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cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) as a part of explosive mixtures

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ABSTRACT

cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) is a relatively available bicyclic nitramine in the present. Due to the high energetic content of its molecule (deformation of valence angles) it has heat of formation higher than β–1,3,5,7-tetranitro-1,3,5,7-tetrazocane (β–HMX) by nearly three times. As a result, it has heat of explosion and relative explosive strength exceed that of β–HMX including their corresponding PBXs. However, penetration abilities of PBXs based on HMX are higher than those based on BCHMX. The relatively high initiation reactivity of BCHMX could be modified in a wide range by its incorporation in a suitable polymeric matrices. Regarding to the performance, coating of BCHMX crystals by 5 wt% Viton A produces the maximum performance while the mixture of BCHMX with polydimethylsiloxane (PDMS) seems to be the optimum composition for the development of PBX with low sensitivity.

1. Introduction

In the eighties of the last century, a number of interesting nitramines specially technical attractive cyclic nitramines were synthesized, one of them is cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) [1–4]. Starting from very complicated syntheses [1], and also with intention to find a new route of the 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (HNIW) preparation, a group of Prof. Sysolyatin from Biysk at Siberia has developed the technological method for preparation of BCHMX with a good yield [4–7]; however, the corresponding results were reserved as a classified patent for a long time and the first short information in face of international audience was presented in 2005 (see quotations in Ref. [4]).

Independently from the Russian colleagues, roughly twenty years later, the same synthesis was developed at University of Pardubice in Czechia [6,7]. Then in the Institute of Energetic Materials at this University, activities were started in the research of possible applications of the BCHMX as a plastic bonded explosives (PBX) (see below). This paper deals with some interesting properties and characteristics of BCHMX and its PBXs.

2. Optimum method for BCHMX synthesis

A survey of synthesis of the interesting new nitramines is presented in Ref. [3]. Also synthesis of BCHMX is mentioned in Refs. [3,4] but the details about the procedure are protected by the open patents [5,7] and are documented by Schemes 1 and 2.

In the sense of Scheme 1, the mutual reaction of glyoxal, formaldehyde and potassium sulfamate is a nucleophilic addition, catalyzed by selected environment; due to the nature of the reactants it takes place in the polar solvent, preferably in an aqueous environment [4,5,7]. TACOS-K separates out as tetrahydrate [8]. The fact that this salt contains crystalline water, leads to its certain instability during lengthy storage due to hydrolytic processes [8]. During the heating of TACOS-K crystals, evaporation of water in the crystals tends to compete with this hydrolysis; the tetrahydrate of TACOS-K should not be produced for storage, even in normal conditions, and during drying process, there is some possibility of its exothermic decomposition [8].

Nitrolysis of TACOS-K realizes in the fuming nitric acid alone [5,7] or in presence of P_2O_5 [7], or N_2O_5 [5], acetic anhydride [5], sulfuric acid or oleum [7]. In addition, the presence of the linear urea-formaldehyde condensate in TACOS-K was tested [7]. Due to content of the 11 % wt. of water in the TASCOS-K crystals, yields of

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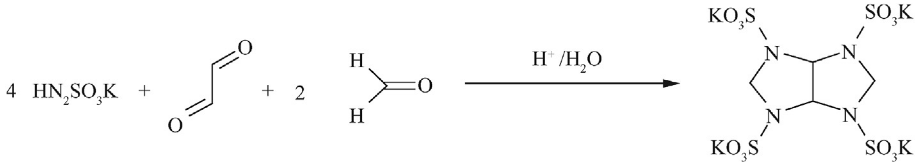
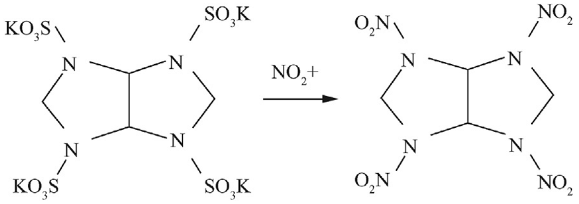


Scheme 1. Synthesis of tetrapotassium salt of octahydroimidazo-[4,5-d]imidazole-1,3,4,6-tetrasulfonic acid (TACOS-K).



Scheme 2. Nitrolysis of tetrapotassium salt of octahydroimidazo-[4,5-d]imidazole-1,3,4,6-tetrasulfonic acid to cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX).

BCHMX do not exceed of 70% toward theory (mostly about 60% of theory [4]).

3. Important properties of BCHMX and some explosive mixtures on its base

3.1. Properties of BCHMX

cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) was predictively considered as a more powerful explosive than β−1,3,5,7-tetranitro-1,3,5,7-tetrazocane (β−HMX) [2]. What is a reality?

