



Synthesis and Study of the Thermal and Ballistic Properties of SMX

Vladimir A. Sizov,^{1*} Dmitriy V. Pleshakov,¹
Andrey F. Asachenko,² Maxim A. Topchiy,² Mikhail S. Nechaev²

¹ *Dmitry Mendeleev University of Chemical Technology of Russia,
9 Miusskaya Sq, 125047 Moscow, Russia*

² *A.V.Topchiev Institute of Petrochemical Synthesis RAS,
Moscow, Russia*

**E-mail: sizovlad@muctr.ru*

Abstract: The high-density tetranitrate ester 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane (SMX) was synthesized. The methods of obtaining and isolating the intermediates were optimized. The differences between the syntheses of SMX by a four- and five-step scheme were investigated. Combustion of SMX and its catalysis was studied. The possibility of replacing NG as the main plasticizer in a double-base propellant composition was demonstrated. SMX particles were shown to have pronounced crystal faceting using scanning electron microscopy. The decomposition rate equation was determined. The amount of SMX decomposed under isothermal conditions (90 °C) was 0.8 wt.% after 60 min. Thermogravimetric analysis demonstrated that heating SMX results in two different processes – decomposition and evaporation, with SMX evaporating faster than it decomposes.

Keywords: tetranitrate ester, burning rate, differential scanning calorimetry, decomposition, thermogravimetric analysis

1 Introduction

The synthesis and properties of a new tetranitrate ester SMX, also known as DNTN (1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane), were first described in 2008 [1]. Its physical and explosive properties (melting point, vapour

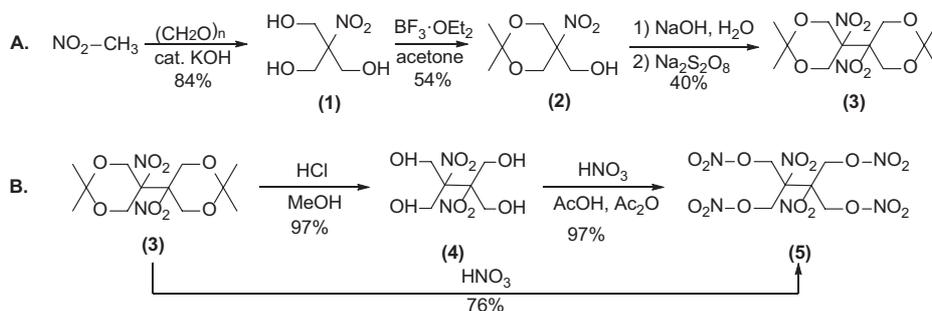
pressure, impact sensitivity) were investigated in [2], along with an attempt to use it as a substitute for ammonium perchlorate (AP) in composite propellants, to reduce environmental toxicity [3]. The melting and decomposition temperatures of SMX were shown to be 85 °C and 170 °C, respectively. The distinguishing feature of SMX is that it possesses the highest density of all known nitrate esters (1.917 g/cm³). It was shown that SMX can be used as a potential component of propellants. Burning rate data for SMX can be found in [4] – $r_b = 0.4p^{0.81}$ (cm/s).

An attempt to use SMX as a replacement for NG in a double-base propellant was made in [5], but there were no results on the burning rate, only on the thermal properties and safety characteristics. The influence of TNT on the properties of SMX was demonstrated in [6].

In [7] the authors calculated the explosive parameters of C₆N₆O₁₆H₈ using quantum chemical methods, and thus demonstrated it is a new high-energy, high-density explosive which properties can match those of HMX. In [8] the heat of formation (–497.8 kJ/mol), explosive energy (4.747 kJ/cm³), shock velocity (9.287 km/s), speed of sound and pressure were calculated for C₆N₆O₁₆H₈. A study of the hydrostatic and uniaxial compression of SMX was reported in [10], a prediction of the isothermal equation of state of SMX was made in [10, 11].

2 Experimental

In the present work we compared the 5- [1, 6] and 4-stage [6-8] synthetic procedures for SMX:



Scheme 1. Synthesis of SMX

Both synthetic procedures, 5 and 4 stages, use nitromethane as the starting compound. During our study we were able to optimize some of synthetic procedures and to increase the yields of the intermediates. Starting from

commercially available nitromethane, we optimized the isolation procedure, which allowed us to increase the product yield of 2-(hydroxymethyl)-2-nitropropane-1,3-diol (**1**) from 66% [11] to 84% (Scheme 1A). Precipitation of the product from the hot reaction mixture with chloroform and refluxing of the reaction mixture for 1 h allowed us to obtain pure 2-(hydroxymethyl)-2-nitropropane-1,3-diol (**1**) *via* simple filtration of the cold suspension.

The deprotection procedure of (**3**) was modified – replacement of gaseous hydrogen chloride with a concentrated aqueous solution of HCl provided a more safe and convenient way to obtain tetra-ol (**4**) [11-13]. In this work the quantities of the reagents were reduced by a factor of 2, but the yield (97%) was not affected.

