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Technologically Attractive High Thermostable Polynitro Arenes

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Abstract: The paper is focused on 2,4,6,4′,6′,2″,4″,6″-octanitro[1,1′,3′,1″]-terphenyl (ONT), 2,2′,2″,4,4′,4″,6,6′,6″-nonanitro[1,1′,3′,1″]-terphenyl (NONA), 2,4,6-tris(2,4,6-trinitrophenyl)-1,3,5-triazine (TPT), *N*,*N*-bis(2,4-dinitrophenyl)-2,4,6-trinitroaniline (NTFA), 2,2′,4,4′,6,6′-hexanitrobiphenyl (HNB), 1,3-dinitrobenzene (1,3-DNB) and 1,3,5-trinitrobenzene (TNB). The initiation reactivity of these substances has been studied by means of the data obtained from non-isothermal differential thermal analysis (DTA), their ignition temperatures, impact sensitivity, the data obtained from the Russian manometric method and the detonation characteristics. For comparison, also the data published about 2,2′,2″,2‴,4,4′,4″,4‴,6,6′,6″,6‴-dodecanitro-[1,3′,1′,1″]quaterphenyl (DODECA) have been included. The paper specifies and discusses the relationships between the results of various methods used, inclusive of the forms of modified Evans-Polanyi-Semenov relationship. It has been stated that the technologically most attractive substances, out of those studied, can be ordered in the sequence ONT-TPT-NONA-NTFA according to their increasing thermal reactivity.

Key words: organic chemstry; DTA; explosives; ignition temperature; impact sensitivity; thermal reactivity; ONT; NONA; NTFA

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1 Introduction

A number of high-energy heterocyclic and carbocyclic substances have been prepared and characterized [1,2] as potential substitutes for 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX), 2,4,6-triamino-1,3,5-trinitrobenzene (TATB) and 2,2′,4,4′,6,6′-hexanitrostilbene (HNS) in weapon systems [1,2] and downhole well [3-5] applications. 2,4,6,4′,6′,2″,4″,6″-Octanitro[1,1′,3′,1″]-terphenyl (ONT) [6,7] and 2,2′,2″,4,4′,4″,6,6′,6″-nonanitro[1,1′,3′,1″]-terphenyl (NONA) [8,9]. belong among them, too, although they were developed earlier. Also earlier, 2,4,6-tris(2,4,6-trinitrophenyl)-1,3,5-triazine (TPT) [10,11] and ONT were registered for spacecraft [12] applications. All these "genuine" high thermally stable polynitro arenes continue to be still very attractive from the point of view of their use as an active part of perforators or detonators in downhole well applications [3-5,13].

We were engaged in a study of some properties based on thermal reactivity of these substances [14] and several new findings from this activity are presented in this paper. For comparison, we have included into this group also *N*, *N*-bis(2, 4-dinitrophenyl)-2, 4, 6-trinitroaniline (NTFA) [15,16] which is a well-known Russian thermostable explosive for downhole well applications [13].

2 Experimental and Data Sources

2.1 Substances

A survey of the substances studied is given in Table 1. Polynitro arenes ONT, NONA and TPT were prepared by known methods [7,8,10] and NTFA was obtained by nitration of triphenylamine in an anhydrous mixture of HNO_3 and H_2SO_4 [19]. As a reference we also used samples of 1,3-dinitrobenzene (1,3-DNB), 2,2′,4,4′,6,6′-hexanitrobiphenyl (HNB) and 2,2′,2″,2‴,4,4′,4″,4‴,6,6′,6″,6‴-dodecanitro-[1,3′,1′,1″]quaterphenyl (DODECA). Purity of the substances studied, with exception of DODECA (the sample of which was not available), was specified by TLC in the systems hexane/acetone (3∶1) and/or hexane/acetone/dichloroethane (8∶3∶1) [14]. According to the TLC analysis, the polynitro arenes examined were practically pure substances.

2.2 Differential thermal analysis (DTA)

We used a DTA 550 Ex apparatus [17] specially modified in our Institute for thermal analyses of explosives. The measurements were carried out at atmospheric

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pressure, the tested sample being in direct contact with the air atmosphere. The sample tested (0.05 g) was placed in a test tube made of Simax glass, 5 mm in diameter and 50 mm in length. The reference standard was 0.05 g aluminum oxide. We used linear rates of temperature increase, *viz.* 5, 10, and 15 ℃ · min^{-1}. The results of these measurements were treated by means of the software delivered with the DTA apparatus. The results obtained were treated using the Kissinger method[18] and the results obtained are presented in Fig. 1. The values E_aR^{-1} (i. e. slope of Kissinger relationship[18]. see in Fig. 1) thus obtained were taken as characteristics of thermal reactivity of the studied substances. A survey of onsets, TD, of thermal decomposition of the studied polynitro arenes is given in Table 2.

