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Research paper

Melt-cast Energetic Matrices with 3-Nitro-1,2,4-triazole Derivatives for Composite Explosives

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Abstract: Safety requirements for the manufacture, use and storage of high-energy materials and explosive substances necessitate a search for new insensitive components of fusible energetic matrices (propellant matrices) in order to completely or partially replace 2,4,6-trinitrotoluene (TNT). 3-Nitro-1,2,4-triazole derivatives and their melt-casts with TNT may be proposed as such replacements. Differential scanning calorimetry was employed to characterize the thermal behaviour of 1-methyl-3-nitro-1,2,4-triazole, 1-ethoxymethyl-3-nitro-1,2,4-triazole, *t*-butyl-3-nitro-1,2,4-triazole and their melt-casts with TNT. This study showed that 1-methyl-3-nitro-1,2,4-triazole and its melt-casts with TNT was the best for explosive systems based on 2,4,6,8,10,12-hexanitro-1,4,6,8,10,12-hexaazaisowurtzitane (HNIW), 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) and guanylurea dinitramide (GUDN).
The present article also presents data for the mechanical sensitivity of these explosives and their calculated detonation characteristics. The composite explosive based on HMX with 1-methyl-3-nitro-1,2,4-triazole has a calculated detonation velocity the same as HMX with TNT, but the sensitivity of HMX/TNT is 1.3-1.7 times higher.

Keywords: melt-cast energetic matrix, 3-nitro-1,2,4-triazole, TNT, composite explosive

1 Introduction

Research and development of yet more powerful energetic compounds and composite explosives has been pursued actively over the last few decades [1, 2]. The design of novel high-energy materials (HEMs) is required for the extraction of natural resources, building work and military purposes. The power increase of explosive materials often impairs their safety during manufacture, storage and use. Explosion safety is known to depend on an HEM's parameters such as mechanical sensitivity, thermal stability and chemical compatibility of the ingredients of an explosive system [3, 4].

A modern explosive system may contain melt-cast substances, for example 2,4,6-trinitrotoluene (TNT), 2,4-dinitro-2,4-diazapentane (DNP), 2,4-dinitrotoluene (DNT), 2,4-dinitroanisole (DNAN), 2,4,6-trinitroanisole (TNAN) *etc.*, and crystalline fillers such as 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (HNIW). The sensitivity of such explosives to mechanical stress is high and does not meet the actual safety requirements. This problem may be solved by the correct selection of the components. For instance, TNT could be used with insensitive fillers: 3-nitro-1,2,4-triazol-5-one (NTO), guanylurea dinitramide (GUDN), 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), or insensitive melt substances (DNAN, TNAN) combined with sensitive fillers (HMX, RDX, HNIW) [5-7]. TNT is a classical, melt-cast energetic matrix for compound explosives as it has been in use for over a century.

Currently, the less sensitive DNAN is often used instead of TNT [7, 8]. The mechanical sensitivity of DNAN is lower than that of TNT by 1.1-1.4 times, however its other important properties (density, melting point, velocity of detonation) are worse. TNAN is more convenient for processing than TNT (melting point TNAN = 68.4 °C) and has a higher velocity of detonation (*VoD*), *i.e.* 7640 m/s at a density of 1.60 g/cm^3. However, molten TNAN has a lower density (1.4 g/cm^3) and is very toxic [2]. Nitroimidazole derivatives are also less sensitive than TNT, and are interesting HEMs [9]. Table 1 lists the properties of TNT and DNAN from the scientific literature [2, 6-8]; the characteristics of 1-methyl-3-nitro-1,2,4-triazole (ME3N) were determined by the authors of the present article. The properties of DNAN and TNAN are well tested, but the properties of nitrotriazole derivatives are insufficiently tested. Therefore, a study of the application of melt-cast nitrotriazole derivatives for explosives should be useful.

Table 1. Properties of melt-cast substances

Compound	Density [g/cm^3]	Melting point [°C]	*VoD* [m/s]
TNT	1.47-1.59	80.1-80.9	6700-6770
DNAN	1.42-1.48	94.5-95.6	5000-5620
ME3N	1.48	65.7-65.9	6900

The impact sensitivity of TNT, as measured by an impact-testing machine (K-44-II, Russia) with a drop weight of 10 kg and a drop height of 250 mm, was 6% [3, 10]. That is to say, the explosive fragments detonated in 6 cases out of 100. In addition, the so-called lower limit (the discharge height of the 10 kg load per 0.1 g sample, when explosion was absent, was 25) according to our data was 200 mm.

The lower limit of sensitivity of TNT (in the so-called shock shift), measured by a friction-testing machine (K-44-III, Russia), was more than 300 MPa [11]. These properties were considered satisfactory. However, an explosive system that consists of TNT together with HMX or HNIW becomes dangerous because the impact sensitivity of these crystalline fillers is increased up to 80%.

The sensitivity of TNT can be reduced by adding less sensitive energetic substances, such as 3-nitro-1,2,4-triazole derivatives. The impact and friction sensitivities of substances of this class are 0% and 981 MPa [12], respectively, *i.e.* are much lower. The positive qualities of 3-nitro-1,2,4-triazole derivatives are simple technological processing and the ability to form simple eutectics with other energetic ingredients. By varying the weight content of the components in a system with a simple eutectic allows energetic matrices with adjustable properties to be made.

