THERMOCHEMICAL PROPERTIES OF N-DIAZOMOSTIC NITROAZOLES

T. S. Kon'kova, Yu. N. Matyushin, E. A. Miroshnichenko, A. B. Vorob'ev, J. O. Inozemtsev, and A. V. Inozemtsev

N. N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

Abstract: Thermochemical characteristics of polyazyrogenous compounds based on pyrazole and triazole containing explozophore nitro- and azo groups have been experimentally determined. Recent studies have demonstrated the high efficiency of designing energy-intensive compounds based on nitrogen-containing heterocycles. The energies of combustion were determined using bomb calorimetry and standard enthalpies of formation (ΔH_f°) for these high-nitrogen substances were calculated. The enthalpy of formation serves as a direct measure of a performance of a compound's energy content; a reliable ΔH_f° value is crusial for accurately assessing the performance characteristics and application prospects of any energy intensive compound.

Keywords: bomb calorimeter; calorimetry; combustion enthalpy; formation enthalpy; nitropyrazoles; nitrotriazoles

DOI: 10.30826/CE26190113 **EDN:** VNZVAW

Figure Caption

Investigated compounds

Table Captions

Table 1 Combustion energies of nitro derivatives of (1H-pyrazole-1-yl)diazene

Table 2 Thermochemical characteristics in the standard state for the studied compounds (I–III)

Acknowledgments

The work was carried out within the framework of the Fundamental Scientific Research Program of the Russian Federation "Chemical Physics of Oxidation, Combustion, and Explosion," registration No. 1024040200065-4, and had budgetary funding.

References

1. Shevelev, S. A., and I. L. Dalinger. 1998. Recent progress in the chemistry of nitropyrazoles. *Russ. J. Org. Chem.* 34(8):1065–1074.
2. Zaitsev, A. A., I. L. Dalinger, and S. A. Shevelev. 2009. Dinitropyrazoles. *Russ. Chem. Rev.* 78(7):593–629.
3. Yin, P., D. A. Parrish, and J. M. Shreeve. 2014. N-diazo–ridged nitroazoles: Catenated nitrogen-atom chains compatible with nitro functionalities. *Chem. — Eur. J.* 20:1–7. doi: 10.1002/chem.201402762.
4. Inozemtsev, Ya. O., A. B. Vorob'ev, A. V. Inozemtsev, and Yu. N. Matyushin. 2014. Kalorimetriya energoemkikh soedineniy [Calorimetry of energetic materials]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* (7): 260–270.
5. Kon'kova, T. S., Yu. N. Matyushin, E. A. Miroshnichenko, and A. B. Vorob'ev. 2009. Thermochemical properties of dinitramidic acid salts. *Russ. Chem. B.* 58(10):2020–2027.
6. Coxm J. D., D. D. Wagman, and V. A. Medvedev, eds.1989. *CODATA key values for thermodynamics. Final Report of the CODATA Task Group on Key Values for Thermodynamics*. New York, Washington, Philadelphia, London: Hemispere Publising Corp. 284 p.
7. Lebedev, V. P., Yu. N. Matyushin, and Ya. O. Inozemtcev. 1998. Thermochemical and explosiv propeties of nitropyrazoles. *Energetic Materials: 29th Annual Conference (International) of ICT*. Karlsruhe: Fraunhofer — ICT. 181–183.
8. Miroshnichenko, E. A., V. P. Lebedev, A. B. Vorob'ev, V. P. Vorob'eva, and Ya. O. Inozemtcev. 2003. Entalpy characteristics of nitro- and fluorinenitro derivatives heterocyclic compounds. *Energetic Materials. 34th Annual Conference (International) of ICT*. Karlsruhe: Fraunhofer — ICT. 122(1)–122(7).
9. Stull, D. R., E. F. Westrum, and G. C. Sinke. 1969. *The chemical thermodynamics of organic compounds.* New York, London, Sydney, Toronto: John Wiley & Sons, Inc. 882 p.

Received October 30, 2025
After revision November 10, 2025
Accepted November 24, 2025

Contributors

Kon'kova Tatiana S. (b. 1941) — Doctor of Science in chemistry, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; taskon@mail.ru

Matyushin Yuriy N. (b. 1940) — Doctor of Science in technology, head of laboratory, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; ynm07@mail.ru

Miroshnichenko Evgeniy A. (b. 1938) — Doctor of Science in chemistry, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; eamir@mail.ru

Vorob'ev Alexey B. (b. 1946) — Candidate of Science in technology, senior research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; vectr1@yandex.ru

Inozemtsev Jaroslav O. (b. 1966) — senior research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; vectr1@yandex.ru

Inozemtsev Alexey V. (b. 1976) — research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; vectr1@yandex.ru