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Application of *cis*-1,3,4,6-Tetranitrooctahydroimidazo-[4,5d] Imidazole (BCHMX) in EPX-1 Explosive

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ABSTRACT

cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5 d]imidazole (BCHMX) has been studied as explosive filler to replace pentaerythritol tetra-nitrate (PETN) inEPX1 explosive. BCHMX with different particle sizes was bonded by thermoplastic binder plasticised by dibutyl phthalate to obtain BCHMX-EPX. Heat of combustion was measured. Impact energy and friction force of initiation were determined. Velocity of detonation was measured, while the detonation characteristics were calculated by thermodynamic code named EXPLO 5. For comparison, the detonation characteristics of some commercial plastic explosives such asEPX-1, SEMTEX 10 and FORMEX P1were also studied. It was concluded that BCHMX-EPX has the highest detonation characteristics of all the studied plastic explosives and its sensitivity is in the same level of the studied traditional plastic explosives. BCHMX-EPX has the highest decomposition temperature of all the studied samples. The mutual relationship obtained from the experimental and calculated results indicates the compatibility of the calculated results with the experimental measurements.

Keywords: BCHMX, plastic explosives, sensitivity, DSC, detonation

1. INTRODUCTION

Several commercial plastic explosives are available and produced by different companies all over the world. Most of the commercially available plastic explosives are based on either RDX (1,3,5-trinitro-1,3,5-tiazinane) or PETN (penterythritoltetranitrate). Semtex 10 is a Czech plastic explosives while Formex P1 is a French plastic explosives, both are based on PETN as energetic filler bonded by different polymeric matrices, they have several applications in the demolition field, underwater explosion and boosters for large caliber warheads.The development in the plastic explosives is based on increasing the performance without significant effect on the cost of the final product. The applications of new highly energetic materials on the commercial available plastic explosives is a topic of interest to several scientists. A new bicyclic compound *cis*-1,3,4,6-Tetranitro-octahydroimidazo-[4,5-d]imidazole (bicyclo-HMX or BCHMX)[1,2] which had been prepared according to Czech patent[3] is attractive explosive. BCHMX has theoretical maximum density (TMD) of 1.86 $g.cm^{-3}$, calculated detonation velocity of 9050 m s^{-1}, detonation pressure of 37 GPa and explosion heat of 6.518 MJ[4] kg^{-1}. The practical studies of BCHMX have been published in several researches. BCHMX had been studied as an energetic filler bonded by C-4 matrix[5,6]. Plastic bonded explosives based on BCHMX and fluorinated binders have been studied[7-9]. Also replacement of PETN by BCHMX in SEMTEX10 has been investigated[10]. The performance and detonation characteristics of BCHMX has been studied and compared with different cyclic nitramines[11].

In this paper, a continuation of the study of BCHMX as explosive filler bonded by available polymeric matrix is presented. EPX-1 is a plastic explosive, based on PETN, produced by Heliopolis Company for Chemical Industries; Egypt[12]. Replacement of PETN by BCHMX in EPX-1 is presented in this study and designated as BCHMX-EPX. Sensitivity, thermal behaviour and detonation velocity of the prepared BCHMX-EPX is determined. The detonation characteristics were calculated using EXPLO5 thermodynamic code[13]. For comparison, the commercial available plastic explosives SEMTEX 10, FORMEX P1 in addition to EPX-1 were also studied.

2. EXPERIMENTAL

2.1 Preparation of BCHMX-EPX

BCHMX was prepared by two steps method according to Czech patent[3] in Military Technical College, Cairo, Egypt. It was recrystallised to obtain two grades (I, II) with meanparticle sizesof 24 µm and 250 µm, respectively. EPX-1 matrix, contains thermoplastic binder (styrene-butadiene rubber) obtained from Heliopolis Company for Chemical Industries, Egypt and plasticised by di-butyl phthalate obtained from Jai Enterprises, Delhi, India, was used to bond BCHMX and form

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BCHMX-EPX. The preparation process is based on direct mixing of BCHMX with the polymeric matrix in stainless steel vertical mixer. BCHMX 86 % wt. (58 % grade II and 28 % grade I) was mixed with the polymeric matrix 14 % wt. at 60 °C for 45 min. under vacuum. The addition of BCHMX to the polymeric matrix was done in three portions each after 15 min. The prepared sample was extruded to obtaincylinders with 21 mm diameter.

