temperature and pressure versus time, c decomposition temperature and pressure versus time, d decomposition temperature and temperature rate versus time Rearranging Eq. (17), we had [14, 16]:

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

where k^* is a pseudo zero-order rate constant at the temperature *T*. According to the Arrhenius equation, one could obtain [14, 16].

$$\ln k^* = \ln C_0^{n-1} A - \frac{E_a}{R} \left[\frac{1}{T} \right]$$
(19)

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

Time to maximum rate (TMR)

According to the literature, the TMR and T have the following relationship [16–18].

$$\ln \text{TMR} = \frac{E_{a}}{R} \left[\frac{1}{T} \right] - \ln A + \ln \frac{RT^{2}}{C_{0}^{n-1} \left[\frac{T_{f} - T}{\Delta T_{ad}} \right]^{n} \Delta T_{ad} E_{a}}$$
(20)

From Table 5, n = 2, E_a was 345.76 kJ mol⁻¹, logA/s⁻¹ was 19.66. Then, the plot of TMR versus *T* was given in Fig. 6.

Self-accelerating decomposition temperature (T_{SADT})

The T_{SADT} is defined as the lowest ambient air temperature at which self-accelerating decomposition may occur within





Fig. 5 Lnk^* versus T^{-1} of DABT

n	$E_{\rm a}/{\rm kJ}~{\rm mol}^{-1}$	$\log A/s^{-1}$	r
1	183.57	8.49	0.9689
2	345.76	19.66	0.9801
3	507.95	30.82	0.9827
4	667.68	41.82	0.9834



Fig. 6 TMR versus T of DABT

a substance in the packaging as used in transport and storage. The adiabatic decomposition kinetics parameters were used for the estimation of the T_{SADT} for DABT in a 50 kg package. Firstly, Eq. (21) was used to get the time constant (τ), 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) [19, 20].

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

$$T_{\rm SADT} = T_{\rm NR} - \frac{{\rm R}T_{\rm NR}^2}{E_{\rm a}}$$
(22)

Table 6	Onset tem	peratures of	DABT	and	DNABT
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Compounds	Onset temperature by DSC ^a	Onset temperature by ARC ^b
DABT	468.23	443.61
DNABT	210.86	200.22

^aOnset temperatures by DSC at 10 $^{\circ}$ C min⁻¹, the value of DNABT is taken from our previous work

^bOnset temperatures by ARC, the value of DNABT is taken from our previous work

where U is the heat transfer coefficient, a is the contact area of the system and environment. Assuming 50 kg DABT 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 m². 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 DABT was calculated as 429.54 °C.

Comparison of onset temperatures of DABT with DNABT

The values of onset temperatures of DABT and its derivative DNABT were listed in Table 6.

From Table 6, it could be concluded that the onset temperatures of DABT were determined in the DSC and ARC experiments were found to be higher than that of DNABT. DABT was a stable compound compared with DNABT

Conclusions

The thermal decomposition behavior of DABT were studied by TG-DTG-DSC, DTA and ARC techniques. The results from TG-DTG-DSC, DTA and ARC all suggested that DABT had an endothermic decomposition of lost DMSO and an exothermic decomposition. The TG-DTG-DSC measurement showed that the endothermic decomposition of lost DMSO started at 388.23 °C and ended at 462.73 °C, and the exothermic decomposition started at 468.23 °C and ended at 535.73 °C. The values of nonisothermal decomposition kinetics and thermodynamics parameters that were obtained by the Ozawa's and Kissinger's methods for DABT showed good correlation. The critical temperature of thermal explosion (T_{bp0}) obtained by the Ozawa's and Kissinger's methods were calculated as 470.46 and 470.73 °C, respectively. The self-heating decomposition parameters, including the T_0 , T_f , T_m , m_m , $\Delta T_{\rm ad}$ and TMR, were obtained and corrected by φ . The self-accelerating decomposition temperature $(T_{\text{SADT}, 50\text{kg}})$ was calculated as 429.54 °C. DABT was a stable compound compared with DNABT.

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