Non-isothermal kinetic studies on thermal decomposition of energetic materials

KNF and NTO

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Abstract Thermal stability and decomposition kinetics for two energetic materials, potassium nitroform (KNF) and 5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO), were investigated to obtain information on their safety for handling, storage, and use. Differential scanning calorimetry (DSC) and simultaneous thermogravimetry-differential thermal analysis (TG-DTA) techniques have been used to study thermal behavior of these energetic compounds. The results of TG analysis revealed that the main thermal degradation for the KNF occurs during two temperature ranges of 270–330 and 360–430 °C. Meanwhile, NTO decomposes completely in temperature range of 250–300 °C. TG-DTA analysis of KNF indicates that this energetic compound dehydrated (at about 108 °C) before its decomposition. However, NTO is thermally stable until its decomposition. The decomposition kinetic of energetic materials was studied by non-isothermal DSC under various heating rates. Kinetic parameters such as activation energy and frequency factor for thermal decomposition of energetic compounds were obtained via the methods proposed by ASTM E696 and Starink. Also, thermodynamic parameters correspond to the activation of thermal decomposition and critical ignition temperatures of the compounds were obtained.

Keywords Decomposition kinetic Thermal stability ·
Non-isothermal · KNF · NTO · Potassium nitroform ·

5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one ·
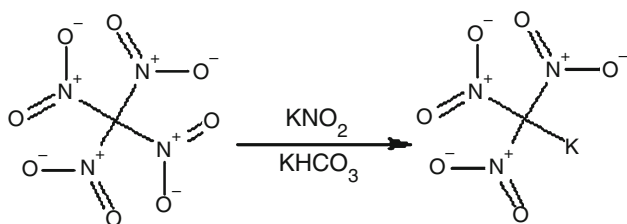Energetic materials

Introduction

KNF or potassium nitroform is a colorless to white crystal or powder. The crystals of this potassium salt are stable and used widely in formulations of energetic materials such as gunpowders, rocket propellants, and fireworks [1]. Although, KNF crystals have considerable stability; but, when ignited they burn violently and rapidly. On the other hand, KNF is easily ignited; however, this nitroform salt undergoes no detonation unless initiated by a primary explosive [2].

KNF could be synthesized (as shown in Scheme 1) via reacting tetranitromethane with potassium nitrite and potassium bicarbonate in a solution of dioxane/water. In the next step of preparation procedure, the resulted mixture is heated, and then cooled in an ice water bath. The precipitated KNF product is then filtered and dried.

5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO) has the chemical structure shown in Scheme 2. This compound posses an appropriate potential for usage as an explosive. Performance characteristics of NTO are similar to those of the widely employed nitramine explosives such as hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX); However, this explosive is considerably less sensitive to accidental ignition by heat, impact, or spark [3, 4].

An important aspect in characterization of energetic compounds includes the measurement of the kinetics and the associated Arrhenius parameters of their thermal decomposition [5–8]. Because such information is valuable for specifying the reaction pathways, the kinetic constants

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Scheme 1 Preparation of KNF by reacting tetranitromethane with potassium nitrite and potassium bicarbonate

Scheme 2 Chemical structure for NTO
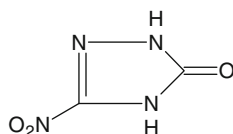
are required to define the burning or explosion process. However, obtaining these data under such conditions is so difficult [9, 10]. Thermal analysis techniques such as differential scanning calorimetry (DSC) and thermogravimetry-differential thermal analysis (TG/DTA) are powerful systems for acquiring thermal decomposition and kinetic data on energetic materials [11].