In the present paper, the properties of melt-cast energetic matrices with 3-nitro-1,2,4-triazole derivatives have been studied. This includes pre-eutectic, eutectic and post-eutectic compositions with TNT, DNT and DNP. The thermal behaviour of these melt-cast energetic matrices was studied by differential scanning calorimetry (DSC). Structural diagrams and state diagrams are shown. These help to select matrices having balanced properties for systems with the fillers GUDN, HMX and HNIW. Experimental data for mechanical sensitivity and calculated detonation characteristics of explosive compositions with nitrotriazole derivatives, TNT and DNT are presented.

2 Materials and Methods

2.1 Materials

The 3-nitro-1,2,4-triazole derivatives were produced in the scientific laboratory of the Institute IPCET SB RAS (Biysk, Russia). Their structural formulas are shown in Figure 1. 1-Methyl-3-nitro-1,2,4-triazole (ME3N), Figure 1(a), was synthesized by alkylation of 3-nitro-1,2,4-triazole with methyl iodide and dimethyl sulfate in the presence of alkali [13]. 1-*t*-Butyl-3-nitro-1,2,4-triazole (TBU3N), Figure 1(b), was produced by alkylation of 3-nitro-1,2,4-triazole with *t*-butyl alcohol in concentrated sulfuric acid [14]. 1-Ethoxymethyl-3-nitro-1,2,4-triazole (EOM), Figure 1(c), was prepared, under acid catalysis, by the interaction of 1-hydroxymethyl-3-nitro-1,2,4-triazole with ethanol in chloroform [15]. For the manufacture of fusible energetic matrices and explosive systems, TNT, DNP, DNT, HMX and HNIW of industrial production (Russia) were used. GUDN was synthesized in the scientific laboratory (Biysk, Russia).

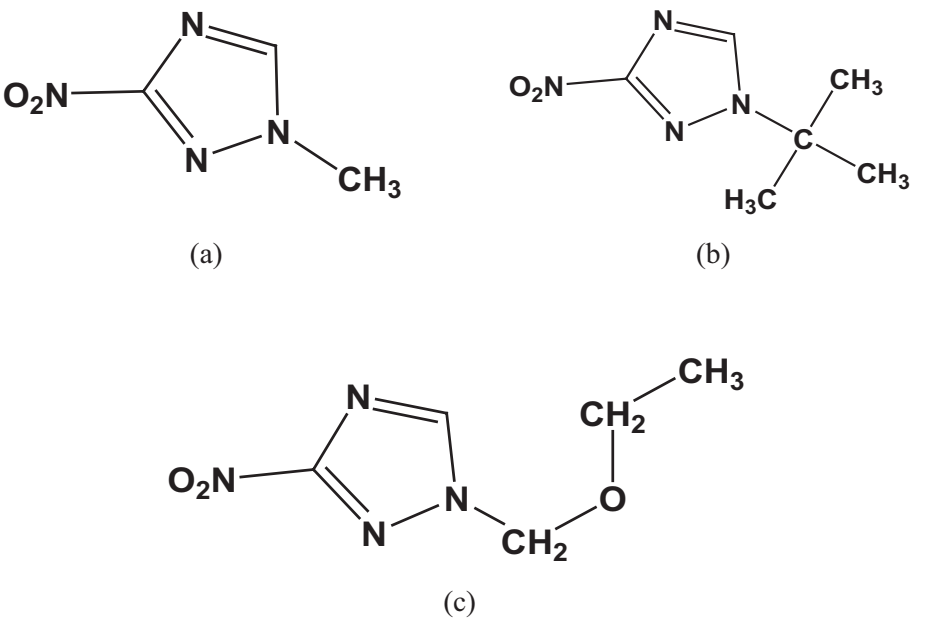
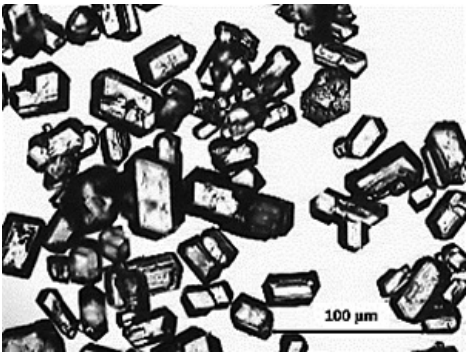


Figure 1. The structural formulas: ME3N (a), TBU3N (b), EOM (c)

2.2 Processing of fusible energetic matrices and explosive systems

Fusible energetic matrixes were prepared by melting mixtures of two substances (original components) of different weight ratios (20/80, 40/60, 50/50, 60/40, 80/20). The melts were cooled to casts at room temperature. After crystallization, they were crushed and stored in glass buckets with lids. Each explosive system contained 50 wt.% energetic matrix and 50 wt.% filler. All of the explosives weighed 5 g and were made in the following way. The melt-cast components were placed inside a steel container equipped with a heated jacket. The mixture was then heated to a temperature exceeding its melting point by 5 °C. A crystalline filler (GUDN, HNIW or HMX) was subsequently added to the melt. The particle size of the filler was 20-100 μm. Figure 2 shows photos of the crystals and their dimensions.



