Investigation of initiating strength of detonators containing TKX-50, MAD-X1, PETNC, DAAF, RDX, HMX or PETN as a base charge

Thomas M. Klapötke[a]*, Tomasz G. Witkowski[a], Zenon Wilk[b]**, Justyna Hadzik[b]

[a] Energetic Materials Research, Department of Chemistry, University of Munich (LMU), Butenandtstr. 5-13, D-81377, Germany

[b] Institute of Industrial Organic Chemistry, Annopol Str. 6, 03-236 Warsaw, Poland

*tmk@cup.uni-muenchen.de, **zenon.wilk@ipo.waw.pl

Abstract

An experimental investigation of the initiating capability of detonators containing as a base charge the following explosives: dihydroxylammonium 5,5'-bis(tetrazolate-1*N*-oxide) – TKX-50, dihydroxylammonium 5,5'-bis(3-nitro-1,2,4-triazolate-1*N*-oxide) – MAD-X1, pentaerythritol tetranitrocarbamate – PETNC and 3,3'-diamino-4,4'-azoxyfurazan – DAAF in comparison with RDX, HMX and PETN was undertaken. In order to estimate the initiating capability of detonators, the underwater explosion test was applied. The total energy as a sum of the primary shock wave and the bubble gas energies was determined by measuring the overpressure of the shock waves generated in water. Furthermore, the complete synthesis for novel explosives is presented. The thermal behavior of the explosives was explored using differential scanning calorimetry. The gas phase absolute molar enthalpies at 298 K and 1 atm were calculated theoretically using the modified complete basis set method (CBS-4M) with the Gaussian 09 software. Gas phase standard molar enthalpies of formation ($\Delta H_{f\,(g)}^{\circ}$) at 298 K were calculated using the atomization energy method. In order to obtain the standard molar enthalpy of formation ($\Delta H_{f\,(s)}^{\circ}$) for the prepared covalent compounds, the values of the standard molar enthalpies of sublimation (applying Trouton's rule) were subtracted from $\Delta H_{f\,(g)}^{\circ}$. In the case of salts, $\Delta H_{f\,(g)}^{\circ}$ of ions and the calculated standard molar lattice enthalpies were used to calculate $\Delta H_{f\,(s)}^{\circ}$. The performance parameters (such as detonation energy, detonation pressure, detonation velocity) based on calculated $\Delta H_{(s)}^{\circ}$ values were computed using the CHEETAH 2.0 software. For the calculations the theoretical maximum densities and densities obtained during the experiments presented in this work were used.

Introduction

Recently, many new types of detonators have been developed and implemented for production. The continuous research for new types of detonators is driven by increasingly strict safety requirements and environmental concerns, protection against unauthorized use, as well as specific requirements set by users. In order to fulfill these requirements, novel explosives with tailored properties which have been recently synthesized, could be used as the base charge in detonators [1-4]. Nevertheless, the shock wave generated during the action of the detonator has to be higher than the initiation pressure of the acceptor explosive charge. If the generated shock wave is not sufficient to initiate the detonation of the explosive, it can result in low-order detonation or misfire [5]. Therefore, the energy output of detonators containing new explosives as a base charge has to be determined and compared with currently used ones.

Materials and Methods

Among the recently developed explosives, the most promising candidates for application based on their performance as well as convenient synthetic method are TKX-50, MAD-X1, PETNC and DAAF (Figure 1).