2.3 Specification of ignition temperature

The ignition temperature was determined by heating a 100 mg sample of the given substance at a heating rate of 5 ℃ · min^{-1}[20] until the point of ignition of the sample. Table 2 presents the corresponding results. It was not possible to determine the ignition temperatures of 1,3-DNB and TNB, because both these substances distilled at the experimental conditions. In the case of TPT, an only not very violent decomposition took place within the temperature range of 350 – 360 ℃.

2.4 Impact sensitivity

The impact sensitivity data (the drop heights) were taken from literature [21, 22]. Most of them were measured at Los Alamos National Laboratory and/or Naval Surface Weapons Center, using the Bruceton method[21, 22]. In this paper, the drop height data were converted into drop energies, E_{dr}. The impact sensitivity data of the studied compounds are presented in Table 2. The impact sensitivity of NTFA was determined in our laboratory.

Table 1 A survey of the studied polynitro arenes, their calculated detonation parameters and Arrhenius parameters of their thermolysis

No.	chemical name	code designation	calculated[a] parameters of detonation for TMD		arrhenius parameters of thermal decomposition by means of the russian manometric method				
			D /km · s^{-1}	Q_{real} /MJ · kg^{-1}	state of decompn.	Temp. region /K	E_a /kJ · mol^{-1}	log$A$ /s^{-1}	Ref.
1	1,3-dinitrobenzene	1,3-DNB	6.38	3871					
2	1,3,5-trinitrobenzene	TNB	7.51	4540	liquid	523 – 583	180.03	10.9	23
3	2,2′,4,4′,6,6′-hexanitrobiphenyl	HNBB	7.48	4654	liquid	513 – 573	207.24	16.1	25
4	2,4,6,4′,6′,2″,4″,6″-octanitro[1,1′,3′,1″]-terphenyl	ONT	7.46	4550	solid	573 – 623	281.58	19.5	26
5	2,2′,2″,4,4′,4″,6,6′,6″-nonanitro[1,1′,3′,1″]-terphenyl	NONA	7.60	4751	solid	523 – 623	236.30[b]	15.2[b]	27
6	2,2′,2″,2‴,4,4′,4″,4‴,6,6′,6″,6‴-dodecanitro-[1,3′,1′,1″]quaterphenyl	DODECA	7.69	4802	solid		217.48[c]	15.2[c]	28
7	2,4,6-tris(2,4,6-trinitrophenyl)-[1,3,5]triazine	TPT	7.08	4324	solid	573 – 623	269.45	18.2	26
8	*N*,*N*-bis(2,4-dinitrophenyl)-2,4,6-trinitroaniline	NTFA	7.19	3994	solid		187.00	11.5	29

Notes: a) a calculation by means of the Kamlet & Jacobs method [31] for the D values and semiempircal Pepekin et. al. method [32] for the Qreal values; b) the value obtained by means by TGA [27]; c) the value obtained on the basis of prediction [28].

Table 2 A survey of sensitivity and detonation characteristics of the polynitro arenes studied

No.	polynitro arene code design.	impact sensitivity /J		velocity of detonation D (km · s^{-1}) experimental for density ρ(g · cm^{-3})			onsets of exothermic decompn. from DTA		ignition temp. /℃	threshold of thermal stability /℃
		d_{dr}	Ref.	D	ρ	Ref.	in state	T_D/℃		
1	1,3-DNB	39.00	30	6.10	1.47	30	liquid	distilled	distilled	
2	TNB	24.64	21,22	7.30	1.71	30	liquid	distilled	347[a]	283
3	HNB	20.92	22	7.10	1.60	13	liquid	282	354	245
4	ONT	15.73	22	7.20	1.72	13	solid	334	370	290
5	NONA	9.10	22	7.30[b]			solid	309	359	280
6	DODECA	9.85	22	7.40[b]						270
7	TPT	22.85	22	6.80[b]			liquid	359[e]	350 – 360[c]	283
8	NTFA	8.92	d	7.20	1.62	13	solid	302	348	285
8	NTFA			6.80	1.45	13				

Notes: a) the value calculated according to the relationship in Fig. 3-published boiling point of TNB is 350 ℃ [34]; b) the value calculated by means of eqn. (1); c) a value of 355 ℃ was taken for construction of relationships, published value is 359 ℃ [33]; d) the value determined in the Inst. of Energetic Matterials; e) the more sensitive DTA has been detected this onset in the solid state at 319.6 – 320.4 ℃ [23].