The key difference between the 5- and 4-stage procedures is the nitration method. The 5-stage procedure uses deprotection of the common intermediate for both procedures, compound 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) (**3**), followed by nitration of the tetra-ol (**4**) obtained, whereas the 4-stage procedure comprises direct nitration of (**3**) to (**5**). The method for nitrating 2,3-bis(hydroxymethyl)-2,3-dinitrobutane-1,4-diol (**4**) to 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane (**5**, SMX) was modified, which allowed us to reduce the synthesis time and the number of reagents used, keeping the yield at the level of 97%, in comparison with [6-8]. Modification of the product isolation procedure (Scheme 1B) for the direct nitration procedure of 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) to the target molecule **5** (SMX) allowed us to increase the yield from 68% [12, 13] to 76%.

As a result of our optimization, it was demonstrated that the 4-step procedure is more environmentally friendly due to the non-use of AcOH, Ac₂O, HCl and MeOH, but the overall yield in the 5-step procedure is 1.24 times higher [1].

In this work the burning rate and the possibility of SMX catalysis is shown. The thermal stability and volatility of the tetranitrate ester was studied. Data on the decomposition products of SMX were obtained.

The reactions were monitored by TLC on Merck TLC Silica gel 60 F₂₅₄ plates. NMR spectra were recorded on a Bruker Avance AV-600 instrument (600 MHz ¹H, 151 MHz ¹³C). Chemical shifts in the NMR spectra were measured in ppm with respect to the solvent signals and recalculated into the δ-scale using standard formulae. The accuracy of the chemical shifts is ±0.01 ppm for ¹H, and ±0.1 ppm for ¹³C. Coupling constants J_{HH} are given with an accuracy of ±0.1 Hz.

The appearance of the SMX powder was characterized by scanning electron microscopy (Helios NanoLab™ 600i, FEI).

Studies of the burning rate were carried out on 7 mm diameter samples armoured in Plexiglas in a constant pressure device (Crawford bomb) under a nitrogen atmosphere. Catalytic action efficiency was estimated as the Z value:

$Z = U_k/U_o$, where U_k – burning rate of SMX with catalyst, U_o – burning rate of pure SMX. When NG was partially replaced by SMX in the double-base propellant – U_k – burning rate of the propellant with NG and SMX, U_o – burning rate of propellant with NG.

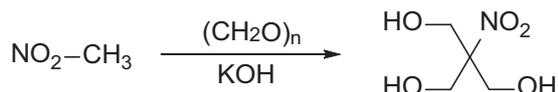
The melting and thermal decomposition of SMX were studied using a Mettler DSC 822^c/500 differential scanning calorimeter (DSC). Measurements were carried out in a nitrogen flow at 50 mL/min. Test samples were sealed in 40 μ L aluminum cells having an orifice of \sim 1 mm diameter. The calorimeter was calibrated against pure metal (zinc and indium) standards.

To study the volatility of SMX, a thermogravimetric analysis module Mettler TMA/SDTA 840 was used. The experiment was carried out in a nitrogen flow at 50 mL/min, in the isothermal mode at a temperature of +90 $^{\circ}$ C, sample weight 13.5 mg.

To study the decomposition of SMX and the analysis of the evolved gases, a combined DSC/TG/IR analysis was performed on a Netzsch STA 449 F3 device with a Bruker Alpha IR attachment. The sample was heated in an argon flow (70 mL/min) at a rate of 10 K/min, sample weight \sim 1 mg.

The five-step synthesis of SMX, modified in comparison with [1, 11] and the four-step method [12, 13] for SMX synthesis are described below.

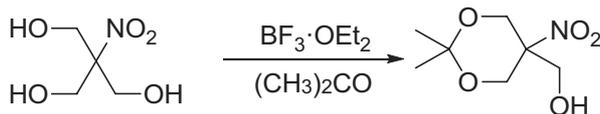
Preparation of 2-(hydroxymethyl)-2-nitropropane-1,3-diol



A 1000 mL round-bottomed flask was charged with nitromethane (73.2 g, 1.2 mol), dry ethyl acetate (600 mL), and paraformaldehyde (108 g, 3.6 mol) followed by the addition 33% aqueous potassium hydroxide (0.5 mL). The reaction mixture was heated under reflux with stirring in an oil bath at 100 $^{\circ}$ C, until all of the solids had dissolved. The resulting mixture was cooled to room temperature and concentrated to 400 mL on a rotary evaporator. Following the addition of CHCl_3 (1200 mL) the reaction mixture was reheated until all of the solids had dissolved and then refluxed for 1 h to obtain a crystalline precipitate. The flask was sealed and placed in a freezer at -18 $^{\circ}$ C for 2 days. The precipitate was then filtered off, washed with CHCl_3 (2×100 mL) and dried *in vacuo* to give 2-(hydroxymethyl)-2-nitropropane-1,3-diol (152.0 g, 84%) as a white solid. M.p. 159 $^{\circ}$ C; ^1H NMR (600 MHz, DMSO-d_6) δ , ppm: 5.12 (t, $J = 5.5$ Hz, 3H), 3.76 (d, $J = 5.5$ Hz, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, DMSO-d_6) δ , ppm: 95.1, 58.5.