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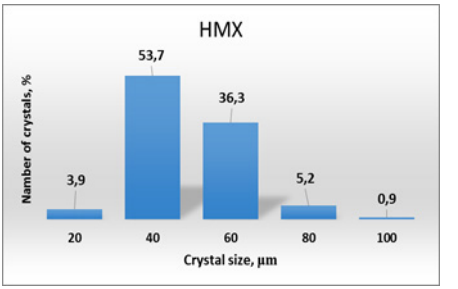

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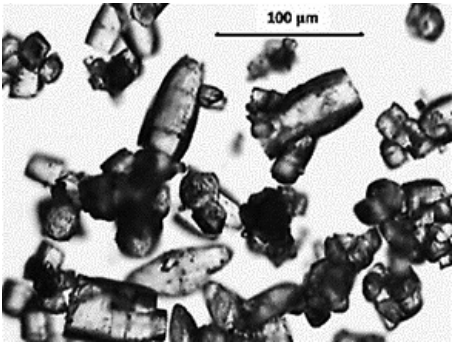

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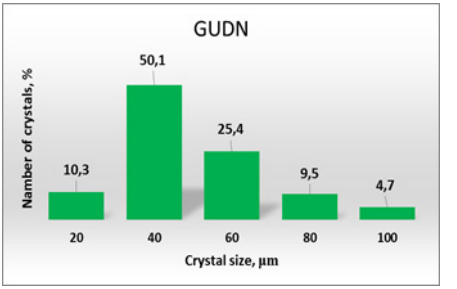

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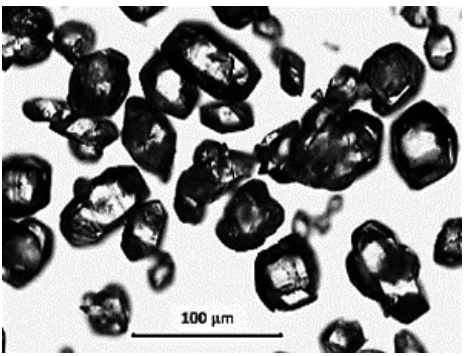
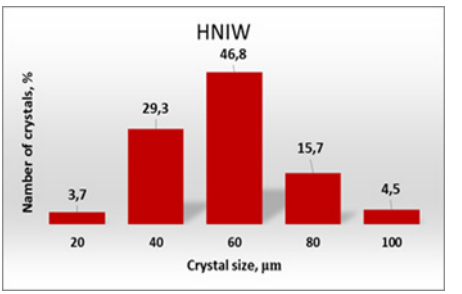




(e) (f)

Figure 2. Crystalline fillers: HMX (a, b), GUDN (c, d), HNIW (e, f)

The mixture was then stirred for 10-15 min until a suspension was obtained. The completed suspension was poured as a thin layer onto a fluoroplastic film. After solidification of the composition, it was ground to a powder with particles of 100 µm. The resulting powder was tested for sensitivity and thermal analysis.

2.3 Sensitivity measurement methods

According to the state standards of Russia, the safety of explosives is determined by special methods on an impact-testing machine K-44-II and a friction-testing machine K-44-III [3]. The impact-testing machine K-44-II consists of a massive steel plate, located on a concrete foundation and three guide rods between which a load is fixed at a certain height. A measure of the shock sensitivity is the lower limit (*LLshock*), that is the maximum drop height of a 10 kg load per 0.1 g sample, located between steel rollers with a diameter of 10 mm in a special clutch. The drop heights of the load are selected. For each drop height, 25 tests are carried out and the number of explosions is noted, then the relative frequency of explosions (in %) is calculated. The minimum height for the absence of explosion is *LLshock*.

The friction-testing machine K-44-III measures the friction at impact displacement. The machine consists of a hydraulic press and a pressure gauge, the body of the device and a lever with the load, which is installed at a certain angle and is discharged to the hammer. A sample weighing 0.02 g is placed between two steel planes, which are shifted by 1.5 mm relative to each other when the hammer falls. The maximum pressure on the sample at which no explosion occurs in 25 tests is the lower limit of friction sensitivity (*LLfriction*). The pressure is determined from special tables according to the angle of deflection of the lever with the load (from 28 to 108°).

2.4 Thermal analysis

The thermal properties of the explosive systems and their ingredients were measured with a thermal analyzer DSC822^e (Mettler Toledo, Switzerland). The measurements were performed in the temperature range 25-100 °C and 25-350 °C, at a heating rate of 10 °C/min in a nitrogen atmosphere (gas flow rate through the measuring cell was 60 mL/min). The samples of the fusible energetic matrices (3.5 mg) and the explosive systems (0.7 mg) were placed in standard aluminum cups with pierced lids. Before measurement, the device DSC822^e was calibrated with special test programs and pieces of indium metal (In, 99.999% pure) and zinc metal (Zn, 99.998% pure). The hardware measurement accuracy was ±0.2 °C. The primary results, as graphical curves, were transformed by STAR^e 14.00 software for interpretation.

2.5 Optical microscopy

The appearance of powdered materials and polished samples was studied by optical microscopy. A Motic DMBA Professional Series digital microscope (China) visualized the samples on the computer monitor at a zoom ranging from ×40 to ×1000. The images and videos were analyzed by Motic Images Plus 2.0 image processing software.

3 Results and Discussion

3.1 Thermal behaviour of melt-cast matrices

Table 2 lists the thermal characteristics of the original melt-cast components. T_b, T_c and T_m illustrate the melting process of the melt-cast substance in the DSC measuring cell. The temperature T_b corresponds to the beginning of melting, T_m is the melting point (the maximum of the endothermic effect in a DSC curve), and T_c is the completion of the melting process (Figure 3). The parameters T_b, T_m and T_c were calculated by the method of tangent lines. Parameter ΔH_m is the measured DSC enthalpy of melting, and is equal to the normalized value of the area of the endothermic effect (Q_m).