2.2 Sensitivity to Impact

A drop hammer test (Julius Peters[14]) was used to determine the impact sensitivity of the samples. The tested sample (50 mm^3) was placed between two pistons and a 2 kg weight was dropped. Probit analysis method[15] was applied to obtain the initiation probability. The impact energy was plotted against the initiation probability. On Table 1, the 50 per cent initiation probability has been reported as impact sensitivity.

Table 1. Formula and measured characteristics of the studied samples

No.	Explosive type	Formula	Mol. Weight ($g\cdot mol^{-1}$)	Heat of combustion ($J\cdot g^{-1}$)	Heat of formation ($kJ\cdot mol^{-1}$)	Impact sensitivity (J)	Friction sensitivity (N)
1	PETN[10]	$C_5H_8N_4O_{12}$	316.15	8182	-538.7	2.9	44
2	EPX-1[12]	$C_{7.88}H_{12.36}N_4O_{12.59}$	364.58	11528	-666.5	13.9	176
4	SEMTEX[10] 10	$C_{8.05}H_{12.64}N_4O_{12.37}$	363.38	11942	-646.8	15.7	204
5	FORMEX P1[18]	$C_{8.26}H_{13.98}N_4O_{11.85}$	358.93	12943	-613.2	13.5	194
6	BCHMX	$C_4H_6N_8O_8$	294.17	9124	236.5	3.2	88
7	BCHMX-EPX	$C_{6.48}H_{10.64}N_8O_{8.62}$	338.53	12366	108.3	15.3	236

2.3 Sensitivity to Friction

Friction sensitivity was determined using A BAM friction test apparatus by applying the standard test conditions[14]. The measurements were based on spreading of 0.01 g of the tested sampleover the porcelain plate as a thin layer. Different weights were added to create different forces between the pistil and the plate. Sound, smoke, or characteristic smell of gaseous products are indication forthe initiation of the tested sample. Probit analysis method[15] was applied to obtain the friction force required for the 50 per cent initiation probability. The results are reported in Table 1.

2.4 Heat of Combustion

Heat of combustion was measured by using Automatic Combustion Calorimeter MS10A. The measurement is based on placing the tested sample on a calorimetric bomb filled with oxygen[16]. Ignition of the sample causes an increase in the temperature of the surrounded water.The obtained measurement was reported in Table 1. The obtained measurementwas appliedto calculate the heat of formation of the plastic explosive in order to beused for the calculation of detonation parameters.

2.5 Thermal Analysis

Differential Scanning Calorimetry (DSC, Q2000, 2000-1334 instrument) was used to study the thermal behaviour and heat flow properties of the prepared sample. 2 mg of the plastic explosive was inserted in an Aluminum pan with a pin-hole cover, and heated by 5 °C min^{-1} heating rate under 0.1 MPa dynamic nitrogen atmosphere from 25 °C to 350 °C. For comparison, EPX-1 explosive and pure BCHMX were tested.Parameters obtained from DSC data was reported in Table 2.