Preparation of (2,2-dimethyl-5-nitro-1,3-dioxan-5-yl)methanol [14]

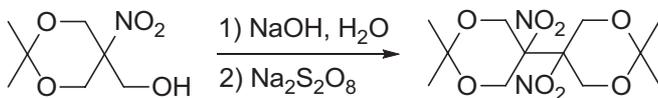


A 1000 mL round-bottomed flask, equipped with a magnetic stir bar, a dropping funnel and a reflux condenser, was charged with 2-(hydroxymethyl)-2-nitropropane-1,3-diol (152 g, 1.0 mol) and freshly distilled acetone (221 mL, 3.0 mol). The mixture was heated until all of the solids had dissolved, then cooled to 15 °C before boron trifluoride etherate (124.2 mL, 1.0 mol) was added dropwise to the resulting suspension. The reaction mixture warmed during this addition. After cooling to room temperature, the reaction mixture was poured in portions into a saturated aqueous solution of NaHCO₃ (1 L) and stirred for 15 min. The resulting white crystals were filtered off, dissolved in methylene chloride (1.2 L), washed with water and dried over anhydrous sodium sulfate. The solvent was distilled off on a rotary evaporator, and the residue was dried *in vacuo* to give (2,2-dimethyl-5-nitro-1,3-dioxan-5-yl)methanol (103.9 g, 54%) as a colorless crystalline powder.

¹H NMR (600 MHz, DMSO-d₆) δ, ppm: 5.48 (t, *J* = 5.8 Hz, 1H), 4.35 (d, *J* = 13.1 Hz, 2H), 4.05 (d, *J* = 13.1 Hz, 2H), 3.73 (d, *J* = 5.8 Hz, 2H), 1.40 (s, 3H), 1.25 (s, 3H).

¹³C{¹H} NMR (151 MHz, DMSO-d₆) δ, ppm: 98.4, 87.5, 62.4, 61.2, 26.8, 20.1.

Preparation of 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane)



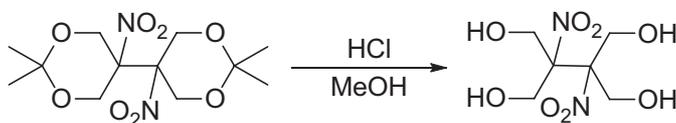
A 1000 mL round-bottomed flask, equipped with a reflux condenser and a magnetic stir bar, was charged with 2,2-dimethyl-5-nitro-1,3-dioxan-5-yl)methanol (41.37 g, 0.216 mol) and a solution of sodium hydroxide (17.31 g, 0.432 mol) in water (542 mL) at ambient temperature. The reaction mixture was heated at 60 °C for 1 h, and then cooled to 20 °C. Portions of solid sodium peroxodisulfate (103.05 g, 0.432 mol) were added and stirred at 20 °C for 20 h. Maintaining a temperature of no higher than 25 °C, 40% aqueous sodium hydroxide solution was added to the resulting mixture to pH > 11, the precipitated crystals were filtered off and washed with water on the filter. The solid was

then dissolved in methylene chloride (200 mL), washed with water [TLC control (CH_2Cl_2) until any impurities had disappeared, approximately 5 times 50 mL each], dried over anhydrous sodium sulfate and concentrated on a rotary evaporator to a volume of 30 mL. The product was purified by chromatography on silica gel (eluent – methylene chloride) to give 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) (13.9 g, 40%) as a colorless fine crystalline powder.

^1H NMR (600 MHz, CDCl_3) δ , ppm: 4.45 (d, $J = 13.6$ Hz, 4H), 4.34 (d, $J = 13.5$ Hz, 4H) 1.42 (s, 6H), 1.36 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ , ppm: 100.8, 90.1, 60.5, 24.1, 21.9.

Preparation of 2,3-bis(hydroxymethyl)-2,3-dinitrobutane-1,4-diol

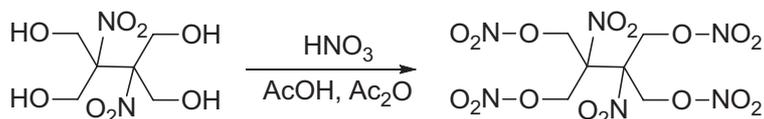


A 2000 mL round-bottomed flask, equipped with a reflux condenser and a magnetic stir bar, was charged with 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) (45.0 g, 140 mmol), methanol (700 mL) and concentrated hydrochloric acid (450 mL). The reaction mixture was heated in a water bath at 60 °C for 2 h. All volatile materials were removed under vacuum. The yellowish solid residue was dissolved in methanol (100 mL) and precipitated by the addition of CHCl_3 (600 mL). The precipitate was filtered off, washed with CHCl_3 (2×100 mL) and dried *in vacuo* to give 2,3-bis(hydroxymethyl)-2,3-dinitrobutane-1,4-diol (27.92 g, 82.7%) as a white microcrystalline solid. The mother liquor was placed in a freezer at -24 °C for 12 h. The second portion of precipitate was filtered off, washed with CHCl_3 and dried *in vacuo* to give more product (4.8 g, 14.3%) as a white microcrystalline solid. Total yield of the product was 32.7 g (97%).

