Journal of Physics:
Conference Series

PAPER • **OPEN ACCESS**

Improving the energetic properties of 1,1-diamino-2,2-dinitroethene in PBX mixture

To cite this article: A K Hussein *et al* 2024 *J. Phys.: Conf. Ser.* **2830** 012029

Improving the energetic properties of 1,1-diamino-2,2-dinitroethene in PBX mixture

A K Hussein[1], M Abdelhafiz[1] and A Elbeih[1]

[1] Military Technical College, Kobry Elkobbah, Cairo, Egypt

elbeih.czech@gmail.com

Abstract: The new eyesight in the energetic materials focuses on reserving high efficiency together with optimization of safe handling. In this study, a novel nitramine, cis1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX), is combined with 1,1diamino-2,2-dinitroethene (FOX7), and bound by a styrene-butadiene rubber fabricating an insensitive plastic bonded explosive (PBX) mixture. The obtained PBX was fully characterized in comparison with the familiar explosives; SEMTEX, EPX1 and other PBXs, filled by RDX (1,3,5trinitro-1,3,5-triazinane), HMX (1,3,5,7tetranitro-1,3,5,7-tetrazine). The related individual fillers were also included. Sensitivities to various stimuli and the velocities of detonation were measured for the composites in comparison with the selected explosives. EXPLO 05 has been applied to obtain the detonation properties of the tested explosives. Different relationships (comparing performance with sensitivities) are stated and discussed. The results showed that BC/FOX7 -SBR has very low sensitivity compared with the studied compositions while its performance has larger values.

Keywords: Explosives; FOX7; EXPLO5 code; performance.

1 Introduction

The evolution of low-vulnerable explosives (LOVA) is a contemporary area of interest for researchers. Its aim is to replace traditional explosives with reserving a high performance [1]. Enhancements in performance are coupled with modifications in sensitivity [2]. Dr. Licht has extensively debated this topic [3],. Nevertheless, this challenge motivated many researchers to achieve exceptions and produce explosives that generates high strength and high-security levels at the same time, as exemplified in Refs. [4]. Therefore, BCHMX, which was successfully fabricated by a simple method patented in refs. [5], is mentioned. It performs interestingly compared to conventional explosives, although it possesses sensitivity that is comparable to PETN [6]. The Thermochemical data and explosives characteristics of PBXs, which are generated from nitramines were utilized to document and research various aspects of this issue. The significant impacts of polymers such as fluorinated, silicone matrix, nitrile rubber and methacrylate matrix on the efficiency of explosives have been published in several manuscripts [7]. Studying BCHMX with its cast compositions take also our interest [8, 9]. Regarding to the recent studies, it is still a motivation to optimize the high performance with the safety characteristics. For this reason, BCHMX and FOX7 were bonded together by styrene butadiene rubber (SBR) forming a modified PBX. As a result, sensitivities and detonation features of this composition are studied. The derived data and traits of this new PBX variant are utilized for comparative analyses against established explosives like SEMTEX10 and EPX1, as well as standard pure explosives.

Journal of Physics: Conference Series **2830** (2024) 012029 doi:10.1088/1742-6596/2830/1/012029

2 Experimental

2.1 Preparation methods

Crystals of BCHMX, the chemical construction is given in Fig. (1.a), BCHMX was made at our department. Crystallization process was performed to produce crystals with a homogeneous shape and tiny particle size. Also, FOX7 crystals with a density of 1.88 g.cm^{-1} were made by nitrating 2-methylpyrimidine-4,6-diol followed by hydrolysis step in the presence of dinitromethane.