2.5 Kinetic parameters of the thermal decomposition

The data obtained from Russian manometric method (SMM)[24-26, 29] have been the main source of the Arrhenius parameters (i. e. E_a and $\log A$) of thermal decomposition of the substances studied. Results of the thermo-gravimetric analysis (TGA) can be converted into compatible values by means of the calibration curves[27]. Also a prediction on the basis of modified Evans-Polanyi-Semenov equation was used[28]. Arrhenius parameters of the substances studied are presented in Table 1. Thermostability thresholds, i. e. the maximum theoretical temperature at which a charge of the given explosive can be heated for the period of six hours without showing changes in its explosive characteristics, were calculated according to Maksimov & Shipitsyn semi-empirical method[29] adopting the Arrhenius parameters; Table 2 presents the resulting values.

2.6 Characteristics of detonation

The values of experimentally determined detonation velocities were taken from literature[13, 30] and they are presented in Table 2. Theoretical detonation velocities, D, for theoretical maximum density (TMD) were calculated by means of Kamlet & Jacob method[31]. and the maximum real heat of explosion, Q_{real}, was obtained by means of semi-empirical Pepekin et. al. method[32]. Table 1 presents the corresponding results.

3 Results and Discussion

The thermal stability of the substances in Fig. 1 is increasing from the right-to left-hand side. This order does not correspond with that of the onsets of their decomposition, T_D (cf. Table 2) and with that of the long-term vacuum stability test at 200 ℃[35] (in the latter case the thermal stability decreases in the order TPT-ONT-NONA-DODECA-HNB).

Fig. 2 presents the interrelationship between the activation energies E_a of thermal decomposition (that correspond to the SMM results) and the slopes of Kissinger relationship, $E_a R^{-1}$. Actually, this is an interrelationship between activation energy values obtained by two different methodologies; therefore, it reflects very close molecular-structure delimitation. Using this relationship, we estimated the value of $E_a R^{-1}$ = 32500 K for TNB, which distils at the DTA conditions.

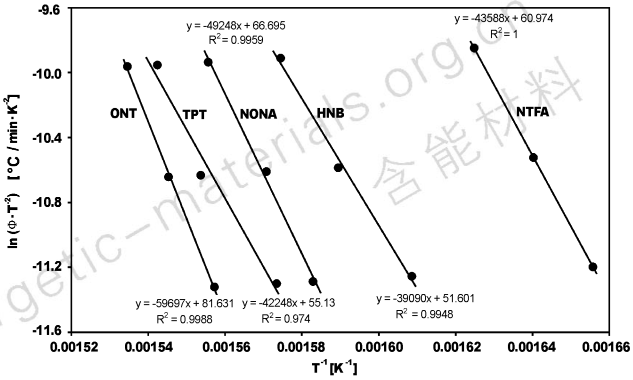

Fig. 1 Evaluation of the DTA outputs by Kissinger method-thermal stability is increasing from the right-to left-hand side

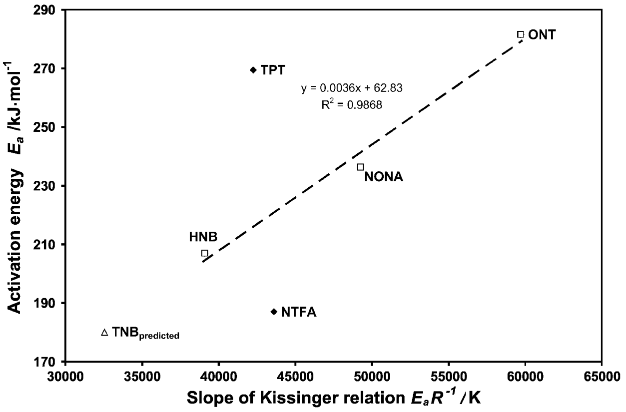

Fig. 2 Relationship between the activation energies E_a of thermal decomposition (that correspond to the SMM results) and the slopes of Kissinger relationship, $E_a R^{-1}$