^1H NMR (600 MHz, DMSO-d_6) δ , ppm: 5.34 (br.s., 4H), 4.07-4.16 (m, 8H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, DMSO-d_6) δ , ppm: 95.4, 59.3.

Preparation of 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane (SMX) [1]



A 1 L round-bottomed flask was charged with glacial acetic acid (136.6 mL) and acetic anhydride (136.6 mL). The mixture was cooled to 0 °C and 98% nitric

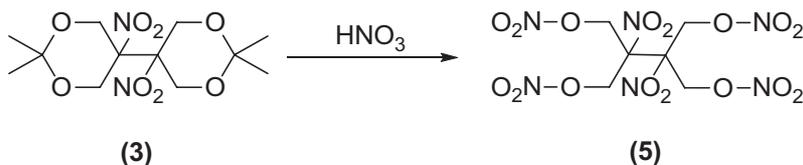
acid (98.9 g) was added dropwise, maintaining the temperature not higher than 5 °C. After the addition of nitric acid was complete, the resulting mixture was stirred for an additional 30 min at 0 °C, and then 2,3-bis(hydroxymethyl)-2,3-dinitrobutane-1,4-diol (27.92 g, 116.25 mmol) in acetic acid-acetic anhydride (1:1, 30 mL) was added dropwise. The reaction mixture was stirred for 0.5 h at 0 °C, and then the temperature was quickly raised to room temperature and stirred for an additional 1.5 h at 25 °C. The resulting mixture was poured into iced water (800 mL) and stirred for an additional 30 min at room temperature in order to crystallize the precipitated oily liquid. The yellowish crystals were filtered off and dissolved in CH₂Cl₂ (1500 mL). The organic phase was washed with saturated aqueous NaHCO₃ (2×500 mL), dried over Na₂SO₄ and evaporated to dryness. The solid residue was transferred to a filter, washed with diethyl ether (2×50 mL) and dried *in vacuo* to give 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene) butane (**5**) (47.1 g, 97%) as a colorless fine crystalline powder.

¹H NMR (600 MHz, CDCl₃) δ, ppm: 5.27 (d, *J* = 12.2 Hz, 4H), 5.10 (d, *J* = 12.3 Hz, 4H).

¹³C{¹H} NMR (151 MHz, CDCl₃) δ, ppm: 88.9, 66.0.

In the case of the 4-step synthesis of SMX, the final stage of the synthesis involved the direct nitration of 2,2,2',2'-tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) (**3**).

Preparation of 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethyl)butane (SMX)



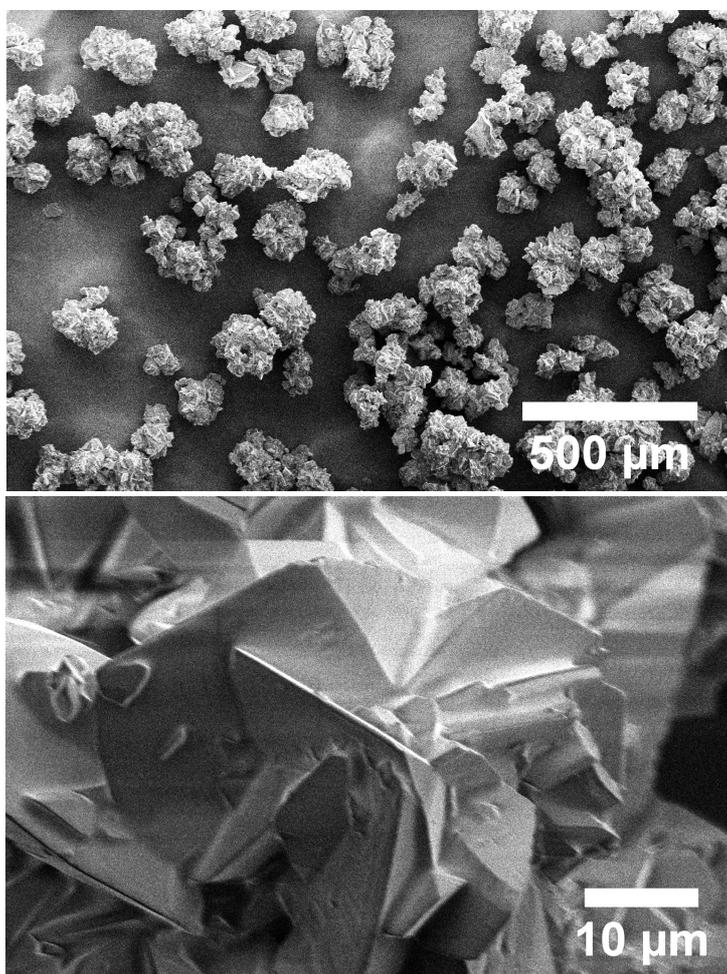
A 50 mL round-bottomed flask, equipped with a magnetic stir bar, was charged with 98% nitric acid (33 mL, 49.5 g, 0.78 mol) and cooled to 0 °C. 2,2,2',2'- Tetramethyl-5,5'-dinitro-5,5'-bi(1,3-dioxane) (2.4 g, 7.5 mmol) was then added at 0 °C. The reaction mixture was stirred for 3 h at 0 °C, then poured into ice water (170 mL) and stirred for an additional 15 min at room temperature to crystallize the precipitated oily liquid. The yellowish crystals were filtered off, dissolved in methylene chloride (50 mL), and the organic phase was washed with a solution of NaHCO₃ (2×50 mL). After drying over Na₂SO₄ the solvent was evaporated *in vacuo*. The resulting product was transferred to a filter, washed with diethyl ether (2×4 mL) and dried *in vacuo* to give 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethyl)butane (**5**) (2.41 g, 76%) as a colorless fine crystalline powder.