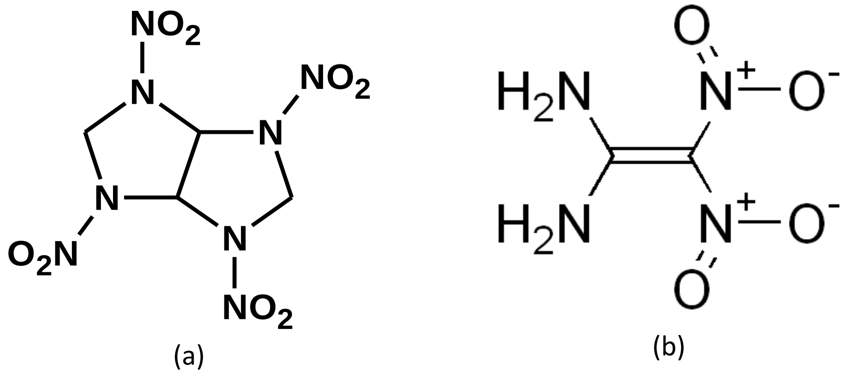

Figure 1. Structures of a) BCHMX and b) FOX7

SBR was prepared by swelling rubber at a 1:3 weight ratio in Dioctyl sebacate, which serves as a plasticizer. The obtained SBR acts as a polymeric binder for explosive mixtures. BCHMX and FOX7 crystals were mixed with a weight ratio of 43.5% and 43.5% respectively utilizing an automated plastographic mixer. The SBR polymeric binder was then added to the explosive crystals' mixture at 25 ^{o}C while continuously mixing for 90 minutes. The final PBX product was obtained in the form of cylinders with a diameter of 24mm using an extruder.

2.2 Impact sensitivity measurements

A changeable drop weight was utilized for precision and consistency measurements [10]. The sample was tested with drop hammers of varying masses to gauge initiation levels. The probit approach [11] was employed to predict the different levels of initiation. Table 1 displays the identified initiation levels that yielded a 50% potential initiation rate or higher.

2.3 Friction sensitivity measurements

The friction sensitivity of the sample was assessed using the BAM test instrument in accordance with standard test conditions [11]. The sample was placed on a porcelain plate, and different masses were employed to vary the normal force acting on the sample. The probit method was employed to predict the 50% successful initiation, which is recorded in table 1 as the friction force.

2.4 Detonation velocity measurements

The BC/FOX7-SBR detonation velocity was assessed using the EXPLOMET-FO-2000 apparatus. A cylindrical specimen with a 24mm diameter was specifically crafted for this Experment. The experiment utilized three optical sensors positioned within the charge. Initially, the first sensor was situated 50mm from the starting point, while the following sensors were spaced 50mm apart from each other, with a distance of 100mm between them. The ignition was initiated through an electric detonator, and the outcomes are detailed in Table 2.

Table 1. The measured values of the samples tested

No	Code designation	Summary formula	Impact sensitivity [J]	Friction sensitivity [N]
1	BCHMX	$C_4H_6N_8O_8$	3.2	88
2	β-HMX	$C_4H_8N_8O_8$	6.4	95
3	RDX	$C_3H_6N_6O_6$	5.6	120
4	FOX7	$C_2H_4N_4O_4$	23.7	>360
5	TNT	$C_3H_7N_3O_6$	39.2	342
6	PETN	$C_5H_8N_4O_{12}$	2.9	46
7	BCHMX -SBR	$C_{7.31}H_{11.72}N_8O_{7.96}$	15.8	228
8	HMX -SBR	$C_{7.16}H_{13.63}N_{8.0}O_{7.94}$	18.2	236
9	RDX -SBR	$C_{5.47}H_{10.1}N_{6.0}O_{5.94}$	21.4	258
10	BC/FOX7-SBR.	$C_{7.17}H_{12.02}N_{7.2}O_{7.3}$	31.2	>360
11	EPX1	$C_{7.88}H_{12.36}N_4O_{12.59}$	13.9	176
12	SEMTEX10	$C_{8.05}H_{12.64}N_4O_{12.37}$	15.7	204

2.5 EXPLO 5 calculations.

The detonation properties were evaluated in this study using the BKW (equation of state) where the heat and pressure of detonation could be calculated in addition to the velocity of detonation which might be compared with the measured values [12]. The selected parameters for the EOS are obtained from BKWN EOS. The values resulted from the calculations are stated in table2.