2.6 Detonation Velocity Measurements

EXPLOMET-FO-2000 produced by KONTINITRO AG was used for measuring the detonation velocity. The tested sample was prepared in the form of cylindrical shape of 300 mm length and 21 mm diameter. Three optical fibers were placed in the sample where the first probe was placed at a distance of 100 mm from the face including the detonator. Each of the other two fibers was placed at a distance of 80 mm from the previous one. Detonator no. 8 was used to set off the charge. Three measurements were performed for the composition and the mean value(max. deviation ± 76 m s^{-1}) is reported in Table 3

Table 2. Parameters obtained from DSC data of BCHMX and its PBX compared with EPX-1 under the heating rate of 5.0 K min^{-1}

Samples	Endothermic peaks			Exothermic peaks		
	T_o (°C)	T_p (°C)	ΔH_1 ($J\ g^{-1}$)	T_o (°C)	T_p (°C)	ΔH_2 ($J\ g^{-1}$)
BCHMX	-	-	-	236.2	249.8	2816
BCHMX-EPX	-	-	-	226.7	242.1	2632
EPX-1	139.6	141.1	107.2	170.8	188.7	2507

Note: T_o: decomposition onset temperature; T_p: the max. peak temperature; T_e: onset temperature of the end decomposition; ΔH_1: heat absorption; ΔH_2: heat release.

2.7 Calculation of the detonation characteristics

EXPLO 5 thermodynamic code[13] was used to calculate the detonation characteristics (detonation velocity (D), heat of detonation (Q), detonation pressure (P)) of all the studied plastic explosives as well as the pure explosives. BKWS set of parameters for the BKW EOS was applied, these parameters are: $\alpha = 0.5$, $\beta = 0.298$, $\kappa = 10.50$, $\Theta = 6620$[10]. The calculated detonation characteristics of all the tested explosives are reported in Table 3.

3. RESULTS AND DISCUSSION

Impact and friction sensitivities of the prepared BCHMX-EPX were measured and compared with the other studied plastic explosives as well as the pure explosive fillers as shown in Fig. 1. It is clear from the figure that the impact sensitivities

Table 3. The calculated detonation characteristics of the studied explosives

Explosive type	Density ($g\cdot cm^{-3}$)	Detonation velocity measured ($m\cdot s^{-1}$)	EXPLO5			
			detonation velocity ($m\cdot s^{-1}$)	D_{calc}-D_{exp} D_{exp}/100 (%)	detonation pressure (GPa)	detonation Heat ($J\cdot g^{-1}$)
PETN[10]	1.70	8400	8350	-0.6	28.62	6258
EPX-1[12]	1.55	7636	7398	-3.1	21.17	5742
SEMTEX[10]	1.52	7486	7370	-1.5	20.89	5708
FORMEX P1[18]	1.53	7544	7346	-2.6	20.03	5411
BCHMX cryst.	1.79*	8650*	8755	+1.2	32.8	6433
BCHMX-EPX	1.59	7910	7861	-0.6	23.9	5874

*BCHMX was measured bonded by 3 per cent viton B[4]

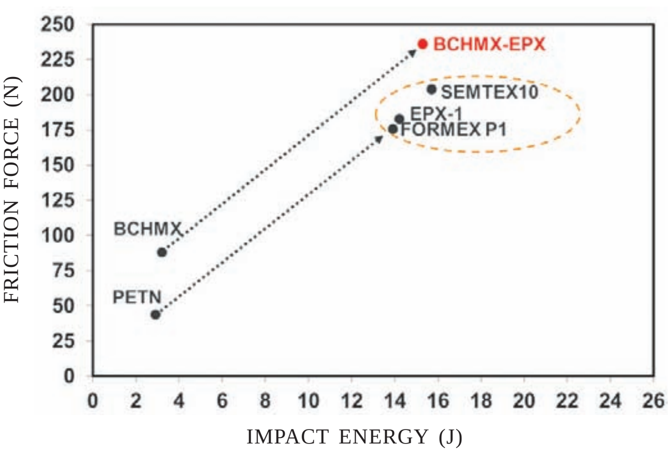

Figure 1. Comparison between the impact and friction sensitivities of all the studied samples.

of all the studied traditional plastic explosives (based on PETN) have close values in the range of 13.5 J to 16 J and the prepared BCHMX-EPX lies on the same range. While the friction sensitivity of BCHMX-EPX is lower than all the studied samples. The results are close to the prediction where the pure BCHMX has impact sensitivity on the same range of pure PETN; while it has lower friction sensitivity than PETN. The results also proved that replacement of PETN by BCHMX in EPX-1 explosive decreased its friction sensitivity without affecting the impact sensitivity.