^1H NMR (600 MHz, CDCl_3) δ , ppm: 5.27 (d, $J = 12.2$ Hz, 4H), 5.10 (d, $J = 12.3$ Hz, 4H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ , ppm: 88.9, 66.0.

3 Results and Discussion

The appearance of SMX powder particles is shown in Figure 1. The particles have pronounced crystalline faceting and form conglomerates about 150 μm in size.



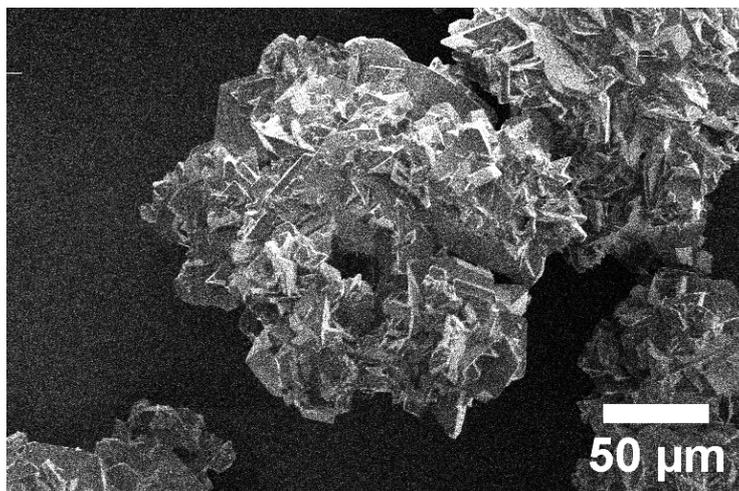


Figure 1. The appearance of SMX powder particles by scanning electron microscopy

Results on the burning rate of SMX are shown in Figure 2. We used copper-lead phthalate (CLP) in combination with carbon black as a catalyst.

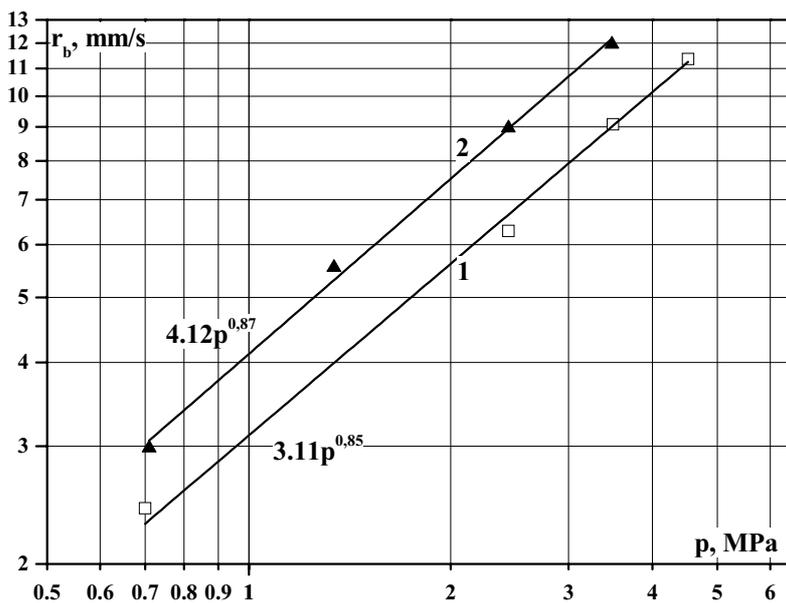


Figure 2. The influence of catalyst on the burning rate of SMX: 1 – SMX, 2 – SMX + 3% CLP + 1.5% C

The burning rate law obtained for SMX was: $r_b = 3.11p^{0.85}$ (mm/s). This is close to the known law from [5]. The addition of catalyst gave a 32-36% burning rate increase over the entire pressure range and a slightly increased pressure exponent, from 0.85 to 0.87. This demonstrated the possibility of using SMX in catalyzed double-base propellants.