3. Results and Discussion

The direct relationship between explosives performance and their sensitivities towards different stimuli has been proven in many academic publications [3]. However, the novel trend in this field was motivated to overcome this issue and achieving a high efficiency while keeping the sensitivity levels at the least values. One of the most promising candidates to achieve this goal is to use the PBXs. Zeman et al deduced a relationship including the influence of different stimuli on the sensitivities of the samples. In this regard, Fig. 2 exhibits a semi-logarithmic relation of the friction sensitivity versus the impact results for the investigated samples. This may be caused by a discrepancy in the manner in which the impulse of initiation is transferred from the aforementioned types of initiation to the center of the reaction of the molecules under study.

The impact sensitivity of different PBXs, including SEMTEX10 and EPX1, was found to be higher than that of BC/FOX7-SBR and TNT. The incorporation of FOX7 and SBR matrix notably decreased the sensitivity of BCHMX [13]. This decrease is evident in the significant reduction in impact sensitivity observed in pure nitramines after the addition of SBR matrix.

Table 2. Detonation characteristics for the investigated samples.

Studied sample		Experimental	Calculated detonation parameters by Explo5 Code				
No	Code of samples	Density ρ [g.cm^{-3}]	Detonation velocity [m.s^{-1}] experimental D_{exp}	Detonation velocity [m.s^{-1}] calculated $D_{cal.}$	Error %	Detonation pressure P [GPa]	Heat of detonation Q [kJ.kg^{-1}]
1.	BCHMX	1.79	8650	8840	+2.2	33.9	6447
2.	β-HMX	1.90	9100	9225	+1.4	38.0	6075
3.	RDX	1.76	8750	8718	-0.4	32.1	6085
4.	FOX7	1.78	8325	8260	-7.8	27.7	4942
5.	TNT	1.60	6900	7126	+3.3	19.5	5101
6.	PETN	1.70	8400	8318	-1.0	28.5	6160
7.	BC-SBR	1.59	7922	7755	-2.1	22.7	6245
8.	HMX –SBR	1.61	7986	7839	-1.8	23.2	5994
9.	RDX –SBR	1.56	7711	7601	-1.4	21.0	5958
10.	BC/FOX7-SBR	1.63	7818	7860	+0.5	23.7	5269
11.	EPX1	1.55	7636	7398	-3.1	21.17	5742
12.	SEMTEX10	1.52	7486	7370	-1.5	20.89	5708

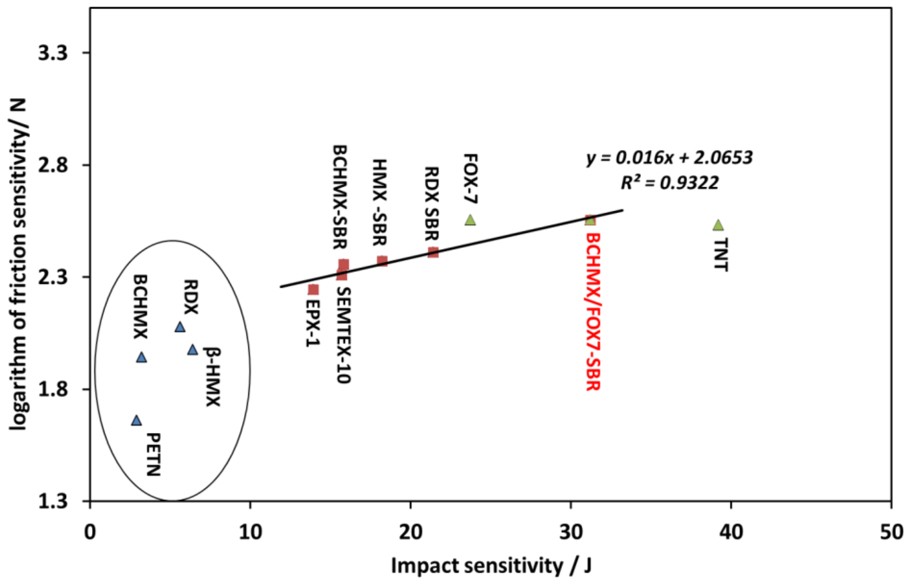

Figure 2. Comparing the impact sensitivity with the logarithm of friction sensitivity

Fig. 3 presents an intriguing link between the volume heat of detonation and the logarithm of impact sensitivity in order to evaluate the performance of the new BC/FOX7-SBR PBX. On this figure, there are two-line groups: the first group has all of the pure nitramines that are sensitive in comparison to the other samples that have been analysed, along with their PBXs that include the SBR matrix in addition to the BC/FOX7-SBR PBX.