Table 2. Thermal properties of the original components

Compound	T_b [°C]	T_m [°C]	T_c [°C]	ΔH_m [J/g]
TNT	77.8	80.1	81.7	102.7
DNP	53.7	55.2	58.1	100.1
DNT	55.5	64.1	67.5	62.0
ME3N	64.1	65.9	68.9	117.4
TBU3N	90.6	93.8	95.8	102.5
EOM	55.1	56.4	59.3	156.1

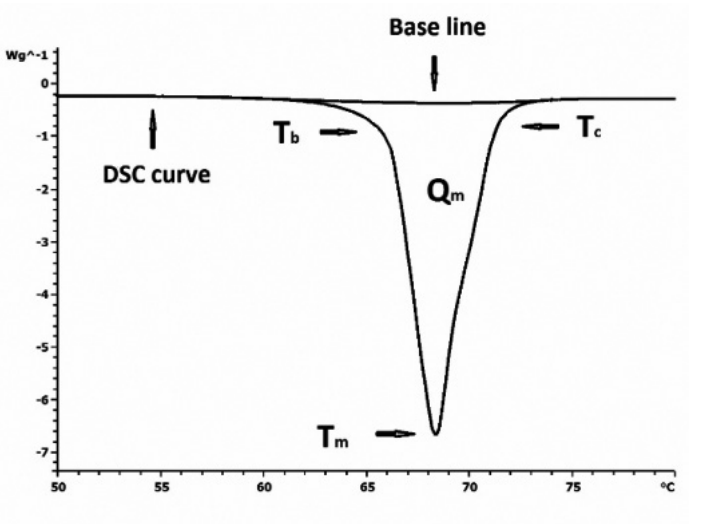


Figure 3. DSC curve of the melting process

Of the 3-nitro-1,2,4-triazole derivatives, TBU3N turned out to be the highest melting; the melting point of ME3N was close to that of DNT; and the melting point of EOM was close to that of DNP (Table 2). All of the original components of the energetic matrices had one melting peak, although their melt-casts can demonstrate two melting peaks.

Figure 4 shows the thermograms of the energetic matrices ME3N/DNT (80/20), ME3N/DNT (40/60), ME3N/DNT (60/40) and ME3N/DNT (20/80). Only the melt-cast ME3N/DNT (40/60) had a single melting peak. The temperatures of the first peaks were close, their average values being 41.5 ±0.3 °C. The temperatures of the second peaks had different values and depended on the proportions of the original components. Identical results were obtained for all of the melt-cast energetic matrices, and are summarized in Table 3.

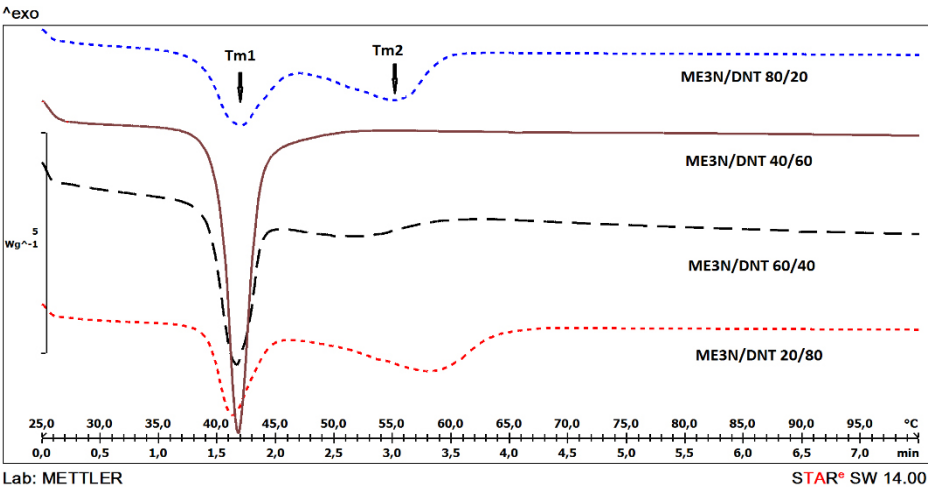


Figure 4. DSC thermograms of ME3N/DNT matrices

The minimum temperatures (Table 3, bold font) corresponded to the melting points of the pure eutectic. The eutectic-casts had one melting peak, and their compositions were determined approximately by experiment. A more accurate content of original components for a pure eutectic can be determined by measuring casts of other proportions or by mathematical calculations. A polynomial approximation could be applied to the ΔH_m parameters that fit the endothermic effects of the second peaks of the energetic matrices. The estimation results are listed in Table 4.

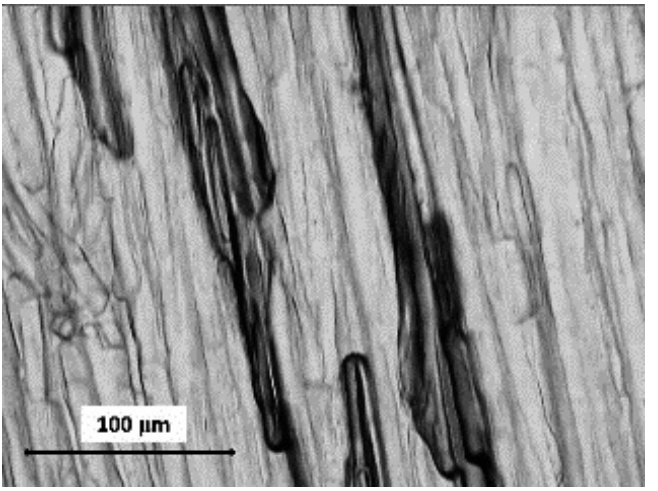
Table 3. Temperature (° C) of the second peak of melt-cast matrices