The double-base propellant composition (Base) contained 50% nitrocellulose (NC) and 50% NG (polymer/plasticizer ratio = 1) and 20% of NG was replaced with SMX. SMX was dissolved in liquid NG at 50 °C and after dissolution that was added to the NC in water. The modified propellant (Base-MX) had degraded technological properties. The specific impulse of the modified propellant (calculated in the "REAL" application [15]) had been increased, by 1 s, as was the volume impulse, because of the high density of SMX compared to NG. The burning rate laws are presented in Table 1. The value "n" in the burning rate law was slightly increased from 0.74 to 0.81, which led to the increase in the burning rate at pressures higher than 4 MPa. At 10 MPa the burning rate was increased from 17.4 mm/s to 18.7 mm/s.

Table 1. Ballistic properties of the double-base propellants

Propellant	I_{sp} [s]	Burning rate law $r_b = ap^n$			r_b^{10} [mm/s]
		a	n	Δp [MPa]	
Base	236	3.17	0.74	1-20	17.4
Base-MX	237	2.89	0.81	1-20	18.7

Now considering the DSC data on SMX thermal decomposition in a closed cell with a hole diameter <1 mm (Figure 3). As the heating rate was increased from 5 °C/min to 20 °C/min, the exothermic peak temperature increased from 178 °C to 197 °C (Table 2).

Table 2. Exothermic peak temperature of SMX decomposition versus heating rate

Heating rate [°C/min]	Peak temperature [°C]
5	178
10	187
15	192
20	197

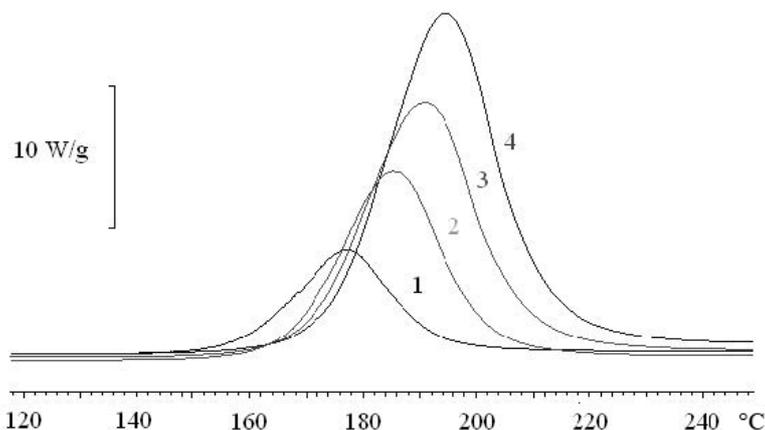


Figure 3. DSC curves for SMX. Heating rate: (1) 5 °C/min; (2) 10 °C/min; (3) 15 °C/min; (4) 20 °C/min. Curves (1), (3) and (4) were obtained in the present paper. (2) – literature data [11]

The equation for the SMX thermal decomposition rate constant derived, according to the procedure described in [16], is:

$$k = k_0 \exp\left(-\frac{E}{8.31 \times T}\right)$$

Here $k_0 = 1.01 \cdot 10^{12} \text{ s}^{-1}$ and $E = 122.7 \text{ kJ/mol}$.

In [17] the thermal decomposition reaction activation energy was calculated in three different ways (Ozawa method, KAS method, Iterative method), and gave the average activation energy as 133.2 kJ/mol, with the pre-exponential factor $k_0 = 3.19 \cdot 10^7 \text{ s}^{-1}$.

The equation for SMX thermal decomposition is:

$$\ln\left(1 - \frac{\Delta m}{m_0}\right) = -k\tau$$

where m_0 is the initial weight of the sample and $(\Delta m/m_0) \times 100$ is the amount of the decomposed material at the time τ (%).

For a comparison of the stability of various energetic materials it is convenient to use the value of $\tau_{0.02\%}$ at 20 °C [18]. The $\tau_{0.02\%}$ value for SMX was calculated and indicated that only 18 days were needed for 0.02% decomposition,

whereas $\tau_{0.02\%}$ for HMX and RDX is hundreds of years. This means that SMX is an unstable substance and its use in any types of propellant is in doubt, except for energetic materials which will not be stored for a long time (~2-3 weeks).

According to the IR spectroscopy of the gas phase products released during heating, it may be seen that the decomposition takes place in two stages. The IR spectra of the decay products at temperatures of 180 °C and 193 °C are shown in Figure 4. Peaks corresponding to CO₂, N₂O, CO, HCN, formic acid and NO₂ were observed. The IR spectrum of neat SMX before decomposition was obtained from [2].