The novel BC/FOX7-SBR PBX performs better than all nitramines in the investigation with SBR polymeric matrix and EPX1 and SEMTEX10 plastic bound explosives while having the lowest sensitivity with the examined plastic explosive. In comparison to the individual explosives, all plastic explosives have a low impact sensitivity. This is because of the influence of the SBR binder. The EPX1 and SEMTEX10 plastic bound explosives and the second line group have the same composition and pure PETN. Fig. 3 supports the overall finding that a rise in performance is generally followed by an increase in explosive sensitivity.

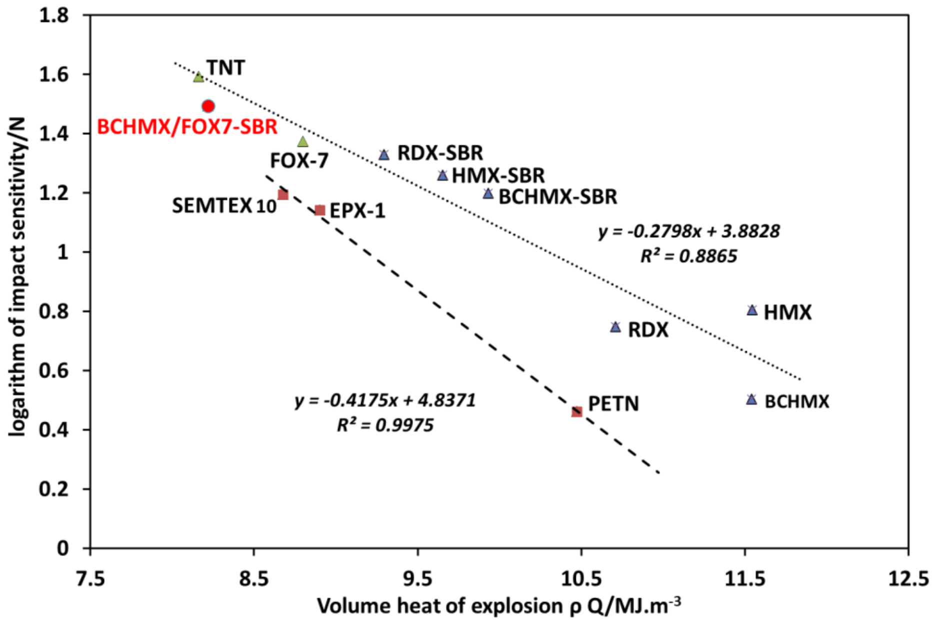

Figure 3. Relationship between impact sensitivity and explosion's volumetric heat.

The equation commonly used to determine the detonation pressure based on detonation velocity was applied to verify the accuracy of the calculations against measured values. The performance data, denoted as ρD2, were plotted against the calculated pressure, demonstrating consistency between the calculated and observed results as shown in Fig. 4. This figure gave a clear ordering of all the studied explosives and their plastic types in comparsion with the new prepared BC/FOX-SBR. It is evident that BC/FOX7-SBR has somewhat better detonation properties than BCHMX-SBR PBX and has greater detonation characteristics than EPX1, SEMTEX10, and RDX-SBR. The findings of the tested samples' sensitivity and performance showed that the fascinating plastic explosive BC/FOX7-SBR performed better than the already in use EPX1 and SEMTEX10 and had less impact sensitivity.