Until today, various reports are published about thermal decomposition process [12–17], explosion properties such as sensitivity and detonation velocity [18, 19], crystalline structure [20], and computational chemistry of pure NTO [21].While the published data on the kinetic parameters of its thermal decomposition are calculated by various methods and techniques; these data do not show a good compatibility together. Therefore, the actual activation energy and other kinetic and thermodynamic parameters corresponding to the thermal decomposition of NTO are still unclear. On the other hand, there is no report on the prediction of thermal decomposition parameters of NTO via non-isothermal methods using DSC data under various heating rates. Thus, in the spirit of reconciling conflicting data on NTO as energetic compound, the objective of this study was to resolve the discrepancy in the kinetic parameters of NTO thermal decomposition by non-isothermal DSC under various heating rates and comparing with previous studies on NTO explosive. Meanwhile, to the best our knowledge there is no data on thermal stability and decomposition kinetic of KNF. Therefore, another aim of the present study is determination of thermal behavior of KNF and prediction of its kinetic parameters by non-isothermal DSC.

Experimental

Both investigated energetic materials (KNF and NTO) were synthesized and purified. KNF was synthesized as

proposed by [22] and purified. Also, NTO was prepared and purified as proposed by [23]. A Stanton Redcroft, STA-780 series was used for TG and DTA. TG/DTA experiments were carried out in an alumina crucible, under heating rate of 10 °C min^{-1} in a temperature range of 30–900 °C. The used atmosphere was nitrogen with the flow rate of 50 mL min^{-1}. While, the sample mass used was about 3.0 mg. A Du Pont differential scanning calorimeter model DSC 910S was used for performing DSC experiments. DSC curves were prepared in temperature rang of 30–800 °C using an alumina crucible, under various heating rates (5, 10, 15, and 20 °C min^{-1}). Nitrogen atmosphere was used with the flow rate of 50 mL min^{-1}.

Results and discussion

The resulted TG/DTA curves for KNF are presented in Fig. 1a. As shown in this figure, an endothermic behavior commencing near 107.7 °C, corresponds to the dehydration of KNF. This result is compatible with TG curve of this sample which shows 3.2% mass loss. Up to the dehydration step, KNF undergoes another endothermic phenomenon at about 138.7 °C due to the evaporation of the remained tetranitromethane in the sample as precursor of KNF during the synthesis procedure. TG curve proves this result and shows 3.3% mass loss for this phenomenon. However, at higher temperatures, KNF presents two significant thermal events in temperature ranges of 270–330 and 360–430 °C. In the first temperature range, $\Delta m_1 = 39.5\%$ and T_{peak} DTA = 318.9 °C. While, in the second temperature range, $\Delta m_2 = 22\%$ and T_{peak} DTA = 435.6 °C. By considering these results it maybe proposed that the first thermal decomposition stage of this compound corresponds to the releasing of the nitro group from the nitroform followed by complete elimination of the nitro groups and consequent formation of KCN as remained material after complete decomposition of KNF in the end of second step.