Nitrotriazole derivative	Content of the original component [wt.%]				
	20	40	50	60	80
	TNT				
ME3N	57.9	49.1	**43.5**	55.1	68.8
TBU3N	84.2	72.2	**59.7**	63.3	71.8
EOM	53.9	**47.1**	58.6	62.3	71.2
	DNP				
ME3N	53.9	38.6	**23.7**	27.8	40.2
TBU3N	83.3	65.2	49.8	**37.8**	46.6
EOM	49.3	**33.8**	39.9	43.6	50.1
	DNT				
ME3N	55.1	**41.5**	47.3	52.4	58.2
TBU3N	84.0	74.4	59.8	**51.1**	64.1
EOM	53.3	**42.8**	45.9	50.1	57.9

Table 4. The contents of the components in the pure eutectics

Original component	Content of 3-nitro-1,2,4-triazole derivative [wt.%]		
	ME3N	TBU3N	EOM
TNT	50.1	51.1	63.6
DNP	47.0	43.2	55.8
DNT	42.9	50.3	49.9

Microscopic imaging of each micrographic sample confirmed that all of the melt-casts were binary systems. Each system consisted of alternating dark and light bands (Figure 5(a)) or bands and grains (Figure 5(b)). Observation of the solidification process helped to describe the formation of the individual solid phases. In all of the experiments, the beginning of crystallization of the energetic matrices is characterized by solidification of the pure eutectic.



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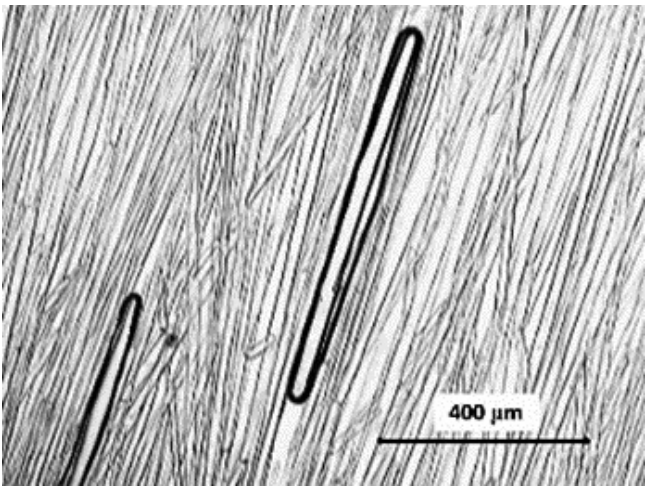
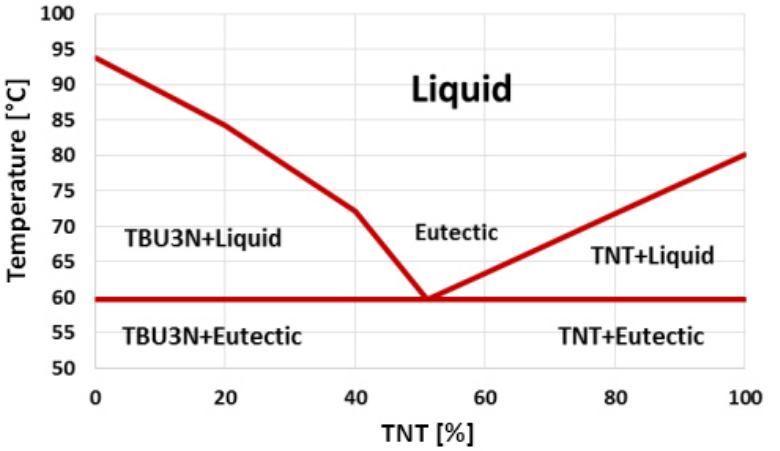


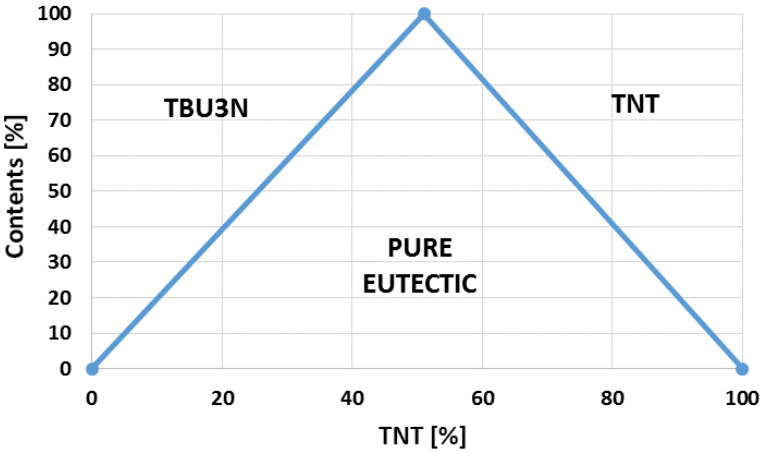
(b)

Figure 5. Energetic matrices EOM/DNP: 20/80 (a) and 40/60 (b)

The data in Tables 2-4 can be used to plot structural and state diagrams. Figure 6 illustrates the diagrams for TBU3N/TNT. Such diagrams allow the determination of the melting point of the energetic matrix, the ratio of the eutectic and the excess component. For example, if TBU3N/TNT is composed of 30 wt.% TBU3N and 70 wt.% TNT, the matrix contains about 59% pure eutectic and 41% TNT (Figure 6(b)); the temperature of transformation into a liquid is about 67 °C (Figure 6(a)).



(a)



(b)

Figure 6. TBU3N/TNT: state diagram (a) and structural diagram (b)

3.2 Thermal characteristics of explosive systems

The technological process of manufacturing, storage and use of explosive systems with melt-cast substances leads to restrictions. The melt point of the melt-cast energy matrix must be more than 50 °C and less than 100 °C. The 3-nitro-1,2,4-triazole derivatives can be used in explosive systems because the melting points of ME3N, TBU3N and EOM correspond to this temperature range (Table 2). It is also possible to use any melt-cast matrices with 20 wt.% TNT, DNP and DNT; all formulations with 60 wt.% TNT and DNT, as well as TBU3N/DNP (60/40) (Table 3).

