

COMBUSTION MECHANISM AND THERMAL DECOMPOSITION OF 4,9-BIS(TRINITROMETHYL)-1,2,4-TRIAZOLO[3,4-d]-1,2,4-TRIAZOLO[3,4-f]-FURAZANO[3,4-b]PYRAZINE

V. P. Sinditskii¹, T. H. Hoang², and A. B. Sheremetev²

¹D. Mendeleev University of Chemical Technology of Russia, 9 Miusskaya Sq., Moscow 125047, Russian Federation

²N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prosp., Moscow 119991, Russian Federation

Abstract: Combustion mechanism and thermal decomposition of 4,9-bis(trinitromethyl)-1,2,4-triazolo[3,4-d]-1,2,4-triazolo[3,4-f]-furazano[3,4-b]pyrazine, which may have potential use as explosive and propellant ingredient, have been studied. Analysis of the gaseous and condensed decomposition products of the studied compound showed that the trinitromethyl groups are decomposed at the initial stage. At temperatures of 100–120 °C, the decomposition stops at intermediate formation of anhydride of carboxylic acid. Thermocouple-aided measurements allowed to determine the vapor pressure and the vaporization heat. In spite of the high combustion temperature, combustion of the tested compound has been shown to obey the mechanism with the leading reaction in the condensed phase, which is due to the high rates of heat release in the molten phase.

Keywords: combustion; thermal decomposition; 4,9-bis(trinitromethyl)-1,2,4-triazolo[3,4-d]-1,2,4-triazolo[3,4-f]-furazano[3,4-b]pyrazine

Acknowledgments

This work was supported by the Russian Science Foundation (grant No. 14-13-01153).

References

1. Kettner, M. A., and T. M. Klapötke. 2017. Synthesis of new oxidizers for potential use in chemical rocket propulsion. *Chemical rocket propulsion*. Eds. L. De Luca, T. Shimada, V. P. Sinditskii, and M. Calabro. Springer Inter. Publishing. 63–88.
2. Fogelzang, A. E., V. Ya. Ajemyan, and B. S. Svetlov. 1977. Issledovanie goreniya svintsovykh soley nitrakarbonovykh kislot i nitroparafinov [Study of combustion of lead salts of nitrocarboxylic acids and nitroparaffins]. *Dokl. Akad. Nauk SSSR* 236(3):688–691.
3. Atwood, A. I., T. L. Boggs, P. O. Curran, T. P. Parr, D. Hanson-Parr, C. F. Price, and J. Wiknich. 1999. Burning rate of solid propellant ingredients. Part 1: Pressure and initial temperature effects. *J. Propul. Power* 15(6): 740–747.
4. Sinditskii, V. P., V. V. Serushkin, S. A. Filatov, and V. Yu. Egorshv. 2002. Flame structure of hydrazinium nitroformate. *Combustion of energetic materials*. Eds. K. Kuo and L. DeLuca. New York, NY: Begell House Inc. 576–586.
5. Khisamutdinov, G. K., V. L. Korolev, T. N. Parkhomenko, V. M. Sharonova, I. Sh. Abdurakhmanov, S. P. Smirnov, and B. I. Ugrak. 1993. Synthesis and properties of 1,2,4-triazolo[4,3-d]-1,2,4-triazolo[3,4-f]furazano[3,4-b]pyrazines. *B. Russ. Acad. Sci. Ch.* 42(10):1700–1702. doi: 10.1007/BF00697044.
6. Sheremetev, A. B., V. L. Korolev, A. A. Potemkin, N. S. Aleksandrova, N. V. Palysaeva, T. H. Hoang, V. P. Sinditskii, and K. Yu. Suponitsky. 2016. Oxygen-rich 1,2,4-triazolo[3,4-d]-1,2,4-triazolo[3,4-f]furazano[3,4-b]pyrazines as energetic materials. *Asian J. Org. Chem.* 5(11):1388–1397.
7. Stepanov, R. S., L. A. Kruglyakova, and A. M. Astakhov. 2007. Structural and kinetic regularities of the thermal decomposition of gem-trinitromethylazoles in the liquid phase. *Russ J. Gen. Chem.* 77(11):1933–1938.
8. Zel'dovich, Ya. B. 1942. Teoriya goreniya porokhov i vzryvchatykh veshchestv [Theory of combustion of powders and explosives]. *Zh. Eksp. Teor. Fiz.* 12(11-12):498–524.

Received December 29, 2016

Contributors

Sinditskii Valeriy P. (b. 1954) — Doctor of Science in chemistry, professor, dean, Institute of Chemical Technology and Engineering, D. Mendeleev University of Chemical Technology of Russia, 9 Miusskaya Sq., Moscow 125047, Russian Federation; vps@rctu.ru

Hoang Trung Huu (b. 1985) — Ph.D. student, D. Mendeleev University of Chemical Technology of Russia, 9 Miusskaya Sq., 125047 Moscow, Russian Federation; hoanghuu264@gmail.com

Sheremetev Alexey B. (b. 1958) — Doctor of Science in chemistry, leading research scientist, N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninskiy Prosp., Moscow 119991, Russian Federation; sab@ioc.ac.ru