The simultaneous TG-DTA curves of the NTO are shown in Fig. 1b. No thermal event was observed before the decomposition of this energetic material. The TG curve exhibits a complete mass loss in 250–300 °C. The mass loss ($\Delta m = 100\%$) occurs rapidly during a single step. By considering the results of TG-DTA studies, it maybe proposed that thermal decomposition for this compound is started by elimination of the nitro group and consequent complete destruction of structure of the compound [12]. The process shows a relatively sharp, rapid, and continuous mass loss observed until 300 °C. According to the DTA data, a sharp exothermic peak was observed about 268.2 °C corresponding to the decomposition of NTO. Table 1 summarizes the experimental results of TG/DTA analysis for both studied energetic materials.
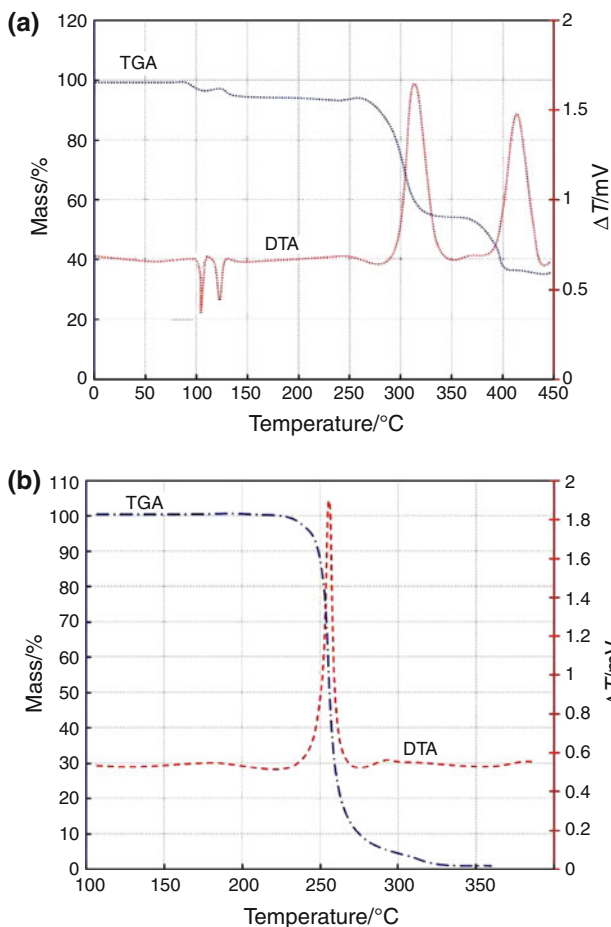
Fig. 1 TG/DTA curves for energetic material samples: **a** KNF and **b** NTO; sample mass 3.0 mg; heating rate 10 °C min^{-1}; nitrogen atmosphere
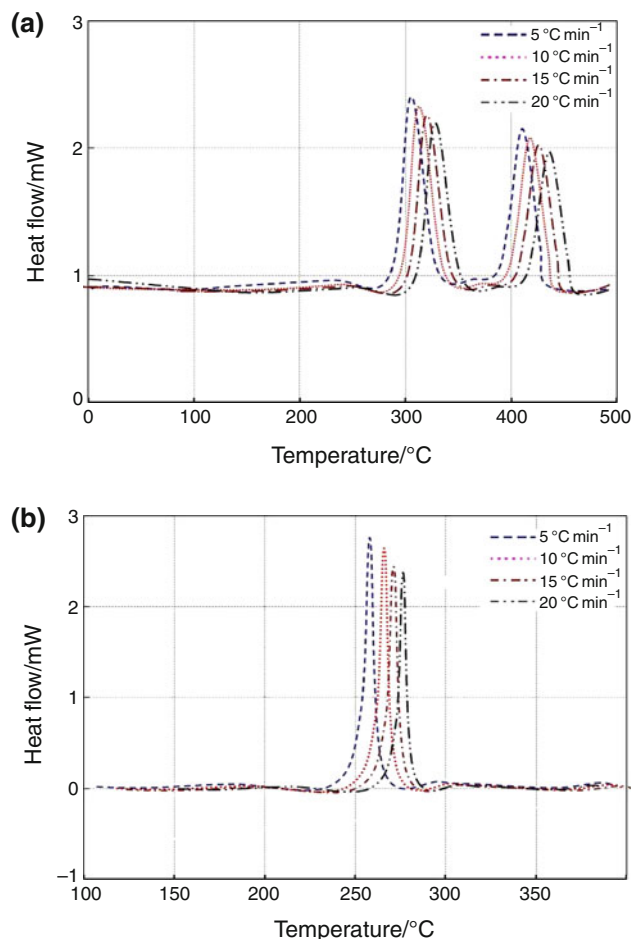
Fig. 2 The effect of heating rate on decomposition temperature of energetic material samples: **a** KNF and **b** NTO; sample mass 3.0 mg; nitrogen atmosphere

Decomposition kinetic studies by DSC

In order to predict kinetic and thermodynamic parameters corresponding to the thermal decomposition of interested energetic materials; their thermal behavior was studied by non-isothermal DSC under various heating rates. Figure 2 shows DSC curves for the decomposition of KNF and NTO

at several heating rates (5, 10, 15, and 20 °C min^{-1}). For both compounds it was found that by increasing the heating rate, the decomposition temperature peaks of the KNF and NTO were shifted to higher temperatures. Also, in order to investigate on self-heating effect, DSC experiments were obtained using three different masses of sample (3, 6, and 9 mg) under heating rate of 20 °C min^{-1} [24]. The results for both energetic compounds show no significant difference (less than 1%) in the peak temperatures when the various sample mass was used for DSC under these heating rates. This data demonstrates that the experiments were out of a self-heating regime.

