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Abstract

The synthesis of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) from trichlorotrinitrobenzene (TCTNB) in toluene and ammonium hydroxide solution under the influence of ultrasonic waves was investigated. When the two-phase reaction mixture was irradiated with high intensity ultrasound at ambient temperature, fine-particle TATB (FP-TATB) was produced. This sonochemically produced TATB powder is lemon color in appearance and was analyzed to have the same explosive properties as reported in the literature.[1] That is, it is insensitive to impact stimuli, and thermally stable. The median particle diameter of FP-TATB was calculated to be around 14 μm, and the powder can be pressed to a density of 1.82 g/cm^3 without a binder. The amination process is simple and requires neither the monitoring of the ammonia gas pressure nor the controlling of the reaction temperature during amination reaction, and we anticipate no problem in large scale production of FP-TATB.

Introduction

TATB is an explosive with a high melting point and thermal stability and has been applied in situation where insensitivity to impact hazards is important. Other potential applications include the use of TATB as the booster or main charge explosives for down-hole oil perforation at elevated temperature surroundings. However, one major problem with the utility of TATB is the resistance to initiation as required. In the past, production grade TATB was prepared by amination of 1,3,5-trichloro-2,4,6-trinitrobenzene (TCTNB) in toluene with anhydrous ammonia gas in a pressurized reactor.[1] TATB thus produced has particle size of 30 micrometres or larger and is suitable for most applications. However, fine-grained TATB is desirable for ease of initiation. TATB powder with an arithmetic mean particle size about 10 micrometres has been produced by LLNL and Pantex that was qualified as an insensitive high explosive (IHE) according to DOE standards. Unfortunately, the processes involved in the production of such TATB (UF-TATB) were complicated and time-consuming.[2]

Ultrasound is sound of a frequency that is beyond human hearing, i.e. above 16 kHz. When ultrasound is applied to liquids of either a homogeneous or heterogeneous reaction system, acoustic cavitation results. That is, the formation, expansion and implosive collapse of microbubbles generated during the high frequency oscillation of liquid molecules. The local temperature and pressure induced during implosion could be as high as 5000 K and 1800 atm respectively, with cooling rates that could exceed 10^9 K /sec. Utrasound is also widely used for promoting dispersion of one liquid phase to another through emulsification. At Los Alamos, chemical reactions were carried out under the influence of ultrasound for both rate enhancement and milder reaction conditions.[3]

Recently, the production of nanostructured inorganic materials by ultrasonication was reported by Suslick and his coworkers.[4]

In this report, the preparation of fine-particle TATB (FP-TATB) from TCTNB in toluene and ammonium hydroxide solution under the influence of ultrasound will be described. Included also are the particle size distribution, and results from small scale snesitivity tests of FP-TATB.

Preparation of Fine-particle TATB (FP-TATB)

Sonication Equipment The ultrasonic liquid processor (Misonix XL2020) equipped with a 0.5-inch probe, operating at 20 kHz with a variable power-supply output was used for the preparation of FP-TATB. The power output was set at 60% of maximum 550 watts.

Procedure A solution of TCTNB in toluene was added to the ammonium hydroxide in a 300 ml beaker (Pyrex No. 1040). The amination reaction began by immersing the horn into the two-phase mixture and the power of the sonicator was turned on. After a reaction time of 40 minutes, the resulting emulsion was left overnight at ambient temperature. FP-TATB thus obtained was collected by fitration, followed by washing the solids sequentially with hot water, toluene and acetone. The solids were then dried at 96°C in a vacuum oven overnight.

Explosive Properties of FP-TATB

The ultrasonically produced FP-TATB powder is lemon color in appearance, and can be pressed to a density of 1.82 g/cm^3 without a binder. Samples of FP-TATB were submitted for small scale sensitivity tests and total inorganic chloride content. Results from these tests are tabulated in Table I. Particle size distribution of FP-TATB was determined by Microtrac analyzer, Figure 1.