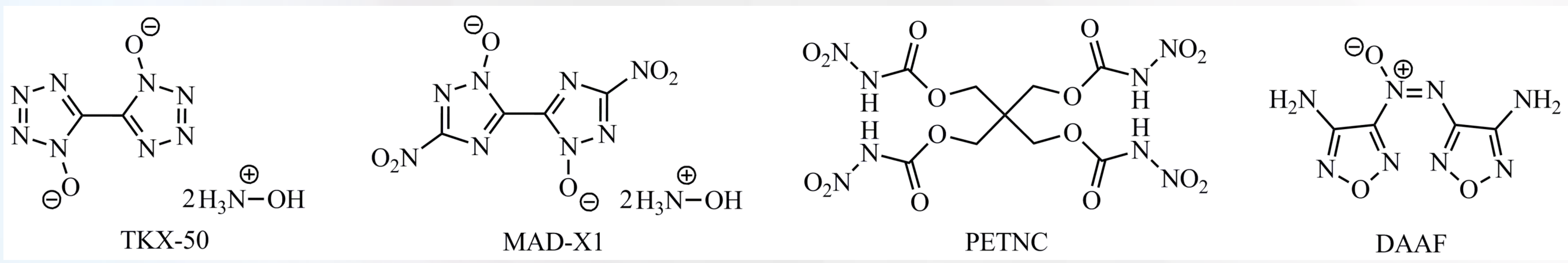

Figure 1. Chemical structures of TKX-50, MAD-X1, PETNC and DAAF.

The explosives (shown in Figure 1) have high decomposition temperatures (≥ 196 °C) and the theoretical maximum densities are between 1.76 and 1.90 g·cm⁻³. TKX-50, MAD-X1 and DAAF are endothermic compounds, while PETNC (similar to its analog PETN) is an exothermic compound, which contains four explosophore nitro functionalities. Theoretically calculated Chapman-Jouguet (C-J) characteristics of these explosives (detonation pressure, 23.47 ÷ 41.89 GPa; detonation velocities, 7639 ÷ 9656 m·s⁻¹), as well as their sensitivity to external stimuli (FS ≥ 120 N, IS ≥ 7 J) also make these species interesting for possible application.

In order to estimate the initiation power of the detonators, the underwater initiating capability test was applied. The primary shock wave energies and the bubble gas energies were determined by measuring the overpressures of the shock waves generated in water. Measurement of the shock wave and the time between the primary shock wave and first pulsation of the gas bubble, allows the energies of the shock wave and gas bubble to be determined. These parameters allow a comparison to be made between the investigated explosives with currently used explosives (RDX, HMX, PETN) [5-9].

Underwater explosion

The initiating capability of detonators containing TKX-50, MAD-X1, PETNC and DAAF as a base charge was measured in underwater explosion test according to the methodology described in European Standard (EN 13763-15, Determination of equivalent initiating capability) [6]. Additionally, commercial available explosives (RDX, HMX, PETN) were used as reference materials. In order to perform the underwater explosion tests, a water tank made from non-reflecting and energy-absorbing material with a positioning system for the sensor and detonator was used (Figure 2).

Figure 2. Model of the water tank showing the location of the detonator and the location of the pressure sensor (a), the arrangement for testing (b), the positioning system with the sensor and detonator (c).

The detonators being tested were placed in the positioning system. Detonation of the explosives generates overpressures in water which were recorded by a piezoelectric transducer. The collected data are presented in two time scales. First one takes into account the presentation of the primary shock wave generated in water (*c.a.* 50 µs) which is used to determine maximum of overpressure (P_{max}) and time at which the sensor output has decreased to $P_{\theta} = P_{max} \cdot e^{-1}$ (θ), and calculation of E_{SW} and E_S (Figure 3a). The second time frame (*c.a.* 30 ms) is used to determine the time interval between the shock-wave pressure peak and the first collapse of the gas bubble (t_b) which is used to calculate E_{BW} and E_B (Figure 3b).