In this study, ASTM method E698 [25] was used to predict the Arrhenius parameters for thermal decomposition of KNF and NTO. Therefore, the values of Ln($\beta \cdot T_m^{-2}$) against $1/T_m$ were plotted; while, β and T_m are DSC heating rate and maximum DSC peak temperatures, respectively. Table 2 shows the maximum peak temperatures (T_m) for each compound under various heating rates (β) which are

Table 1 Summary of TG/DTA results for investigated energetic compounds

| Compound | Transition temperature/°C | | | Mass loss/% |
	Dehydration	Decomposition	T^*	Δm
KNF	107.7	318.9	T_1^*: 270–330	39.5
			T_2^*: 360–430	22
NTO	–	268.2	250–300	100

T^* is the temperature range when there is fall in a sample's mass

Table 2 Dehydration and decomposition temperature of KNF and NTO obtained by DSC at various heating rates.

Compound	KNF			NTO
Heat flow/ °C min^{-1}	Dehydration/ °C	Decomposition temperature/°C		Decomposition temperature/ °C
		First step	Second step	
5	102.3	314.4	432.2	260.7
10	107.7	318.9	435.6	268.2
15	111.5	321.5	437.9	272.2
20	114.2	323.2	440.0	275.8

used to perform the kinetic parameters calculations by the ASTM E698 method.

The plot of $Ln(\beta \cdot T_m^{-2})$ against $1/T_m$ was straight lines for KNF ($r = 0.999$) and NTO ($r = 0.999$), which indicated that the mechanism of thermal decomposition of these energetic materials did not vary during the decomposition under various heating rates [26]. Then, slopes of the lines ($-E_a/R$) were used to calculate the activation energy. These values of obtained activation energies were used for computing the logarithm of pre-exponential factor, log (Z/s^{-1}), according to the following expression, given in ASTM E698:

$$Z = \beta \left(E_a/RT_m^2\right)\exp(E_a/RT_m) \tag{1}$$

By using the ASTM method values of activation energy and frequency factors for both energetic materials were calculated and the results are presented in Tables 3 and 4 for KNF and NTO, respectively. Meanwhile, activation energy (E_a) for these energetic compounds was calculated by Starink method. In Starink method, activation energy could be determined from plots of the $Ln(\beta \cdot T_m^{-1.92})$ versus the inverse of the temperatures at the maximum reaction rate during constant heating rate experiments. The activation energy can be determined by this method without a precise knowledge of the reaction mechanism, using the following equation [27]:

$$Ln\left(\beta/T_m^{1.92}\right) + 1.0008 E_a/RT_m = C \tag{2}$$

The plots of $Ln(\beta/T_m^{1.92})$ versus reciprocal of the absolute peak temperature for KNF and NTO were straight lines with $r = 0.999$. This linearity of these plots indicated that the mechanism of thermal decomposition of these energetic materials over this heating rate range is constant and undergoes no considerable change during various heating rates [26]. In the next step of this study, values of frequency factor (Z) correspond to the activation energies obtained by this method for both energetic compounds were calculated using the Eq. 1 [28]. All of the calculated Arrhenius data are summarized in Tables 3 and 4.

Comparing the results obtained via applying two methods shows that value of activation energy calculated for NTO energetic material by ASTM method is slightly lower than those of Starink method. However, activation energy for KNF obtained by ASTM method is similar than those of Starink method. This trend in activation energy values shows that ASTM and Starink method have a good agreement with each other. Meanwhile, comparing thermal stability of two energetic materials shows that KNF as a salt with three nitrate groups in its structure has the higher activation energy for its decomposition reaction. However, thermal decomposition parameters of NTO show that activation energy for the decomposition reaction of this organic energetic compound is considerably lower in spite of its lower nitrate content. The result of thermal stability investigation on KNF and NTO as energetic materials is valuable in usage of these compounds in future for energetic formulations; because in comparison between thermal stability data for these energetic compounds with conventional materials, one of these energetic compounds (KNF) has considerably higher thermal stability; but another compound (NTO) has lower activation energy for initiation of its thermal decomposition reaction.

