## **ENERGETIC PROPERTIES OF DERIVATIVES OF 1,2,4-TRIAZOLE**

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**Abstract:** Energies of combustion of dinitropyrazole, modelling and energy-intensive derivatives of 1,2,4-triazole have been measured by the method of bombing calorimetry. On the basis of experimental data, the enthalpies of formation of the specified compounds in a standard condition have been determined. The obtained data along with available data in the literature allowed the values of contributions of 1,2,4-triazole and functional groups in the enthalpy of formation of compounds to be calculated. In the literature, there are publications in which synthesis of salt structures on the basis of 1,2,4-triazole is described, their enthalpies of formation and explosive characteristics are calculated. In authors' opinion, for some compounds, the resulted enthalpies of formation are considerably overestimated that has led to appreciable exaggeration of the explosive properties. Using the determined contributions for the same salt compounds, the enthalpies of formation have been calculated and based on the obtained values, their explosive characteristics have been estimated. The obtained results are compared with the data from the literature.

**Keywords:** calorimetry; combustion enthalpy; enthalpy of formation; derivative of 1,2,4-triazole; explosive characteristics

**DOI:** 10.30826/CE18110410

## Acknowledgments

This work was supported by the subsidy given to N. N. Semenov Institute of Chemical Physics of the Russian Academy of Sciences to implement the state assignment on the topic 44.8 (theme 0082-2014-0012, registration No. AAAA-A17-117040610346-5, theme 0082-2018-0004, registration No. AAAA-A18-118031590088-8, and theme 0082-2018-0002, registration No. AAAA-A18-118031490034-6).

## References

- 1. Fraunhofer Institut Chemische Technologie. 2004. The ICT-Datebase of thermochemical values and the ICT-thermodynamic code. Pfinztal, Berghausen.
- 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.
- Kon'kova, T.S., Yu. N. Matyushin, E.A. Miroshnichenko, and A. B. Vorob'ev. 2009. The thermochemical properties of dinitramidic acid salts. *Russ. Chem. B.* 58(10):1–8.
- Cox, J. D., D. D. Wagman, and V.A. Medvedev, eds. 1989. CODATA key values for thermodynamics. New York, Washington, Philadelphia, London. Final Report of the CODATA Task Group on Key Values for Thermodynamics.
- Hermann, T., T. M. Klapötke, B. Krumm, and J. Stierstorfer. 2016. Highly energetic 3-trinitromethyl-5-nitramino-1H-1,2,4-triazole — synthesis and investigation. 19th Seminar on New Trends in Research of Energetic Materials Proceedings. Pardubice: University of Pardubice. 2:583–590.

- Klapötke, T. M., P. C. Schmid, and J. Stierstorfer. 2016. Investigation on the energetic performance and thermal stability of N-bonded nitramines. *19th Seminar on New Trends in Research of Energetic Materials Proceedings*. Pardubice: University of Pardubice. 2:635–641.
- Klapötke, T. M., T. G. Witkowski, Z. Wilk, and J. Hadzik. 2016. Investigation of initiating of detonators containing TKX-50, MAD-XI, PETNC, DAAF, RDX, HMX or PETN as a base charge. *19th Seminar on New Trends in Research of Energetic Materials Proceedings*. Pardubice: University of Pardubice. 2:642–656.
- Fischer, N., D. Fischer, and T. M. Klapötke. 2012. Pushing the limits of energetic materials — the synthesis and characterization of dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate. *J. Mater. Chem.* 22:20418–20422.
- Konkova, T. S., J. N. Matjushin, E. A. Miroshnichenko, A. F. Asachenko, and P. B. Dzhevakov. 2016. Thermochemical properties TKX-50 (Dihidroxylammonium-5,5-bistetrazole-1,1-diolate). 47th Annual Conference (International) of ICT. Karlsruhe, Germany. 90/1–90/8.
- Kamlet, M. J., and S. J. Jacobs. 1968. Chemistry of detonation. I. A simple method for calculating detonation properties of C-H-N-O explosives. *J. Chem. Phys.* 48:23–35.

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- 11. Makhov, M. N., and V. I. Arkhipov. 1989. Velocity of shell dispersion. *Combust. Explo. Shock Waves* 25:343–345.
- 12. Orlenko, L. P. ed. 2002. *Fizika vzryva* [Physics of explosion]. 3rd ed. Moscow: Fizmatlit. Vol. 1. 832 p.
- Makhov, M. N. 2001. Explosion heat and metal acceleration ability of high explosives. *32nd Annual Conference* (*International*) of *ICT Proceedings*. Pfinztal, Germany. 1/97–11/97.

Received November 12, 2018

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