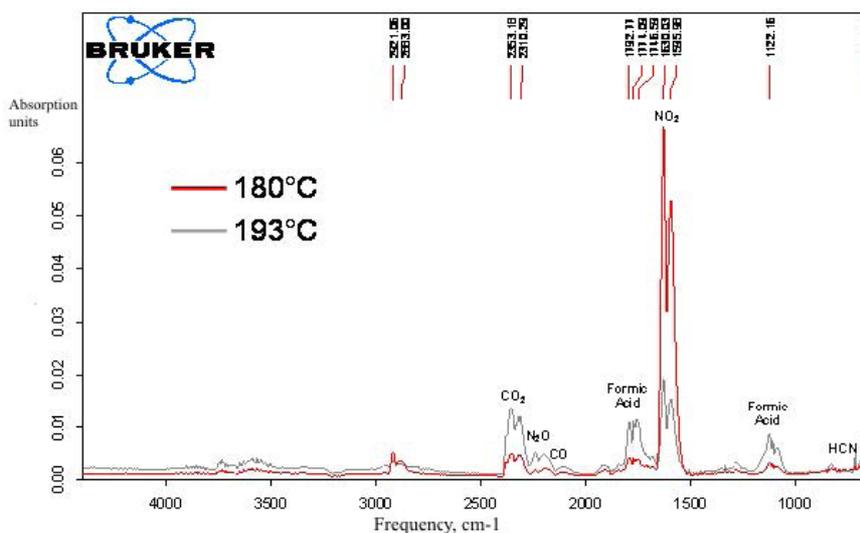


Figure 4. IR spectra of the decay products at 180 °C (red curve) and 193 °C (gray curve)

The dependence of the concentration of the released gases on the temperature of the sample is shown in Figure 5, where the concentrations of the gases are plotted in relative units of the CO₂ concentration.

It may be seen that in the first stage of the decomposition, which begins at 154 °C, a large amount of NO₂ is released, which indicates cleavage of NO₂ groups at the beginning of SMX decomposition. In the second stage of the decomposition (173 °C), the cleavage of C–C bonds with the formation of CO₂, N₂O, CO, HCN and formic acid occurs. The peak of the main energy release falls precisely at this stage.

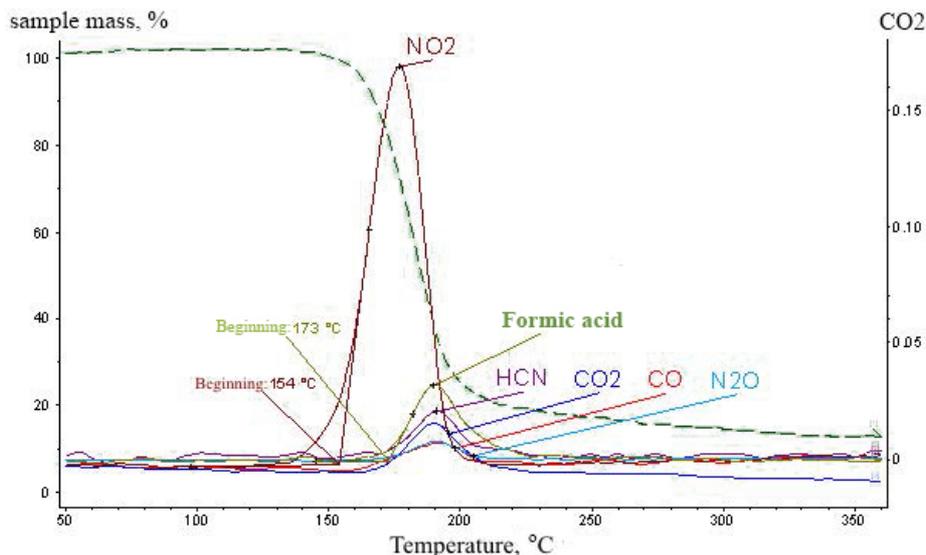


Figure 5. Concentrations of gases in the decomposition products. Green dotted curve is the loss of sample mass

Table 3 shows the amount of SMX decomposed as a function of time in a closed cell with a 1-mm hole at 90 °C in an isothermal experiment. The results compiled in Table 3 were obtained on the assumption that the SMX decomposition reaction is first-order. Autocatalysis is known to be typical behaviour for nitroesters [18]. In the case of SMX, however, the reaction products exit through the orifice in the cell, being entrained with the nitrogen flow, and do not affect the reaction mechanism.

Table 3. Amount of SMX decomposed versus time at 90 °C

Heating time [min]	Decomposed SMX [%]
1	0.013
5	0.065
10	0.13
15	0.2
30	0.4
60	0.8

The temperature of 90 °C was chosen as the presumed temperature of granulation (production of spherical particles) of SMX. It should be noted that it is necessary to obtain two types of spherical crystalline particles of SMX: fine and coarse fractions. In this case, at temperatures below the melting point of SMX, the tetranitrate ester can be used as a solid filler.