Thermodynamic parameters corresponding to the activation of thermal decomposition reaction of these energetic compounds could be predicted by the following equations; while the kinetic data obtained by ASTM and Starink methods are used as input data. The values for entropy of activation ($\Delta S^{\#}$), enthalpy of activation ($\Delta H^{\#}$), and free energy of activation ($\Delta G^{\#}$) were obtained by Eqs. 3–5 [29–31]:

$$A \exp\frac{-E}{RT} = v \exp\frac{-\Delta G^{\neq}}{RT} \tag{3}$$

$$\Delta H^{\neq} = E - RT \tag{4}$$

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

In these equations, $\Delta G^{\#}$, $\Delta H^{\#}$, and $\Delta S^{\#}$ are Gibbs energy, enthalpy, and entropy of the activation, respectively. Also, $v = K_B T/h$ (where K_B and h are Boltzmann and Plank constants, respectively). Tables 3 and 4 give the values of calculated thermodynamic parameters for the studied energetic materials. The thermodynamic values presented in these tables were calculated at the maximum peak temperatures (T_m) in DSC curves; which makes these thermodynamic parameters valuable; because T_m characterizes the highest rate for thermal decomposition of the energetic materials. Comparison of these thermodynamic parameters pointed out the following results: As can be seen from Table 3, the value of $\Delta S^{\#}$ for the KNF is considerably higher than NTO (Table 4). It means that the corresponding activated complexes for KNF decomposition has a lower degree of arrangement (higher entropy)

Table 3 Comparison of kinetic parameters for the first step of KNF thermal decomposition obtained by ASTM and Starink methods.

Method	Activation energy/kJ mol^{-1}	Frequency factor log Z/s^{-1}	Linear regression	$\Delta G^{\#}$/kJ mol^{-1}	$\Delta H^{\#}$/kJ mol^{-1}	$\Delta S^{\#}$/J mol^{-1}	Log k	T_b/°C
ASTM	446.8	39.6	0.999	131.9	441.6	499	−37.5	335.5
Starink	446.8	39.6	0.999	131.9	441.6	499	−37.5	335.5

Table 4 Comparison of kinetic parameters for the first step of NTO thermal decomposition obtained by ASTM and Starink methods.

Method	Activation energy/ kJ mol^{-1}	Frequency factor log Z/s^{-1}	Linear regression	$\Delta G^{\#}$/kJ mol^{-1}	$\Delta H^{\#}$/kJ mol^{-1}	$\Delta S^{\#}$/J mol^{-1}	Log k	T_b/°C
ASTM	216.9	20.9	0.999	135.5	212.4	142	−16.5	247.8
Starink	217.0	20.9	0.999	135.6	212.5	142	−16.5	247.8

than its initial state; while for the NTO this was vice versa. According to the theory of activated complex (transition theory) [29] thermal decomposition of NTO maybe interpreted as a fast reaction while the KNF as a slow reaction rate. The positive values of $\Delta H^{\#}$ and $\Delta G^{\#}$ for both energetic materials showed that they are dependent to the introducing heat and their decompositions are non-spontaneous reactions. The value of $\Delta G^{\#}$ for the decompositions of KNF energetic compound is considerably higher than NTO. On the other hand, the value of the activation enthalpies ($\Delta H^{\#}$) for the decompositions of NTO is lower in comparison with KNF energetic material.

Reaction rate constant determination

By assuming the mechanism of the decomposition reactions for the studied energetic materials as first-order reactions, the rate constant (k) for decomposition reaction could be calculated by the following equation [32]:

$$\text{Log } k = \text{Log } Z - E_a/2.3RT \tag{6}$$

Under the temperature of 30 °C and using the values of activation energies (E_a) and frequency factors (Z) obtained by ASTM and Starink methods; the equation was solved for determination of decomposition reaction rate (k). Tables 3 and 4 listed the values of log k for KNF and NTO, respectively. By considering reaction rate constant calculated for these energetic material samples using kinetic parameters obtained by different methods, KNF reaction rate constant was compared with NTO reaction rate constant. It was found that the reaction rate constant of NTO was higher than that calculated for the KNF. This lower reaction rate constant for KNF shows that this energetic material has a considerable higher half-life rather than NTO in identical condition of storage.

