

THERMAL DECOMPOSITION OF CYANURIC TRIAZIDE

V. V. Nedelko¹, B. L. Korsunskiy^{1,2,3}, T. S. Larikova¹, S. V. Chapyshev¹,
N. V. Chukanov¹, and Y. Shu⁴

¹Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation

²N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

³National Research Nuclear University MEPhI, 31 Kashirskoye Sh., Moscow 115409, Russian Federation

⁴Xi'an Modern Chemistry Research Institute, Xi'an, Shanxi, China

Abstract: Thermal decomposition of cyanuric triazide in melt and in dinonyl phthalate solution has been studied by means of thermogravimetry, manometry, mass spectrometry, and infrared spectroscopy. Kinetic and activation parameters of the processes have been determined. Nitrogen is the only gaseous product of the reaction. This fact as well as the structure of the condensed residue after cyanuric triazide thermal decomposition in melt indicate elimination of nitrogen molecules from azide groups at the initial stage of reaction followed by subsequent reactions resulting in the formation of flat networks with polyconjugated bonds between C and N atoms. For thermal decomposition of cyanuric triazide in solution, preexponential factor of $10^{12.8} \text{ s}^{-1}$ and activation energy of 34100 cal/mol have been found. These values are typical for thermal decomposition of the majority of organic azides. Anomalously high values of effective activation parameters for the reaction in melt (accordingly, $10^{17.4} \text{ s}^{-1}$ and 42300 cal/mol), are explained in frames of the mechanism of polymerization (polycondensation) with formation of two-dimensional networks in the rate-determining stage. The conclusion is drawn that high impact sensitivity of cyanuric triazide has the kinetic nature.

Keywords: cyanuric triazide; thermal decomposition; kinetics; sensitivity

Acknowledgments

The work was supported by the Russian Foundation for Basic Research, project No. 15-53-53004 GFEN a.

References

1. Finger, H. 1907. Uber Abkommlinge des Cyanurs. *Z. prakt. Chem.* 75:103–104.
2. Keßenich, E., T. Klapotke, and J. Knizek. 1998. Characterization, crystal structure of 2,4-Bis(triphenylphosphanimino)tetrazolo[5,1-a]-[1,3,5]triazine, and improved crystal structure of 2,4,6-Triazido-1,3,5-triazine. *Eur. J. Inorg. Chem.* 12:2013–2016.
3. Andreev, K. K. 1966. *Termicheskoe razlozhenie i gorenje vzryvchatykh veshchestv* [Thermal decomposition and combustion of explosives]. Moscow: Nauka. 346 p. (In Russian.)