TGA and SDTA thermograms of SMX are shown in Figure 6. It may be seen that SMX melts at 81 °C, evaporates in the temperature range 85-145 °C (an elongated endothermic peak) and decomposes at 145-210 °C.

The SMX thermogram in the isothermal mode in an open cell at 90 °C, obtained by thermogravimetric analysis, is shown in Figure 7.

The mass loss in 60 min was ~4 wt.%. This is ~5 times higher than the value indicated in Table 3. Thus, when SMX is heated, two processes occur: decomposition of the substance and its evaporation. SMX evaporates faster than it decomposes.

The SMX friction sensitivity test was carried out on the pendulum on the drop-hammer K-44-III (according to the Russian standard). The lower limit P_0 (the lack of explosions in 20 parallel experiments) and 50%-point P_{50} (50% explosion frequency in 20 parallel experiments) were determined as $P_0 = 240$ MPa, $P_{50} = 260$ MPa.

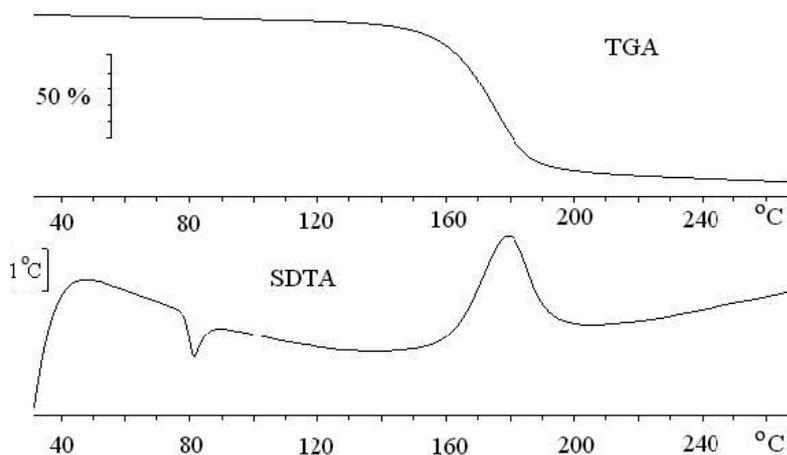


Figure 6. Dependence of mass loss of SMX in an open cell (%) on temperature (TGA) and SDTA curve. Heating rate, 10 °C/min

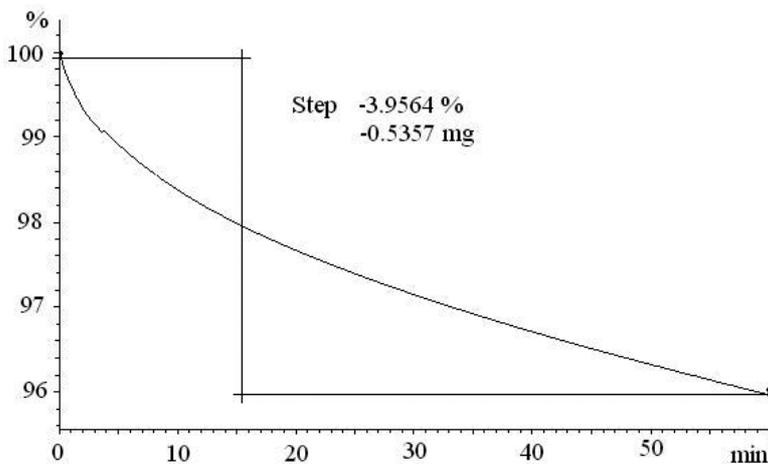


Figure 7. Dependence of mass loss of SMX (%) on time, obtained by thermogravimetric analysis in an open cell. Isothermal mode. Temperature 90 °C. Heating time 60 min

As a comparison, for PETN $P_0 = 170$ MPa, $P_{50} = 300$ MPa; for RDX $P_0 = 240$ MPa, $P_{50} = 420$ MPa; for tetryl $P_0 = 300$ MPa, $P_{50} = 470$ MPa. Thus, SMX is at the same level as RDX in its propensity for initiation to explosion, but is superior to the other explosives in its ability to develop from the source of initiation, and in this sense SMX is at the level of quickmatch explosives and compositions.

4 Conclusions

In this work two synthetic procedures for SMX preparation were compared. It was shown that the one-pot deprotection/nitration procedure gives 1.24 lower yield than the consecutive deprotection and nitration method.

It was shown that SMX may be subjected to the catalysis by various salts, *e.g.* organic copper salts such as phthalates. On this basis SMX may be used in catalyzed double-base propellants as a partial substitution for NG. Due to its rather high density and its enthalpy of formation value that is considerably higher than that of NG, SMX can also increase the ballistic properties of propellants. At 20 °C, 0.02% of SMX decomposes during 2-3 weeks, which makes it an unstable substance and can be used only in energetic materials which are not

stored for a long time. It follows from the friction sensitivity test that SMX is a quite dangerous energetic material for handling and requires special precautions.

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