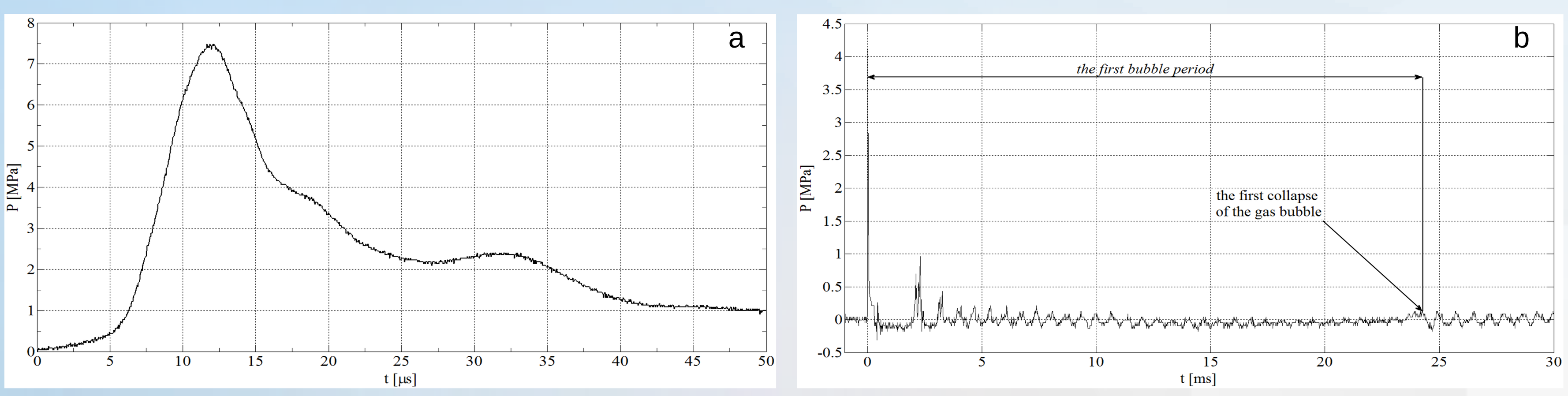

Figure 3. The primary shock wave (a) and the overpressure (b) generated in water by firing detonator filled in with 0.7 g of DAAF.

The following oscillograms present the primary shock wave for reference explosives (RDX, HMX, PETN) and novel ones (TKX-50, MAD-X1, PETNC, DAAF) (base charges: 0.2 g (a), 0.5 g (b), 0.7 g (c)).

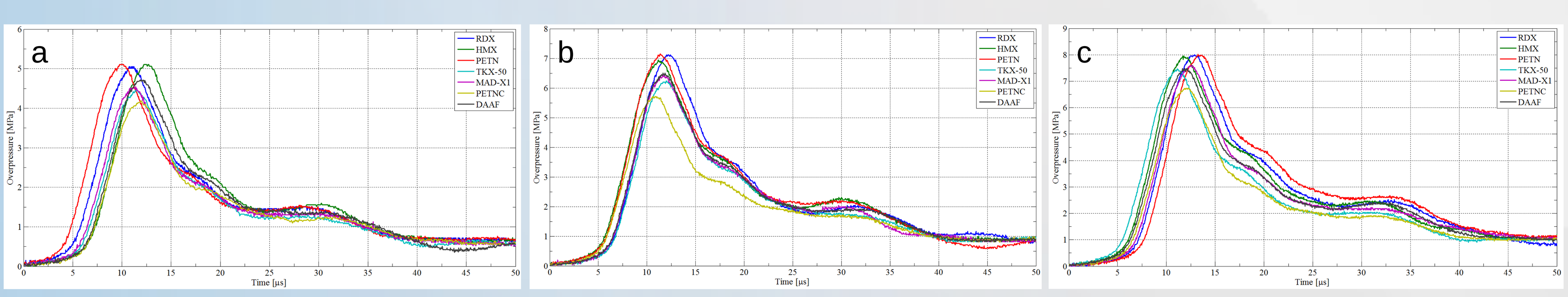

Figure 4. The primary shock waves generated in water by firing detonators filled in with investigated explosives.

The following oscillograms present the period of the first bubble pulsation for reference explosives (RDX, HMX, PETN) (base charges: 0.2 g (a), 0.5 g (b), 0.7 g (c)) and novel ones (TKX-50, MAD-X1, PETNC, DAAF) (base charges: 0.2 g (d), 0.5 g (e), 0.7 g (f)).