From the point of view of molecular structure, the relationship between ignition temperatures and activation energies E_a (Fig. 3) is more universal. From the solution to the problem of thermal explosion during linear temperature increase[36] it follows that the dependence of critical temperature on the activation energy of decomposition of the given energetic material is virtually linear. If in the first approximation the ignition temperature is considered as the critical temperature, then the dependence in Fig. 3 is logical. Almost the same can be stated also about the dependence in Fig. 4. Using this relationship, we estimated the ignition temperature of TNB (347 ℃), which is practically identical with its boiling temperature (350 ℃[34]). The data of TPT do not correlate with this dependence, because the E_a value used corresponds to its decomposition in the solid phase. The correlation would be complete if the predicted value $E_a = 225.8\ \mathrm{kJ \cdot mol^{-1}}$ [23] ($\log A = 15.2$; which perhaps corresponds to its decomposition in the liquid phase) was considered. The decomposition of TPT during determination of its ignition temperature takes place in its liquid state (its melting point is 352 – 353 ℃[33] and the published ignition temperature is 359 ℃[33]). The DTA method using a more sensitive registration of temperature differences recorded the onset of exothermal decomposition of TPT in the solid state at 319.6 – 320.4 ℃ [23]. The thermal reactivity of TPT is strongly increased by the presence of substances having the character of a solvent of this polynitro arene [39, 41] (in TNB solution, the decrease in the onset of its exothermic decomposition is 143 ℃[41]).

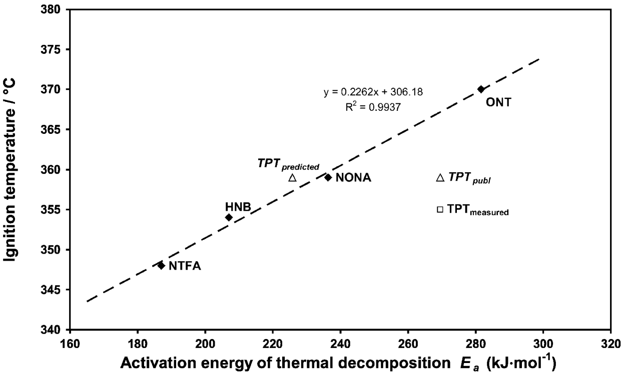

Fig. 3 Relationship between ignition temperatures and the activation energies E_a (that correspond to the SMM results): for a point TPT predicted the published value $E_a = 225.8\ \mathrm{kJ \cdot mol^{-1}}$ [23] was used

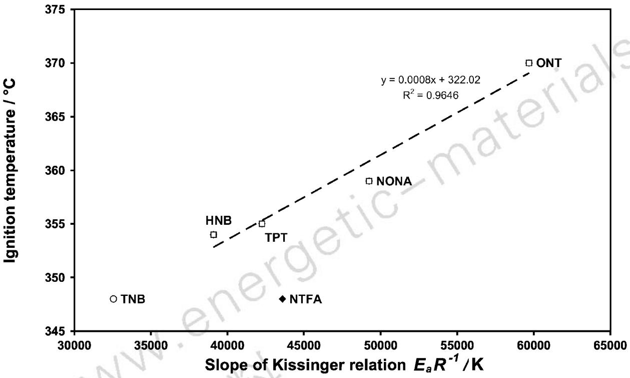

Fig. 4 Relationship between ignition temperatures and the slopes of Kissinger relationship, E_aR^{-1}

From the standpoint of temperature threshold, the most stable of the polynitro arenes studied is ONT. There is a relationship between these thresholds and the onsets of exothermic decomposition (Fig. 5); while the data of TPT decomposition in liquid phase fall outside the relationship, the data published [23] about its decomposition in solid phase correlate very well. In the case of a much more extensive set of polynitro arenes and application of a markedly more sensitive detection of temperature difference in their DTA, this dependence has a semi-logarithmic form [41].

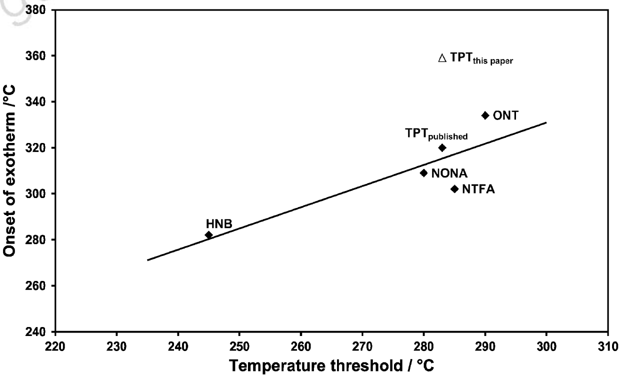

Fig. 5 Approximate relationship between temperature thresholds and the onsets of exothermic decomposition