Journal of Physics: Conference Series **2830** (2024) 012029 doi:10.1088/1742-6596/2830/1/012029

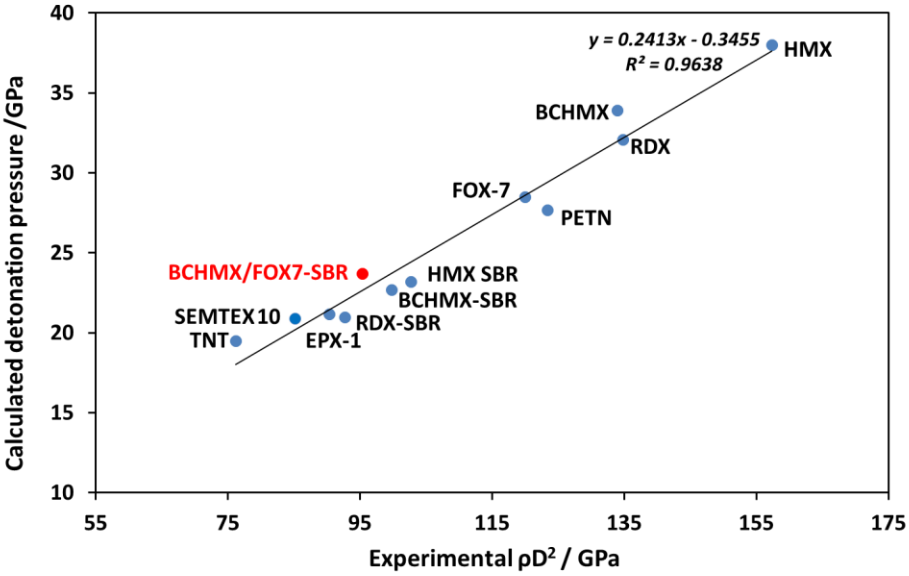

Figure 4. Relationship between the experimental detonation velocity squared times the loading density and the estimated detonation pressure.

4. Conclusion

The newly fabricated PBX based on FOX7/BC/SBR was found to exhibit the least sensitivities, either to impact or to friction, among the whole investigated samples. The studied nitramine explosives' impact and friction sensitivity have a semi-logarithmic connection that represents the significant influence of the presence of insensitive high explosive FOX7 and in application polymeric matrix SBR matrix on decreasing the sensitivity of BCHMX. The intriguing correlation between explosive sensitivity and its performance emphasizes the high performance of the new BC/FOX7-SBR PBX with reserving low sensitivity to impact compared with the in-service plastic explosives EPX1, SEMTEX10 and RDX-SBR. The BC/FOX7-SBR is considered a promising composition optimize between the high performance with low sensitivity which can be significantly be used in future applications.

Reference

[1] Klapötke T M 2015 Chemistry of high-energy materials, Walter de Gruyter GmbH & Co KG.

[2] Trzciński W, Cudziło S, Dyjak S and Nita M 2014, *Central European Journal of Energetic Materials,* **11**, 443.

[3] Licht H-H 2000 *Propellants Explosives, Pyrotechnics* **25** 126.

[4] Talawar, M 2015 *Journal of hazardous materials* **300** 307-321.

[5] Klasovity D *et al* 2010 *Czech Pat.* 302068.

[6] Mayseless, M. 2011 *Journal of Applied Mechanics* **78(5)** 051006.

[7] Weinheimer R 1992 *Properties of selected high explosives in: Proc. of the 18th Int. Pyrotechnics seminar* 13.

[8] Elshenawy T, Elbeih A and Li QM 2016, *Central European Journal of Energetic Materials* **13** 927.

[9] Elbeih A, Abd-Elghany M and Klapötke T M 2017 *Propellants, Explosives, Pyrotechnics* **42** 468.

[10] Suceska M 1995 *Test methods for Explosives* Springer Heideleberg.

[11] Finney D J 1971 *Probit analysis* Cambridge University **3**.

[12] Sućeska M 2001 *Int. Annual Conference of ICT, Karlsruhe, Germany* **32**.

[13] Simková L, Liska F and Ludvik J 2011 *Current Org. Chem.* **15** 2983.