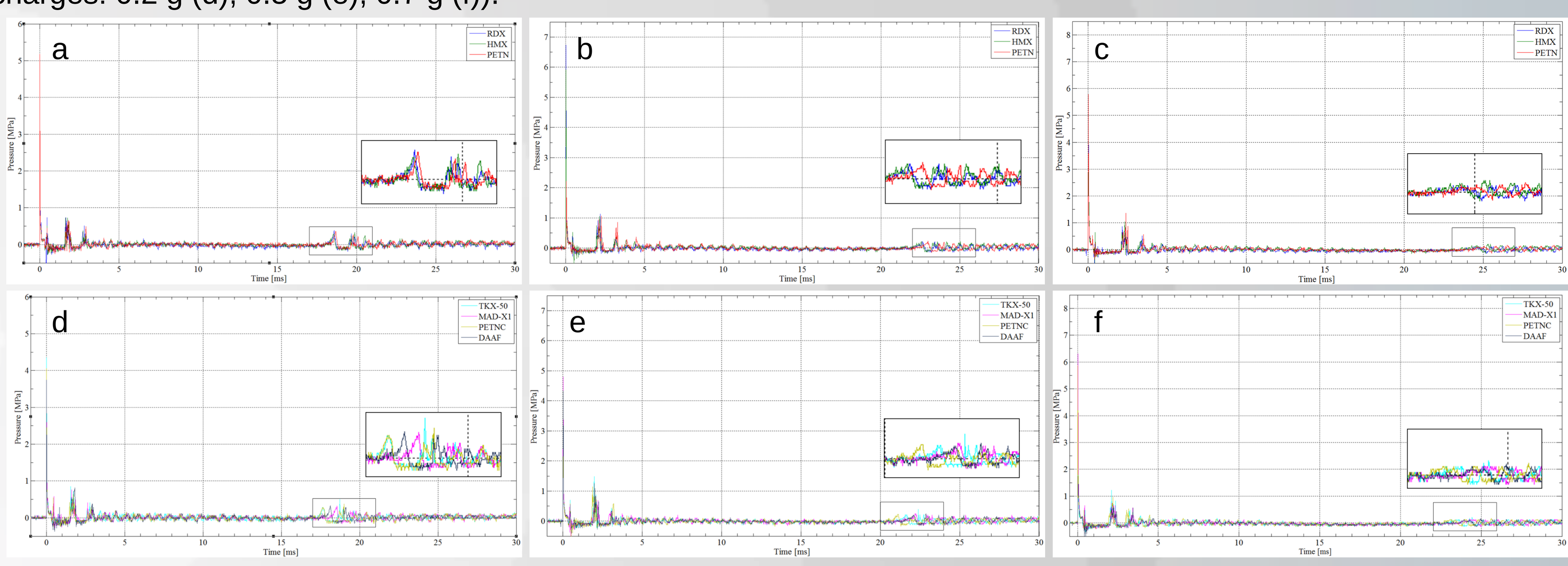

Figure 4. Overpressure generated in water by firing detonators being investigated.

Based on the obtained data, P_{max}, P_{θ}, θ, t_b, were determined and E_S, E_{SW}, E_B, E_{BW} and the total energies (E) were calculated for the detonators being investigated. The calculated total energies as a sum of the shock wave and bubble energies generated in water for the explosives which were investigated are summarized graphically (Figure 5).