More than thirty energy systems were investigated by the DSC method. The thermograms of most of the explosive systems had a clear endo-effect of the melt-cast matrix melting and an exo-effect of the energy system decomposition (Figure 7). Energy systems with 3-nitro-1,2,4-triazole derivatives, DNT and HMX had an exo-effect of complex form (Figure 8).

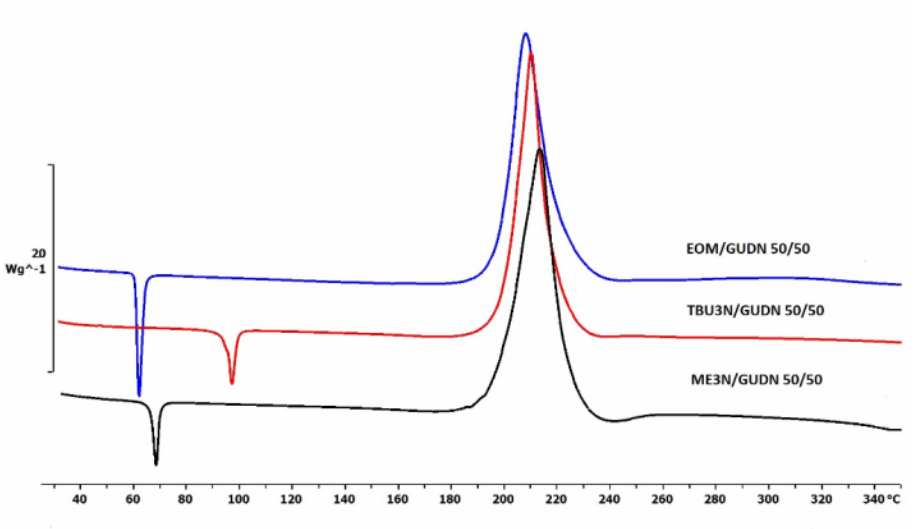


Figure 7. DSC thermograms of explosive systems with GUDN

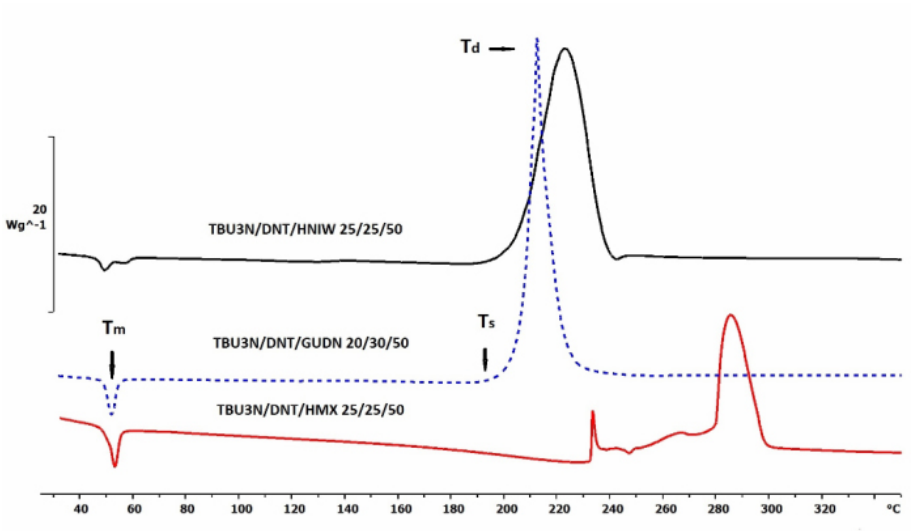


Figure 8. DSC thermograms of explosive systems with DNT

Table 5 lists the thermal characteristics of some explosive systems. The parameter T_m corresponds to the melting point of the melt-cast matrix; T_s is the beginning of the pyrolysis process; T_d corresponds to the decomposition temperature of the explosive system. The parameter ΔH_d is the enthalpy

of decomposition as measured by DSC. ΔH_d is equal to the normalized value of the exothermic effect area (Q_d).

Table 5. Thermal parameters of explosive systems

Formulation (ratio [wt.%])	T_m [°C]	T_s [°C]	T_d [°C]	ΔH_d [J/g]
HMX	281.4	281.4	293.5	1714
TNT	80.1	325.7	333.6	178
TNT/HMX (50/50)	83.5	250.1	270.6	396
ME3N/HNIW (50/50)	68.7	204.4	225.1	1859
ME3N/HMX (50/50)	68.8	259.8	275.7	1006
ME3N/GUDN (50/50)	68.2	197.9	214.2	1320
ME3N/TNT/HMX (20/30/50)	43.9	254.3	281.1	1286
ME3N/TNT/GUDN (20/30/50)	44.9	202.9	210.5	1489
ME3N/DNT/HMX (20/30/50)	43.6	280.2	286.5	890
ME3N/DNT/GUDN (20/30/50)	43.7	197.1	209.2	1144
TBU3N/HMX (50/50)	91.9	278.9	284.9	1014
TBU3N/GUDN (50/50)	52.1	200.7	211.1	1067
TBU3N/DNT/HMX (20/30/50)	76.2	279.2	285.8	663
TBU3N/DNT/GUDN (20/30/50)	75.9	206.1	214,5	1082
EOM/HMX (50/50)	54.1	268.3	278.9	1027
EOM/GUDN (50/50)	53.9	198.1	209.1	1176
EOM/TNT/HNIW (20/30/50)	48.1	206.1	225.2	1831
EOM/TNT/HMX (20/30/50)	49.3	258.3	278.9	1282
EOM/TNT/GUDN (20/30/50)	48.6	202.9	211.5	1524