Fig. 6 graphically presents the forms of modified Evans-Polanyi-Semenov (E-P-S) equation [37,38] for the substances studied. In this case, for the dependence of polynitro arenes exhibiting a very strong stabilising effect of crystal lattice (for TPT and NONA see Ref. [39]) this equation has a positive slope [37]. The category of modified E-P-S relationships also includes the relation between drop energies, E_d, and heats of explosion in Fig. 7, which was derived for the first time on the basis of quantum-chemistry methods for nitramines [40]. In Fig. 7 the substances of lower physical stability (i. e. TNB and HNB) are distinctly separated. According to the dependences given in this figure, the increasing energy content of the polynitro arenes studied is associated with increase in their impact sensitivity. Both the relationships (i. e. in Figs 6 and 7) are valid for narrow sets of substance structures and they document that the strength of bond being split is a decisive factor in the given reaction [37, 38].

Literature often gives the so-called maximum values of experimentally determined detonation velocities of explosives without specifying the charge densities at which these velocities were determined. For TPT, NONA and DODECA, these velocities can be estimated on the basis of the relationship between the maximum theoretical values of detonation velocities, D_{theor}, and the maximum values published, D_{publ}, in the following form:

$$D_{publ} = 0.9845\ D_{theor} - 0.1447 \qquad (1)$$

with the coefficient $r^2 = 0.9044$.

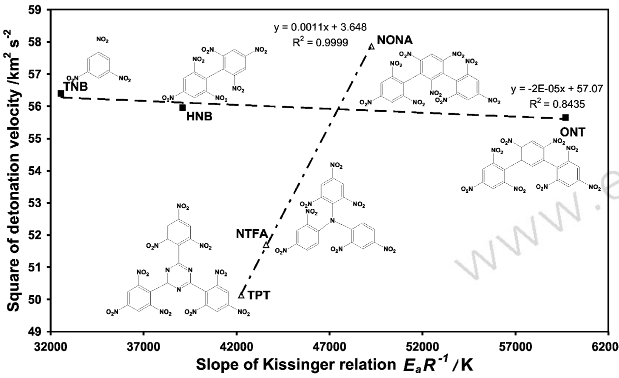

Fig. 6　Relationship between squares of detonation velocities and the slopes of Kissinger relationships-a form of modified Evans-Polanyi-Semenov equation

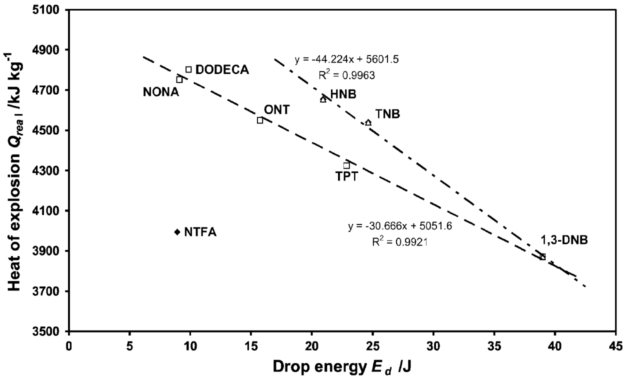

Fig. 7　Relationship between heats of explosion and the drop energies-another form of modified Evans-Polanyi-Semenov equation

4　Conclusions

As expected, the relative thermal reactivity of polynitro arenes studied depends upon the method of its specification. Interrelationships can be found between the results of individual methods of specification or evaluation of this reactivity. From the point of view of molecular structure, a clearly demarcated relationship exists for these substances between the activation energies obtained from the Russian manometric (isothermal) method and slopes of the Kissinger equation. This delimitation is practically identical with that obtained from modified forms of Evans-Polanyi-Semenov equation for these compounds. In addition, the forms of this equation also reflect the stabilising effect of crystal lattice. The relationship between the ignition temperatures and the activation energies of decomposition obtained from the Russian manometric method is unambiguous for these substances in contrast to the analogous relationship of slopes of the Kissinger equation: the kinetic data obtained from isothermal methods of investigation of thermal reactivity of energetic materials are markedly closer to reality than are the corresponding data obtained from non-isothermal methods. On the basis of the results obtained here and those published earlier about the studies of initiation reactivity of the polynitro arenes studied, it is possible to arrange the most (technologically) attractive of them in the order of their increasing thermal reactivity as follows: ONT-TPT-NONA-NTFA.

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