Thermal study of the prepared BCHMX-EPX compared with EPX-1 explosive using DSC technique is presented in Fig. 2. It is clear from the figure that BCHMX-EPX has exothermic peak temperature higher than EPX-1.

The exothermic maximum peak temperature of BCHMX-EPX is 242 °C, which is higher than that of EPX-1 by 53 °C. Also BCHMX-EPX has lower exothermic peak than the pure BCHMX, which means that EPX polymeric matrix decreased the exothermic peak of pure BCHMX. This result might be attributed to the presence of polar plasticiser on EPX matrix, which acts as a solvent for BCHMX and decreased its thermal stability as reported by Elbeih[17], *et al*. The thermal behaviour parameters of the prepared PBX by the DSC studies are presented in Table 3. Endothermic peak was observed in EPX-1 at 139.6 °C due to the presence of PETN as explosive filler; while BCHMX and BCHMX-EPX have only one step exothermic peak.

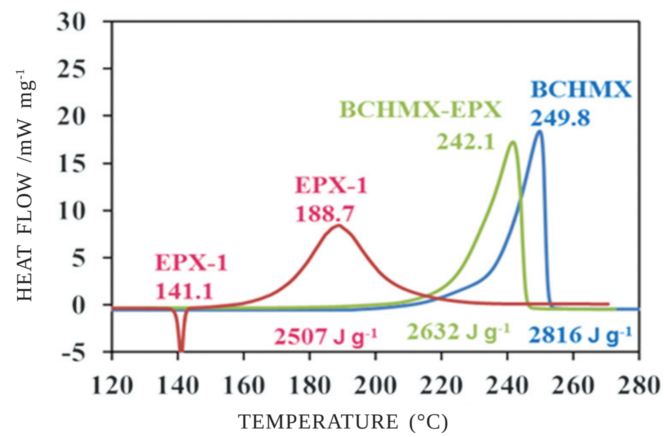

Figure 2. DSC curves for BCHMX and BCHMX-EPX.

The peak intensity of heat release of BCHMX has been decreased by the effect of EPX matrix. Also, in case of EPX-1, a wider overlapped peak was observed due to the greater interfacial interaction of PETN with EPX matrix. The EPX matrix could decrease the heat release of BCHMX. Besides, the heat released by BCHMX-EPX is higher than that of EPX-1 explosive.

Regarding to the performance of the prepared BCHMX-EPX compared with the other studied plastic explosives, the well-known dependence of detonation velocity on loading density is presented in Fig. 3. It is clear that BCHMX-EPX has the highest detonation velocity of all the studied plastic explosives. It has detonation velocity higher than EPX-1 by

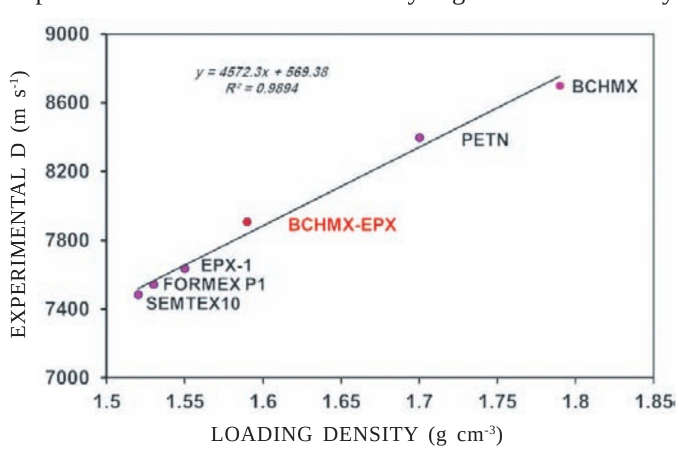

Figure 3. Relationship between the loading density and experimental detonation velocity of the studied samples.

more than 250 ms^{-1}. This result prove the high efficiency of BCHMX compared with PETN.