Table 5 shows that the melting point of each melt-cast matrix has changed due to the filler. The melting temperatures shifted 1-3 °C higher, which is probably due to the structure of the sample. Decomposition of the formulation occurs at a lower temperature than that of the corresponding filler. For compositions with GUDN, this displacement is 7-16 °C compared to the decomposition temperature of pure GUDN (T_s = 213.9 °C, T_d = 220.7 °C); the shift of the exothermic effect for formulations with HNIW reaches 37-51 °C compared to pure HNIW (T_s = 255.7 °C, T_d = 262.2 °C). The exo-effects of compositions based on HMX (without DNT and TBU3N) were shifted by 13-31 °C. The decomposition temperature of formulations with HMX, DNT and TBU3N exhibited the smallest offset (1-9 °C) compared to the other compositions (Table 5).

3.3 Sensitivity and detonation characteristics of the formulations

Table 6 lists the results of measurements of the sensitivity of the explosive systems. The higher the lower limits are, the better and safer is the system. Table 7 lists the calculated density of the explosive compositions, their detonation velocities and pressures.

Table 6. Sensitivity of explosive systems

Formulation (ratio [wt.%])	*LLshock* [mm]	*LLfriction* [MPa]
HMX	50	240
TNT	200	650
TNT/HMX (50/50)	120	500
ME3N/HNIW (50/50)	150	600
ME3N/HMX (50/50)	200	650
ME3N/GUDN (50/50)	>500	800
ME3N/TNT/HMX (20/30/50)	200	600
ME3N/TNT/GUDN (20/30/50)	400	800
ME3N/DNT/HMX (20/30/50)	200	650
ME3N/DNT/GUDN (20/30/50)	>500	1000
TBU3N/HMX (50/50)	200	750
TBU3N/GUDN (50/50)	>500	>1177
TBU3N/DNT/HMX (20/30/50)	300	750
TBU3N/DNT/GUDN (20/30/50)	>500	>1177
EOM/HMX (50/50)	250	750
EOM/GUDN (50/50)	>500	>1177
EOM/TNT/HNIW (20/30/50)	300	450
EOM/TNT/HMX (20/30/50)	250	700
EOM/TNT/GUDN (20/30/50)	>500	1000

Table 7. Detonation characteristics of explosive systems

Formulation (ratio [wt.%])	Density [g/cm^3]	*VoD* [m/s]	Pressure [kbar]
HMX	1.910	9083	397
TNT	1.654	6773	188
TNT/HMX (50/50)	1.773	7971	284
ME3N/HNIW (50/50)	1.730	8162	290
ME3N/HMX (50/50)	1.680	7984	272
ME3N/GUDN (50/50)	1.618	7630	226
ME3N/TNT/HMX (20/30/50)	1.735	7978	280
ME3N/TNT/GUDN (20/30/50)	1.668	7614	234
ME3N/DNT/HMX (20/30/50)	1.668	7708	253
ME3N/DNT/GUDN (20/30/50)	1.625	7218	195
TBU3N/HMX (50/50)	1.528	7195	196
TBU3N/GUDN (50/50)	1.476	6608	145
TBU3N/DNT/HMX (20/30/50)	1.623	7231	205
TBU3N/DNT/GUDN (20/30/50)	1.565	6817	165
EOM/HMX (50/50)	1.634	7650	240
EOM/GUDN (50/50)	1.575	7270	196
EOM/TNT/HNIW (20/30/50)	1.767	7936	275
EOM/TNT/HMX (20/30/50)	1.715	7773	256
EOM/TNT/GUDN (20/30/50)	1.649	7390	210

The results of Table 7 were obtained using the equation of state BKW-NV [16] under the assumption of graphite formation in the explosion products, the equation of state of which was borrowed from article [17]. The enthalpies of formation of the nitrotriazole derivatives that were required for the calculations were obtained by the method of [18]. The enthalpy of ME3N was 208.2 kJ/mol; the enthalpy of TBU3N was 137.5 kJ/mol; the enthalpy of EOM was 34.7 kJ/mol. The calculation of the detonation characteristics of the source explosives (HMX, GUDN, DNT, TNT, *etc.*) was based on reference data of density and enthalpy of formation [19]. The densities of the materials listed in Table 7 were determined by hydrostatic weighing. The enthalpy of formation each composition was calculated using an additive scheme.

According to the results, the sensitivity of the composition ME3N/HMX (50/50) was significantly less than that of TNT/HMX (50/50) and was equal to that of TNT; the sensitivity of ME3N/HNIW (50/50) was less than that of TNT/HMX (50/50), and the detonation velocity was higher (Tables 6 and 7). TNT improves the density of ME3N/TNT/HMX (20/30/50) compared

to ME3N/HMX (50/50), but increases the sensitivity to friction. Since these compositions had approximately the same values of detonation velocity, the formulation without TNT is preferable. Formulations with EOM/HMX and TBU3N/HMX (50/50) were less sensitive than ME3N/HMX (50/50), however, the density of these compositions and their detonation velocities were also less. The sensitivity of ME3N/DNT/HMX (20/30/50) was equal to the sensitivity of ME3N/HMX (50/50), but had a lower density and *VoD*. Compounds with GUDN were the least sensitive, due to the insensitivity of GUDN itself. When using this filler, compositions with melt-casts ME3N and ME3N/TNT had the same detonation velocities, but differed in density and sensitivity to impact.