4. Gal'perin, L. N., Ju. R. Kolesov, and N. A. Zelenov. 1981. Avtomaticheskie vesy s magnitoelektricheskim kompensatorom [Automatic thermobalance with magnitoelectric compensator]. *Izmeritel'naya Tekhnika* 4:23–27. (In Russian.)
5. Gillan, E. 2000. Synthesis of nitrogen-rich carbon nitride networks from an energetic molecular azide precursor. *Chem. Mater.* 12:3906–3912.
6. Nedelko, V. V., N. V. Chukanov, A. V. Raevskii, B. L. Korsunskii, T. S. Larikova, O. I. Kolesova, and F. Volk. 2000. Comparative investigation of thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane (CL-20). *Propell. Explos. Pyrot.* 25(5):255–259.
7. 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 ditetrazol-5-ilamina [Synthesis and thermal decomposition of ditetrazol-5-ylamine]. *Izvestiya RAN. Ser. Khimicheskaya* 7:1660–1664. (In Russian.)
8. Dyll, L. K., and J. E. Kemp. 1968. Neighbouring-group participation in pyrolysis of arylazides. *Chem. Soc. B* 9:976–979.
9. Dyll, L. K. 1975. Pyrolysis of aryl azides. III. Steric and electronic effects upon reaction rate. *Aust. J. Chem.* 28(10):2147–2159.
10. Stepanov, R. S., L. A. Krugljakova, and E. S. Buka. 1986. Kinetika termicheskogo razlozheniya zameshchennykh alkil- i arilazidov [Kinetics of thermal decomposition for substituted alkyl and aryl azides]. *Kinetika i Kataliz* 27(2):479–482. (In Russian.)
11. Nedel'ko, V. V., B. L. Korsunskii, T. S. Larikova, Yu. M. Mikhaylov, S. V. Chapyshev, and N. V. Chukanov. 2011. The thermal decomposition of azidopyridines. *Russ. J. Phys. Chem. B* 5(2):244–249.
12. Walker, P., and W. A. Waters. 1962. Pyrolysis of organic azides: A mechanistic study. *J. Chem. Soc.* 5:1632–1638.
13. Afanas'ev, G. T., and V. K. Bobolev. 1968. *Initsirovanie tverdykh vzryvchatykh veshchestv udarom* [Initiation of solid explosives by impact]. Moscow: Nauka. 172 p. (In Russian.)
14. Dubovik, A. V. 2011. *Chuvstvitel'nost' tverdykh vzryvchatykh sistem k udaru* [Sensitivity of solid explosives to impact]. Moscow: RHTU im. D. I. Mendeleeva. 276 p. (In Russian.)
15. Bagal, L. I. 1975. *Khimiya i tekhnologiya initsiruyushchikh vzryvchatykh veshchestv* [Chemistry and technology of initiating explosives]. Moscow: Nauka. 456 p. (In Russian.)
16. Dubihin, V. V., V. G. Matveev, and G. M. Nazin. 1995. Termicheskoe razlozhenie 2,4,6-trinitrotoluola v rasplave i rastvorakh [Thermal decomposition of 2,4,6-trinitrotoluene in melt and solution]. *Izvestiya RAN. Ser. Khimicheskaya* 2:266–270. (In Russian.)
17. Burov, Ju. M., G. B. Manelis, and G. M. Nazin. 1985. Termicheskii raspad 1,3,5,7-tetranitro-1,3,5,7-tetrazaciklooktana v tverdom sostoyanii [Thermal decomposition of 1,3,5,7-tetranitrooctahydro-1,3,5,7-tetrazacine in solid state]. *Khim. Fizika* 4(7):956–962. [In Russian.]
18. Dubovik, A. V., and M. V. Lisanov. 1985. Raschet kriticheskikh parametrov initsirovaniya tverdykh VV udarom na kopre [The calculation of critical parameters of initiation for solid explosives by impact on impact testing machine]. *Fizika Goenija i Vzryva* 21(4):87–93. (In Russian.)

Received November 17, 2015

Contributors

Nedelko Vadim V. (b. 1943) — Doctor of Science in chemistry, leading research scientist, Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation; vnedelko@icp.ac.ru

Korsunskiy Boris L. (b. 1936) — Doctor of Science in chemistry, chief research scientist, N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; leading research scientist, Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation; professor, National Research Nuclear University MEPhI, 31 Kashirskoe Sh., Moscow 115409, Russian Federation; kors@polymer.chph.ras.ru

Larikova Tatiana S. (b. 1947) — research scientist, Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation; vnedelko@icp.ac.ru

Chapyshev Sergey V. (b. 1958) — Doctor of Science in chemistry, chief research scientist, Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation; chap@icp.ac.ru

Chukanov Nikita V. (b. 1953) — Doctor of Science in physics and mathematics, head of laboratory, Institute of Problems of Chemical Physics, Russian Academy of Sciences, 1 Acad. Semenov Av., Chernogolovka, Moscow Region 142432, Russian Federation; chukanov@icp.ac.ru

Shu Yuanjie (b. 1969) — Doctor of Science in chemistry, chief research scientist, Xi'an Modern Chemistry Research Institute, Xi'an, Shanxi, China; 1204172675@qq.com