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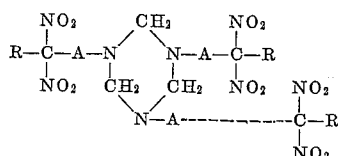
3,000,889

**TRIS N-ALKYLENEPOLYNITRO HEXAHYDRO  
S-TRIAZINES**

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16 Claims. (Cl. 260—248)

This invention relates to new compositions of matter and a method for their preparation. In particular this invention relates to 1,3,5-triazines having the general formula:

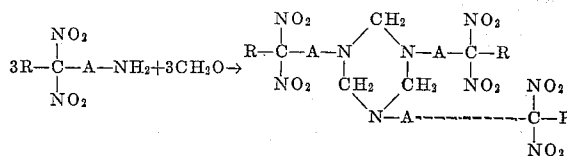


wherein A is an alkylene radical and R is a nitro or alkyl radical.

This application is a continuation in part of my co-pending United States patent application No. 408,608 filed February 5, 1954, now abandoned.

The compositions of this invention are useful as high explosives and can be used in any conventional explosive missile, projectile, rocket, or the like, as the main explosive charge. An example of such a missile is disclosed in United States Patent No. 2,470,162, issued May 17, 1949. One way of using the high explosives of this invention in a device such as that disclosed in United States Patent No. 2,470,162, is to pack the crystalline explosive in powder form into the warhead of the missile. Alternatively, the crystals can be first pelletized and then packed. A charge thus prepared is sufficiently insensitive to withstand the shock entailed in the ejection of a shell from a gun barrel or from a rocket launching tube under the pressure developed from ignition of a propellant charge, and can be caused to explode on operation of an impact- or time fuse-mechanism firing a detonating explosive such as lead azide or mercury fulminate.

The compounds of this invention are prepared by condensing a primary amine with formaldehyde, in accordance with the general reaction scheme set forth below:



wherein A is an alkylene radical and R is a nitro or alkyl radical.

The amines used as starting materials in this invention are prepared by reacting a strong mineral acid with a polynitro isocyanate, which may be prepared by reacting a polynitro acid halide with sodium azide, as disclosed in assignee's copending application No. 405,515, now abandoned, filed January 21, 1954.

To more fully illustrate this invention, the following examples are presented. It is to be understood, however, that these examples are presented merely as a means of illustration, and are not intended to limit the scope of the invention in any way.

**EXAMPLE 1**
**Preparation of 1,3,5-tris(3',3'-trinitropropyl)-hexahydro-1,3,5-triazine**

In a flask, fitted with a mechanical stirrer and dropping funnel, was placed 34.5 gm. (0.15 mole) of 3,3,3-trinitropropyl amine hydrochloride, 75 ml. of water, and 12.1

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gm. (0.15 mole) of sodium acetate in 50 ml. of water. A yellow solid was immediately precipitated, which was collected, washed with water, and dried, to give 30.7 gm. (99.4%) of product. The product exhibited an impact stability of 9 cm./2 kg. Recrystallization from a large volume of methanol gave yellow plates, M.P. 121–123° C. dec. The elemental analysis of the product is as follows:

Calculated for  $C_{12}H_{18}N_{12}O_{18}$ : Percent C, 23.31; percent H, 2.93; percent N, 27.19. Found: Percent C, 23.78; percent H, 2.88; percent N, 27.21.

The explosive power of the compound is as follows:

Lead block value 130\_\_\_\_\_ T.N.T.=100  
Ballistic mortar value 140\_\_\_\_\_ T.N.T.=100

**EXAMPLE II**
**Preparation of 1,3,5-tris(3',3'-dinitrobutyl)-hexahydro-1,3,5-triazine**

Twenty gm. (0.1 mole) of 3,3-dinitrobutylamine hydrochloride, 25 ml. of water, and 8.1 gm. (0.1 mole) of 37% formalin was placed in a 300 ml. 3-necked flask, fitted with a mechanical stirrer and dropping funnel. To this solution was added dropwise a solution of 8.2 gm. (0.1 mole) of sodium acetate in 15 ml. of water. A yellow solid was immediately precipitated. After the addition was complete, stirring was continued for an additional 30 minutes. The product was collected, washed with water, and dried; the yield was 17 gm. (97%). Two recrystallizations from ethyl acetate yielded a product having a M.P. of 131–132° C. (dec.), and an impact stability greater than 100 cm./2 kg. The elemental analysis of the product is as follows:

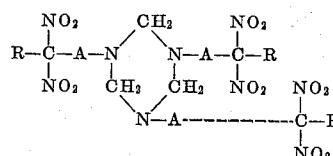
Calculated for  $C_{15}H_{27}N_9O_{12}$ : Percent C, 34.29; percent H, 5.18; percent N, 23.99. Found: Percent C, 34.76; percent H, 5.36; percent N, 24.62.

I have also found that related amines, namely, 4,4,4-trinitrobutyl amine, 3,3-dinitropentyl amine, and 4,4-dinitropentyl amine will also condense with formaldehyde to produce the corresponding triazines, namely, 1,3,5-tris(4',4',4'-trinitrobutyl)-hexahydro-1,3,5-triazine, 1,3,5-tris(3',3'-dinitropentyl)-hexahydro-1,3,5-triazine, and 1,3,5-tris(4',4'-dinitropentyl)-hexahydro-1,3,5-triazine.