4 Conclusions

The results of experimental studies have confirmed that the use of pure 3-nitro-1,2,4-triazole derivatives and their melt-casts with TNT are promising energetic matrices for explosive systems. The most interesting of the tested compositions were those with 1-methyl-3-nitro-1,2,4-triazole. Complete or partial replacement of TNT by 1-methyl-3-nitro-1,2,4-triazole will reduce the risks due to the mechanical sensitivity of powerful explosives. In this case, the detonation characteristics of such compositions will remain the same as those of similar formulations with TNT.

References

[1] Talawar, M.B.; Sivablan, R.; Anniyappan, M.; Gore, G.M.; Astana, S.N.; Gandhe, B.R. Emerging Trends in Advanced High Energy Materials. *Combust., Explos. Shock Waves* **2007**, *43*(1): 62-72.

[2] Zhukov, B.P. *Energetic Condensed. Systems*. (in Russian) Moscow, **1999**, pp. 80-116; ISBN 5-8037-0031-2.

[3] Fomicheva, L.V. *Explosives. Basic Properties. Production and Processing Technology*. (in Russian) All-Russian Scientific Research Institute of Experimental Physics, Sarov, **2007**, pp. 7-131; ISBN 978-9515-0078-8.

[4] Badgujar, D.; Talawar, M. Thermal Analysis and Sensitivity Studies on Guanylurea Dinitramide (GUDN or FOX-12) Based Melt Cast Explosive Formulations. *Cent. Eur. J. Energ. Mater.* **2017**, *14*(2): 296-303.

[5] Pepekin, V.I. Tendencies in the Development of Studies of High Explosives. *Russ. J. Phys. Chem. B.* **2011,** *5*(1): 41-44.

[6] Davies, P.J.; Provatas, A. *Characterisation of 2,4-Dinitroanisole: An Ingredient for*

Use in Low Sensitivity Melt Cast Formulations. DSTO, Technical Report DSTO-TR-1904, Australia, **2006**, pp. 1-5, 20.

[7] Mishra, V.S.; Vadali, S.R.; Bhagat, A.L.; Garg, R.K.; Kugaonkar, V.M.; Raman, S.; Sinha, R.K.; Asthana, S. Studies on NTO-, FOX-7- and DNAN-based Melt Cast Formulations. *Cent. Eur. J. Energ. Mater.* **2017**, *14*(2): 403-417.

[8] Miao, F.; Zhang, X.; Zhou, L.; Wu, X.; Jiang, T.; Xing, R. Hugoniot and Mie-Grüneisen Equation of State of Unreacted 2,4-Dinitroanisole (DNAN). *Int. J. Impact Eng.* **2019**, *134*: 103369.

[9] Lei, F.-B.; Zhu, J.-P.; Cao, D.-L. Theoretical Research on Structures and Detonation Performance for Nitro Derivatives of Triazole. (in Chinese) *Binggong Xuebao (Acta Armamentarii)* **2011**, *32*(1): 8-16.

[10] Nesterenko, D.A.; Garanin, V.A.; Kazakov, A.I.; Korepin, A.G.; Romanova, L.B. Energetic Properties and Impact Sensitivity of Crystalline Explosives. *Russ. J. Phys. Chem. B.* **2014**, *8*(5): 46-57.

[11] Dubnov, L.V.; Bakharevich, A.I.; Romanov, A.I. *Industrial Explosives*. (in Russian) Nedra, Moscow, **1988**, pp. 325-332; ISBN 5-247-00285-7.

[12] Komarova, M.V.; Vakutin, A.G.; Kozyrev, N.V.; Il'yasov, S.G. Binary Systems Based on Nitrotriazole Derivatives and Nitrofurazanyl Furoxane. (in Russian) *South-Siberian Scientific Bulletin* **2018**, *23/3*: 33-38.

[13] Sukhanov, G.T.; Lukin, A.Yu. Reaction of 3-Nitro-1,2,4-triazoles with Alkylating Agents. 1. Alkylation in the Presence of Alkali. *Chem. Heterocycl. Compd.* **2005**, *41*(7): 861-865.

[14] Sukhanova, A.G.; Sakovich, G.V.; Sukhanov, G.T. Reaction of 3-Nitro-1,2,4-triazoles with Alkylating Agents. 6. Alkylation of a Neutral Heterocycle by Alcohols in Acid Media. *Chem. Heterocycl. Compd*. **2008**, *44*(11): 1368-1373.

[15] Sukhanov, G.T.; Pivovarova, E.V.; Digo, T.A.; Filippova, Yu.V.; Sukhanova, A.G.; Bosov, K.K. Synthesis of Simple Mixed Esters of Heterocyclic and Aliphatic Alcohols. (in Russian) *South-Siberian Scientific Bulletin* **2017**, *20/*4: 182-184.

[16] Kozyrev, N.V. Reparametrization of the BKW Equation of State for CHNO Explosives which Release no Condensed Carbon upon Detonation. *Cent. Eur. J. Energ. Mater.* **2015**, *12*(4): 651-669.

[17] Cowan, R.D.; Fickett, W. Calculation of the Detonation Properties of Solid Explosives with the Kistiakowsky-Wilson Equation of State. *J. Chem. Phys.* **1956**, *24*(5): 932-939.

[18] Joback, K.G.; Reid, R.C. Estimation of Pure-component Properties from Group-contributions. *Chem. Eng. Commun.* **1987**, *57*(1-6): 233-243.

[19] Meyer, R.; Köhler, J.; Homburg, A. *Explosives.* 6th ed., WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, **2007**, pp. 106-336; ISBN 978-527-31656-4.

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