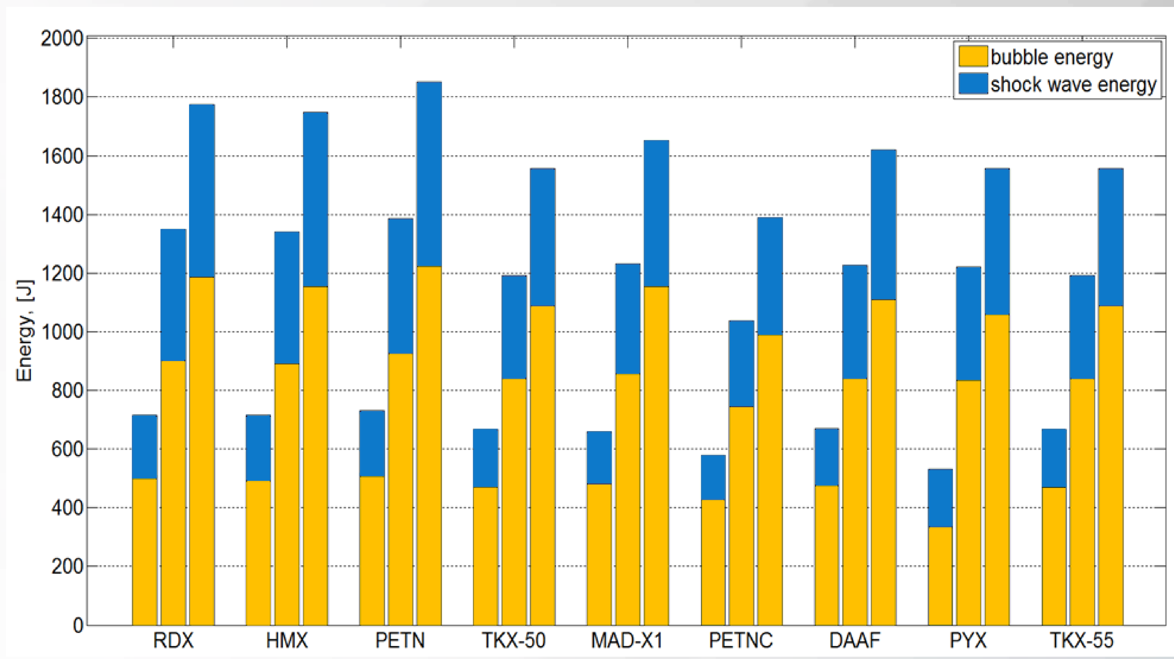

Figure 5. Total energy (E) generated in water for investigated explosives (0.2 g, 0.5 g, 0.7 g).

Conclusions

The initiating capability of detonators containing as base charge TKX-50, MAD-X1, PETNC, DAAF in comparison to RDX, HMX or PETN using an underwater explosion test was determined. Densities obtained during the experiments are lower than TMD. The lowest values of densities in comparison to TMD are obtained for base charges equal 0.2 g of studied explosives (between 51.05 % TMD for MAD-X1 and 80.14% TMD for DAAF). The highest values of densities obtained among investigated explosives were those of commercially available explosives PETN, HMX and DAAF (86.29, 84.56, 83.00% TMD, respectively). The differences in the densities obtained are due to the methodology used, which is described in the European Standard [6], *i.e.* the same pressing pressure (4.40 MPa) for all investigated explosives. That has direct impact on the primary shock wave generated in water, maximum of overpressure, the time interval between the shock-wave pressure peak and the first collapse of the gas bubble as well as calculated on those data values *i.e.* the shock wave and bubble energies generated in water. Nevertheless a constant value of pressing pressure was used for comparative reasons. Therefore additionally, underwater test results are supported by calculated detonation parameters at obtained densities.

Reference explosives (RDX, HMX and PETN) possess the highest values of the peak overpressure. Nevertheless novel explosives are characterized by slightly lower values of the recorded maximum overpressure (DAAF > 92.89, MAD-X1 > 89.93%, TKX-50 > 86.97%, PETNC > 81.81%, of RDX). Similar tendency appears for the time of decreasing of the overpressure to $P_{max} \cdot e^{-1}$. Those factors show that primary shock waves generated by investigated explosives possess similar nature.

The highest values of time of the first bubble collapse are also obtained for reference explosives; however, new explosives differs from RDX not more than 7% of t_b (MAD-X1 > 98.31%, DAAF > 97.47, TKX-50 > 95.04%, PETNC > 93.76 of RDX). That indicates also good action of mentioned explosives at longer distance from the point of initiation.

The total energies as sum of primary shock wave energies and the bubble gas energies were determined. The highest value of the total energy acquired for 0.7 g base charge mass was for PETN (104.32% RDX), the lowest for PETNC (78.82% RDX). MAD-X1, DAAF and TKX-50 possess also high values of the total energy (93.04%, 91.19%, 84.97% of RDX, respectively). The primary shock wave energy (which corresponds to brisance of explosive) for investigated explosives is between 26.18% (PETNC, 0.2 g of base charge) and 33.97% (HMX, PETN 0.7 g of base charge) of the total energy. Endothermal explosives show following contribution of shock wave energy to the total energy: DAAF > 29.03%, TKX-50 > 28.05%; MAD-X1 > 26.98,. The second part of the total energy namely bubble energy, which correlates with heaving power of explosive, is for investigated species higher than 66.01% of the total energy.

Moreover, presented technique can be also used as a comparative method; therefore the shock wave and bubble energies equivalents are also given. Thus the small scale underwater test can be useful tool for determining and comparing blast parameters (brisance, heaving power) of different explosives. It is characterized by using small amount of tested species, and a great amount of information which can be obtained from the tests.

Therefore we can conclude that the data obtained are consistent and show that the explosives presented can be used as based charges in detonators. They meet requirements which are demanded from energetic materials intended for use in detonators. In order to maximize performance parameters pressing pressure should be optimized for every explosive separately.

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