Table I. Explosive Properties and Chloride Content of FP-TATB

DTA Exotherm (°C)	>350
Impact Sensitivity (type 12, cm)	>320
Total Inorganic Chloride (wt%)	0.070

It can been seen that FP-TATB is insensitive to impact stimuli and is thermally stable. Based on the particle size distribution, the mean particle diameter of FP-TATB was calculated to be about 14 micrometres.

Conclusion

A simple and efficient method for the production of fine-particle TATB from TCTNB and ammonium hydroxide by ultrasonication has been developed. The process requires no special reaction vessel and there is no need to monitor either the ammonia gas pressure or the amination temperature, and we anticipate no problem in large scale production of FP-TATB.

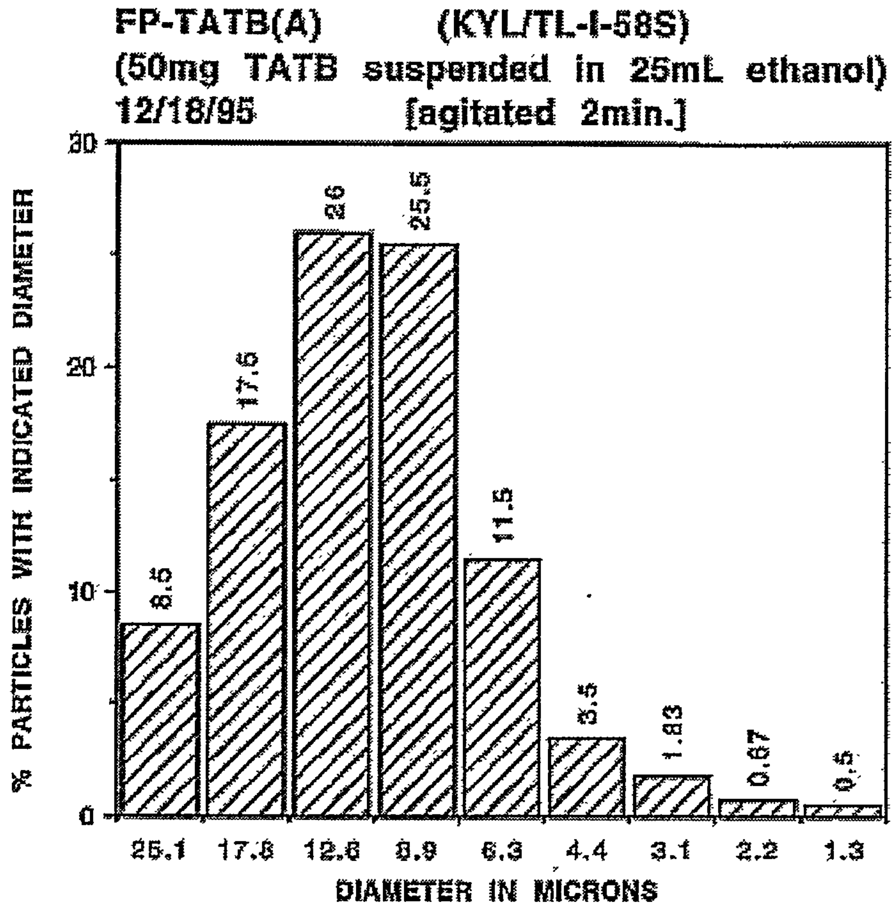

Fig. I Particle size distribution of FP-TATB

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References

1. B. M. Dobratz, "The Insensitive High Explosive Triaminotrinitrobenzene (TATB): Development and Characterization -- 1888 to 1994", Los Alamos National Laboratory, LA-13014-H, August, 1995.

2. R. Lee, et al.,"The Relationship Between the Shock Sensitivity and the Solid Pore Sizes of TATB Powders Pressed to Various Densities", Proc., Eighth Symposium (Intl.) on Detonation, pp 3-14, NSWC MP 86-194, Albuq., NM, July, 1985.

3. K.-Y. Lee, "Study of Chemical Reactions under the Influence of Ultrasound", Ultrasonics International 93 Conference Proceedings, pp 743-746, Vienna, 1993.

4. K. S. Suslick, et al.,"Sonochemical Synthesis of Nanostructured Catalysts", Mater. Sci. Eng., A204 (1-2), pp 186-92, 1995.