As a result of the C2−C4 bond creation in case of BCHMX (see Fig. 1) from the skeleton of HMX (see Fig. 2), the deformation of the valence angles of the original HMX molecule is changed to form BCHMX molecules in a certain internal tension [6]. This tension is proved in higher energetic content of the BCHMX molecule in comparison with the HMX one (roughly three time higher heat of formation of BCHMX-see in Table 1). The mentioned skeleton deformation is visible on the angular conformation of the BCHMX molecule and relatively very long length of the N3−N7 bond while the other N−N bond lengths are comparable with those in the HMX molecule [6]. The longest N−N bond is a bearer of initiation reactivity of this nitramine [6] (see higher sensitivity data of BCHMX compared with HMX in Table 1). In the impact sensitivity, BCHMX is roughly in the same level of pentaerythritol tetranitrate (PETN) [9].

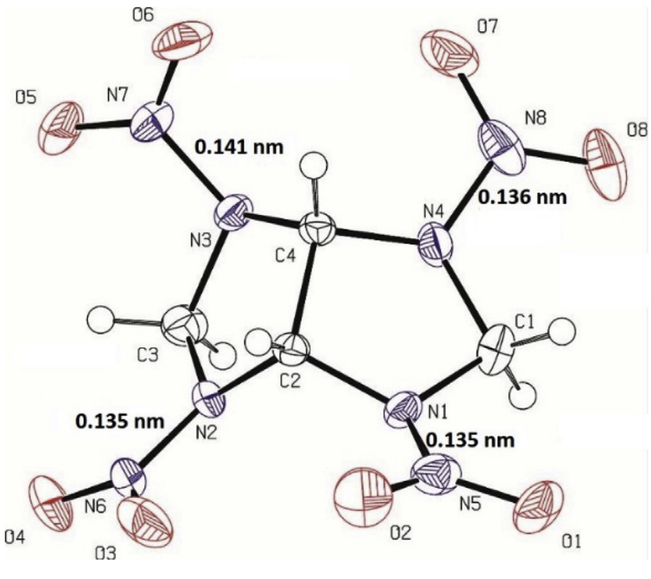


Fig. 1. cis-1,3,4,6-Tetranitrooctahydroimidazo- [4,5-d]imidazole (BCHMX).

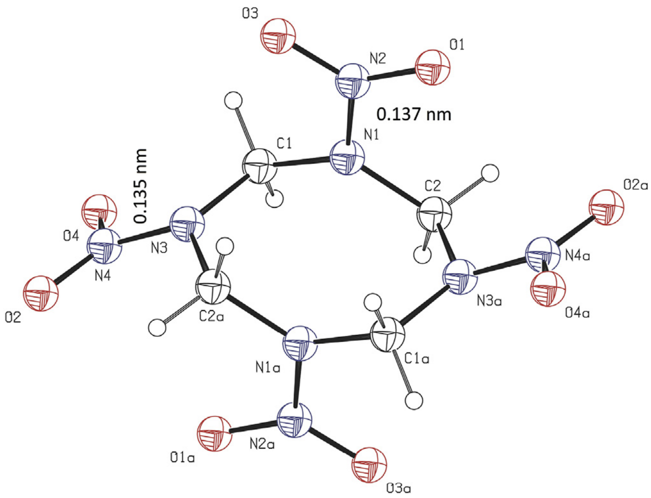


Fig. 2. β−1,3,5,7-tetranitro-1,3,5,7-tetrazocane (β−HMX).

Due to angular conformation and lower molecular symmetry, the BCHMX molecule cannot be as perfectly placed into crystal lattice, as in the case of HMX analogue, and its maximum theoretical density is thus lower in comparison with HMX. On the other hand, the maximum heat of explosion is higher (by 4.7%) compared to HMX, and that is due to the higher heat of formation of BCHMX. This difference is transferring into the explosion heats of their corresponding PBXs (see Fig. 3).

3.2. Properties of some explosives based on BCHMX

Already Qui and Xiao published a molecular dynamic study of the plastic bonded explosives (PBXs) containing BCHMX and polyfluorinated binders [12]. They claim that BCHMX is suitable for special plastic bonded explosives (PBXs) or applications in propellants [12]. Several of our publications presented the effect of different polymeric matrices on the performance of the BCHMX, such as polystyrene-butadiene rubber (SBR) [13], Viton A 200 [8,14,16], polydimethylsiloxane (PDMS) [10,17−19], acrylonitrile-butadiene rubber (NBR) [8,15,16], polyisobutylene (PIB) [8,17], poly-(methyl methacrylate) (PMMA) [8], TNT [19], GAP [21] and HTPB [22]. For comparison also PBXs with these binders were studied which were filled by 1,3,5-trinitro-1,3,5-triazinane (RDX), β-1,3,5,7-tetranitro-1,3,5,7-tetrazocane (β-HMX) and ε-2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (ε-HNIW). Regarding to the recent studies [9,10,18,19], it was concluded that the PDMS matrix considers one from the optimum

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