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Review

2,4,6-Triamino-1,3,5-trinitrobenzene (TATB) and TATB-based formulations—A review

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ABSTRACT

This paper reviews the research and development work on 2,4,6-triamino-1,3,5-trinitrobenzene (TATB), and TATB-based formulations of other explosives. Syntheses including the production of nano-sized particles, analytical methods, thermophysical properties, performance, formulations, toxicity and safety of TATB are reviewed in this work.

Contents

1. Introduction

There has been a renewed interest in the synthesis and characterization of new energetic materials during the past two to three decades. This is due in part to find materials of better performance, but also to reduce the loss of lives and property due to accidental explosions that could occur during the different stages of explosive preparation, manufacture, formulations, load assemble and package operations, and use. Information on thermophysical properties of energetic materials is essential for:

1. Military needs to minimize the collateral damage to all sites other than the targeted sites,
2. Determining the fate of these chemicals in the environment,
3. Detecting hidden explosives—extremely accurate data on vapor pressure are required for development of sensors,

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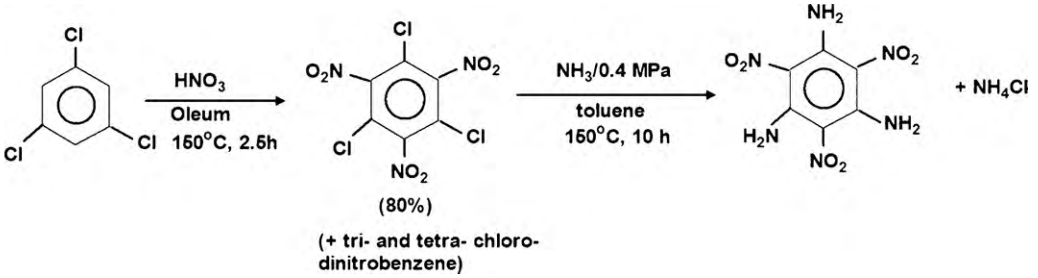

Fig. 1. Synthesis of TATB using 1,3,5-trichlorobenzene.
Reproduced from Ref. [5].

4. Proper disposal of these hazardous materials,
5. Preventing smuggling of these materials in their original form or as bombs, etc.,
6. Testing predictive methods associated with the testing and fielding of new energetic materials to minimize the cost and time associated with an experimental program. For example, the prediction of crystal density paves the way in predicting detonation velocities. Enthalpies of formation and sublimation are critical in assessing the potential energy release and performance in a gun or a warhead,
7. Developing models to predict accurately physicochemical properties. In the present collection of properties, it has become evident that models currently used to predict properties are far from satisfactory. Many examples can be cited, and
8. Studying syntheses pathways, reaction mechanisms and products, and exhaust plume signature, etc.

Among the various insensitive high explosives, 2,4,6-triamino-1,3,5-trinitrobenzene, commonly known as TATB, is an attractive insensitive explosive as it satisfies the safety requirements at high temperatures and its resistance to accidental initiation and explosion. In addition, it readily forms eutectics with other explosives such as 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX), trinitrotoluene (TNT), and several others. This paper should be viewed as a companion review to the excellent review by Dobratz [1]. TATB is perhaps the most thermo-resistant insensitive explosive known to date. Although TATB contains an amino group, it is much more stable compared to a nitro compound such as trinitrobenzene.

The potential of TATB as an insensitive explosive was realized during the 1960s. TATB is used in modern nuclear warheads in the military, deep oil well explorations in the civilian community, and as a reagent in the manufacture of liquid crystal displays. It is used extensively in the USA. In recent years it is the preferred conventional secondary high explosive in nuclear weapons [2].

Dobratz [1] cites Jackson and Wing as the earliest workers to mention TATB in 1888, although it was left to Flurscheim and Holmes [3] to synthesize pure TATB by ammoniation of pentanitroaniline. Many processes yield TATB with a small percentage of chlorine but recent attempts to make chlorine-free TATB have been documented. TATB exhibits both monoclinic and triclinic crystal structures and is classified as a heat resistant explosive.

2. Synthesis and manufacturing

The current industrial method is to nitrate 1,3,5-trichlorobenzene to give 2,4,6-trichloro-1,3,5-trinitrobenzene. Nitration is carried out at 423 K using a mixture of nitric and sulfuric acids. It is reacted with ammonia in a toluene medium to yield the product. Other methods of synthesis of TATB have been described in Ref. [1]. The current cost of TATB prohibits its use for civilian applications but new routes for its synthesis could reduce the cost of production. One such route is patented by Mitchell et al. [4] who used picramide as the starting material. Bellamy et al. [5] have described a new route starting with 1,3,5-trihydroxy benzene for the synthesis of TATB. Although the direct nitration of 1,3,5-trihydroxy benzene can be carried out, Bellamy et al. [5] have suggested a number of modifications. Some of these modifications are shown below.

The authors give details of the above syntheses methods, claim improved yields and report other starting materials. They also show the synthesis of TATB by vicarious nucleophilic substitution [VNS]. Pagoria et al. [6] claim considerable reduction in the cost of production of TATB based on the VNS Process. In this process, TATB is synthesized starting with 4-nitroaniline and converting it to trinitroaniline. Trinitroaniline is then converted to TATB using trimethylhydrazinium iodide in a mixture of dimethylsulfoxide and sodium methoxide. The inventors claim the cost of production to be less than $90/kg and a reduction of 40% in time.

Thiokol Corporation, Brigham City, Utah, has set up a pilot-plant for the production of TATB as described by Dressen et al. [7]. This process is based on the synthetic route proposed by Bellamy et al. [5]. The overall process yield was 81%. The syntheses routes are shown in Figs. 1 and 2. A similar synthesis method as shown in Fig. 3 was followed by researchers at Pantex, Amarillo, Texas, to reduce chlorine contamination. Aniline was used as a starting material to synthesize 1,3,5-trichlorobenzene by Urbansky and Vasudeva [8] in their attempts to synthesize TATB. TNT was the starting material for Atkins et al. [9] to form 2,3,4,5,6-pentanitroaniline using H_2S and NH_4OH, which was converted to TATB after adding NH_3, toluene, and CCl_4. High purity TATB was synthesized by Ott and Benzinger [10] by ammonolysis of 3,5-dichloro-2,4,6-trinitroanisole in toluene at room temperature.

Recently, Yang et al. [11], and Nie et al. [12] have prepared nanoparticles of TATB by amination of TCTNB [2,4,6-trichloro-1,3,5-trinitrobenzene] in toluene medium. The surface area of the particles was 22 m^2/g and the pore diameter was 1.7 nm. X-Ray Diffraction (XRD) patterns of nano- and micron-sized TATB are shown in Fig. 4. XRD studies showed that particles were about 60 nm in size. The size of these particles may be small for certain formulations, and by changing the experimental parameters it is possible to obtain larger particles. Nevertheless, nanoparticles would give higher surface energy and higher detonation energy.

Pagoria et al. [13] and Agrawal [14] provide excellent reviews of the synthesis of several energetic explosive materials. These two reviews complement one another in discussing the current state of knowledge in the synthesis of explosive and propellant materials. Shorky et al. [15] synthesized TATB starting with TNT in p-dioxane and reducing with hydrogen sulfide to give 4-amino-2,6-dinitrotoluene. It is then nitrated with a mixture of nitric and sulfuric acids to yield 2,3,4,5,6-pentanitrobenzenamine and reacted with ammonia in methylene chloride to give TATB. Mitchell et al. [16] describe the use of recycled explosives as starting materials for the synthesis of high value products. The authors have