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## Synthesis of a new energy-intensive crystalline compound 3,6-bis(2,2,2-trinitroethylnitramino)-1,2,4,5-tetrazine

Anatoly G. Korepin, Galina V. Lagodzinskaya, Gennady V. Shilov,  
Natalya M. Glushakova, Vera P. Kosilko, Valentina S. Malygina,  
Vera P. Lodygina, David B. Lempert,\*<sup>+</sup> and Sergey M. Aldoshin

*Institute of Problems of Chemical Physics Russian Academy of Sciences.  
Acad. Semenov Ave., 1. Chernogolovka, 142432. Moscow Region. Russia.*

*Fax: +7 (496) 522-19-99. E-mail: lempert@icp.ac.ru*

\*Supervising author; <sup>+</sup>Corresponding author

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### Abstract

The process of nitration of 3,6-bis(2,2,2-trinitroethylamino)-1,2,4,5-tetrazine (C<sub>6</sub>H<sub>6</sub>N<sub>12</sub>O<sub>12</sub>, BTAT) was investigated. It was found that when a mixture of 99% nitric acid with trifluoroacetic anhydride was used as a nitrating agent, a new energetic compound 3,6-bis(2,2,2-trinitroethylnitramino)-1,2,4,5-tetrazine (C<sub>6</sub>H<sub>4</sub>N<sub>14</sub>O<sub>16</sub>, NBTAT) was formed. In the case of using only 99% nitric acid as a nitrating agent, the mono-*N*-nitro derivative 3-(2,2,2-Trinitroethylnitramino)-6-(2,2,2-trinitroethylamino)-1,2,4,5-tetrazine (MNBTAT) is formed, but it is readily denitrated. It was found that for a successful synthesis of NBTAT, the nitration of BTAT should be carried out in exactly two stages, first the reaction is carried out in 99% nitric acid, with the amount of the latter being greater than that required for the nitration of both amino groups in BTAT, after which trifluoroacetic anhydride should be added to the reaction mixture and then the nitration of the second amino group already proceeds. The synthesis of BTAT, MNBTAT and NBTAT are described in detail. The structure of NBTAT has been reliably confirmed by various physical methods (NMR, IR, X-ray diffraction). Interest in the study of the synthesis and properties of NBTAT is due to the fact that it can become a very effective oxidizer of solid composite propellants (SCP), since the combination of a high estimated (above 1000 kJ/kg) value of the standard enthalpy of formation, high density (1.94 g/cm<sup>3</sup>), and the oxygen coefficient  $\alpha$  equal to 1.14, makes it possible to create on its basis metal-free SCP-compositions with the specific impulse exceeding the compositions based on ammonium perchlorate, ammonium salt of dinitramide and to

reach the ballistic level of compositions based on hexanitrohexaazaisowurtzitane (CL-20), recently one of the most promising components for SCP.

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