From this it is apparent that any 1,3,5-triazine of this series can be prepared by merely condensing an appropriate nitro-containing amine with formaldehyde, in accordance with the teachings of this invention.

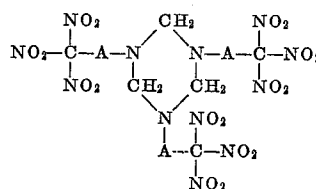
I claim:

1. As compositions of matter, the N-nitroalkyl-1,3,5-triazines having the formula:



wherein A is a lower alkylene radical and R is a radical selected from the group consisting of lower alkyl and nitro radicals.

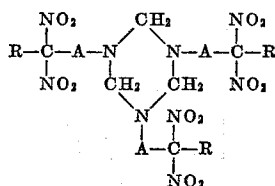
2. As compositions of matter, the N-nitroalkyl-1,3,5-triazines having the formula:



wherein A is a lower alkylene radical.

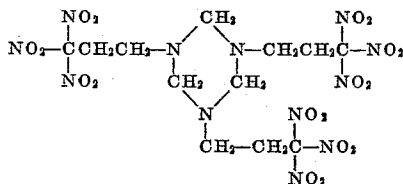
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3. As compositions of matter, the N-nitroalkyl-1,3,5-triazines having the formula:

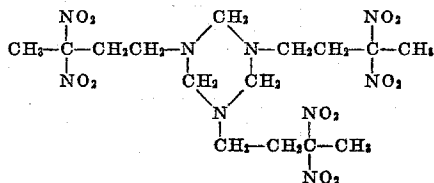


wherein A is a lower alkylene radical and R is a lower alkyl radical.

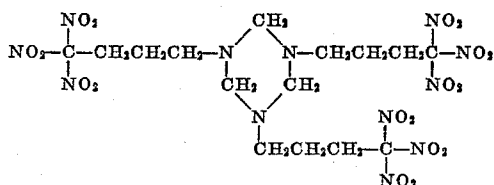
4. As a composition of matter, 1,3,5-tris(3',3',3'-trinitropropyl)-hexahydro-1,3,5-triazine, having the structural formula:



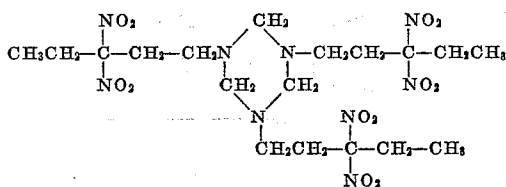
5. As a composition of matter, 1,3,5-tris(3',3'-dinitrobutyl)-hexahydro-1,3,5-triazine, having the structural formula:



6. As a composition of matter, 1,3,5-tris(4',4',4'-trinitropentyl)-hexahydro-1,3,5-triazine having the structural formula:



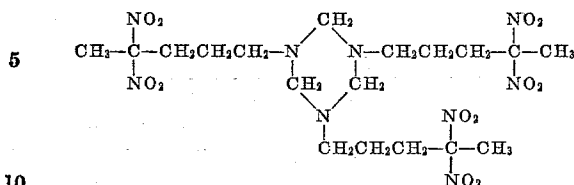
7. As a composition of matter, 1,3,5-tris(3',3'-dinitropentyl)-hexahydro-1,3,5-triazine, having the structural formula:



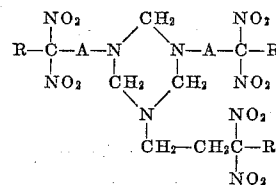
8. As a composition of matter, 1,3,5-tris(4',4'-di-

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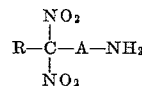
nitropentyl)-hexahydro-1,3,5-triazine, having the structural formula:



9. The method of preparing N-nitroalkyl-1,3,5-triazines having the formula:

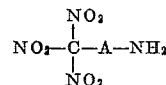


which comprises condensing formaldehyde with a nitro-containing amine having the formula:



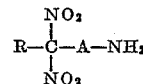
wherein A is a lower alkylene radical and R is a radical selected from the group consisting of lower alkyl and nitro radicals.

10. The method of preparing N-nitroalkyl-1,3,5-triazines which comprises condensing formaldehyde with an amine having the formula:



wherein A is a lower alkylene radical.

11. The method of preparing N-nitroalkyl-1,3,5-triazines which comprises condensing formaldehyde with an amine having the formula:



wherein R is a lower alkyl radical and A is a lower alkylene radical.

12. The method of preparing 1,3,5-tris(3',3',3'-trinitropropyl)-hexahydro-1,3,5-triazine, which comprises condensing 3,3,3-trinitropropyl amine with formaldehyde.

13. The method of preparing 1,3,5-tris(3',3'-dinitrobutyl)-hexahydro-1,3,5-triazine, which comprises condensing 3,3-dinitrobutyl amine with formaldehyde.

14. The method of preparing 1,3,5-tris(4',4',4'-trinitrobutyl)-hexahydro-1,3,5-triazine, which comprises condensing 4,4,4-trinitrobutyl amine with formaldehyde.

15. The method of preparing 1,3,5-tris(3',3'-dinitropentyl)-hexahydro-1,3,5-triazine, which comprises condensing 3,3-dinitropentyl amine with formaldehyde.

16. The method of preparing 1,3,5-tris(4',4'-dinitropentyl)-hexahydro-1,3,5-triazine, which comprises condensing 4,4-dinitropentyl amine with formaldehyde.

No references cited.