Critical ignition temperature

The critical ignition temperature (T_b) is an important parameter required to insure safe storage and process operations especially for energetic compounds. T_b is defined as the lowest temperature to which a specific charge maybe heated without undergoing thermal runaway [33–35]. Inflammation theory is able to predict this parameter using appropriate thermokinetic parameters such as activation energy, pre-exponential factor, and heat of reaction. In our study, critical temperature of thermal ignition (T_b) for KNF and NTO was obtained by following equations [32]:

$$T_e = T_{e0} + b\phi_i + c\phi_i^2, \quad i = 1 - 4 \tag{7}$$

$$T_b = \frac{E - \sqrt{E^2 - 4ERT_{e0}}}{2R} \tag{8}$$

Where in these equations, b and c are coefficients, R is the gas constant, and E is the value of activation energy obtained by kinetic method. The values (T_{e0}) for the onset temperature (T_e) corresponding to $\varphi \rightarrow 0$ obtained by Eq. 7 were 328.6 and 237.4 °C for KNF and NTO, respectively. These temperatures were used for prediction of critical temperatures for thermal explosion (T_b) for KNF and NTO by Eq. 8. The results of these calculations are shown in Tables 3 and 4.

Comparison of NTO kinetic data

The values of activation energies, reported in the literature, for thermal decomposition of NTO are obtained by various methods and scattered from about 130 to 340 kJ mol^{-1} [4]. This wide difference in Arrhenius parameters maybe attributed to differences in the sample characteristics

(originality, purity, crystallinity, etc.) and experimental conditions (used analysis technique, non-isothermal or isothermal measurement, atmosphere and its pressure, etc.) [4, 15]. In this study, the values of activation energy obtained by ASTM and Starink methods showed good agreement and have values between 216.9 to 217.0 kcal - mol^{-1}. Kondrikov et al. [14] measured kinetics of thermal decomposition of NTO in temperature interval from 200 to 260 °C using a glass Bourdon gauge. Their finding showed that E_a for decomposition reaction is close to the values usually observed for nitro-compounds: $E_a = 173$ kJ - mol^{-1}. Also, they reported the value of Log k as 12.5 which in comparison with our results (16.5) is lower. On the other hand, Long et al. [15] used isoconversional DSC analysis in closed pan for exothermic decomposition of NTO. They showed that $E_a = 273$ kJ mol^{-1} for $\alpha = 0.01$ increased to a plateau of 333 kJ mol^{-1} for $\alpha = 0.17$ to 0.35; then, it decreases to 184 kJ mol^{-1} for $\alpha = 0.99$. The decreasing of E_a with α during the latter stages of decomposition was agreed with previous reports of autocatalytic behavior. Also, the chemiluminescence (CL) method [16] was used for determination of NTO activation energy and the frequency factor. The results showed the values of $E_a = 140$ kJ mol^{-1} in the temperature interval 100–140 °C. By considering the value of activation energy obtained in our study with previous studies, the following terms could be explained as main source for differences in the value of kinetic parameters of NTO: the used technique for measurements, properties of the compound such as particle size and purity [36], applied method for prediction of the kinetic parameters and reaction conditions such as atmosphere pressure and etc.

Conclusions

Thermal decomposition of two energetic materials was investigated via DSC and simultaneous differential thermal analysis and thermogravimetry (TG/DTA). Also, DSC curves of the compounds obtained under different heating rates were used for prediction of kinetic and thermodynamic parameters of the thermal decomposition reaction. Meanwhile, activation energies and frequency factors for the decomposition of both energetic compounds were calculated via different methods. TG/DTA data indicated that the thermal decomposition of KNF started at 140 °C after its dehydration temperature at 107.7. However, NTO was decomposed completely at temperature of 268.4 °C without undergoing melting. Based on the TG/DTA and kinetic data obtained from decomposition reactions of both energetic compounds, KNF is about 79 °C more stable than NTO.

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