

KINETIC AND THERMOCHEMICAL PROPERTIES OF TRINITROMETHYL DERIVATIVES OF 1,3,5-TRIAZINE

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Abstract: Thermochemical and kinetic properties of some 1,3,5-triazines containing trinitromethyl and azide substituents have been studied. The formation enthalpies of these compounds have been determined. The kinetics of thermal decomposition of 2,4-diazido-6-trinitromethyl-1,3,5-triazine and its derivatives has been described by the equation of the first order. The rate constants, activation energies, and preexponential factors of these reactions have been calculated. The dissociation energies of C–NO₂ have been found. The rate determining stage of the reactions is decomposition of trinitromethyl group. In nonisothermic conditions, thermal decomposition proceeds in two macroscopic stages. The first stage of the process is decomposition of trinitromethyl group. Energetic characteristics of 2,4-diazido-6-trinitromethyl-1,3,5-triazine as possible component of propellants have been estimated.

Keywords: energetic compounds; thermal decomposition; kinetics; nitrocompounds; azides; triazines; formation enthalpy

References

1. Stepanov, R. S., L. A. Kruglyakova, and A. M. Astakhov. 2007. Strukturno-kineticheskie zakonmernosti termoraspada gem-trinitrometilazolov v zhidkoy faze [Structural and kinetic regularities of thermal decomposition of gem-trinitromethylazoles in liquid phase]. *Zh. Obshch. Khimii* 77(11):1881–1886. (In Russian.)
2. Shastin, A. V., T. I. Godovikova, S. P. Golova, L. I. Khmel'nitskiy, and B. L. Korsunskiy. 1995. Reaktsii nukleofil'nogo zameshcheniya 2,4,6-tris(trinitrometil)-1,3,5-triazina. Vzaimodeystvie 2,4,6-tris(trinitrometil)-1,3,5-triazina so spirtami, diolami, ammiakom i vtorichnymi aminami [Reactions of nucleophilic substitution of 2,4,6-tris(trinitromethyl)-1,3,5-triazine. Interaction 2,4,6-tris(trinitromethyl)triazine with alcohols, diols, ammonia, and secondary amines]. *Khimiya Geterotsiklicheskih soedineniy* 5:674–678. (In Russian.)

3. Nedel'ko, V. V., A. V. Shastin, B. L. Korsunskiy, N. V. Chukanov, T. S. Larikova, and A. I. Kazakov. 2005. Sintez i termicheskoe razlozhenie 5,5'-bis(tetrazolil)amina [Synthesis and thermal decomposition of 5,5'-bis(tetrazolyl)amine]. *Izv. AN. Ser. Khim.* 7:1660–1664. (In Russian.)
4. Shastin, A. V., T. I. Godovikova, and B. L. Korsunskiy. 2011. Novyy metod polucheniya 2,4-diazido-6-trinitrometil-1,3,5-triazina [Novel method of preparation of 2,4-diazido-6-trinitromethyl-1,3,5-triazine]. *Izv. RAN. Ser. Khim.* 6:1194–1196. (In Russian.)
5. Inozemtsev, Ya. O., A. B. Vorobjov, A. V. Inozemtsev, and Yu. N. Matyushin. 2014. Kalorimetriya energoemkikh soedineniy [Calorimetry of energetic materials]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 7:260–270.
6. Kon'kova, T. S., Yu. N. Matyushin, E. A. Miroshnichenko, and A. B. Vorobjov. 2009. Termohimicheskie svoystva dinitrazovoy kisloty [Thermochemical properties of hydrogen dinitramide]. *Izv. RAN. Ser. Khim.* 10:1958–1965.
7. Manelis, G. B., G. M. Nazin, Yu. I. Rubtsov, and V. A. Strunin. 1996. *Termicheskoe razlozhenie i gorenje vzryvchatykh veshchestv i porokhov* [Thermal decomposition and combustion of explosives and powders]. Moscow: Nauka. 223 p.
8. Trusov, B. G. 2002. Program system TERRA for simulation phase and thermal chemical equilibrium. *14th Symposium (International) on Chemical Thermodynamics Proceedings*. St. Petersburg, Russia. 483–484.

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