As a result of the difficulty to determine the detonation pressure of the studied samples experimentally, results of EXPLO5 thermodynamic code has been used and compared with the experimental measured data. According to the physics of explosion theories, the detonation pressures of explosives are correlated with the products of the square of the experimental detonation velocities and their loading densities. Here, a linear relationship was observed between the calculated detonation pressure and the experimental ρD^2 as shown in Fig. 4. The results confirms the compatibility of the calculated results with the experimental measurements. BCHMX-EPX has detonation pressure of 23.9 GPa which is the highest value of all the studied plastic explosives.

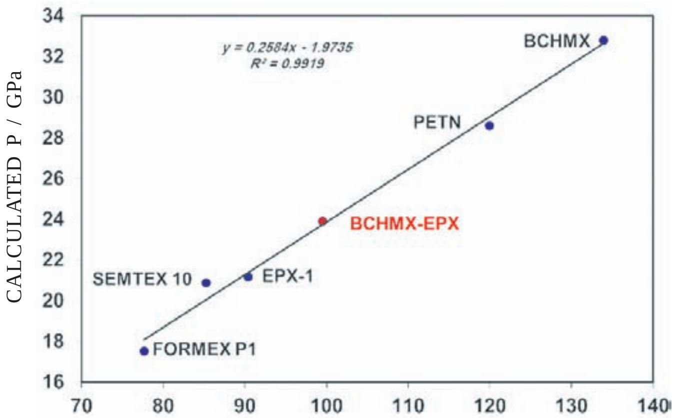

Figure 4. Relationship between the calculated detonation pressure and the experimental ρD^2 (ρ-loading density, D- experimental detonation velocity).

Another relationship between the calculated heat of detonation and the measured heat of combustion is presented in Fig. 5. An inverse proportional relationship between the heat of detonation and the heat of combustion of the studied samples was observed. These results confirm the prediction that the presence of the polymeric matrices with the explosives increase their heat of combustion and decrease their heat of detonation. Also the heat of detonation is based on the type of explosive as well as the polymeric matrix used. BCHMX-EPX has the highest heat of detonation of all the studied plastic explosives.

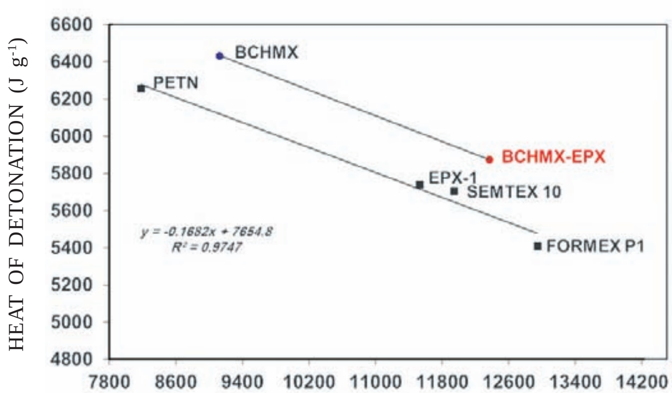

Figure 5. Relationship between the calculated heat of detonation and the measured heat of combustion of the studied samples.

4. CONCLUSION

From this study, it was concluded that BCHMX-EPX has impact sensitivity in the same range of the studied traditional plastic explosives, while its friction sensitivity is lower. BCHMX-EPX has higher thermal decomposition temperature compared with the original EPX-1 explosive. The presence of EPX matrix decreased the decomposition temperature of the pure BCHMX. BCHMX-EPX has the highest detonation parameters of all the studied plastic explosives. Several relationships has been studied and proved the good agreement of the calculated detonation parameters by EXPLO5 code with the measured parameters. BCHMX is therefore the candidate to replace PETN in traditional plastic explosives.

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In the current study, his contribution was studied the polymeric matrix used in the manuscript.