THE FORMATION ENTHALPIES AND RADICALS REORGANIZATION OF AZIDO-CONTAINING COMPOUNDS

E. A. Miroshnichenko[1], Yu. N. Matyushin[1], T. S. Kon'kova[1], Y. D. Orlov[2], A. B. Vorob'ev[1], V. P. Vorobeva[1], and J. O. Inozemtsev[1]

[1]N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation
[2]Tver State University, 33 Zhelyabova Str., Tver 170100, Russian Federation

Abstract: Standard formation enthalpies of some azido-containing compounds in standard state and in gas phase are determined. The bond dissociation energies C–N are determined. Using fundamental equations of chemical physics, the calculation scheme of energies of reorganization of molecule fragments into radicals by a method of "double difference" is suggested. The new calculation method is proposed to determine the energies of reorganization of molecule fragment N_3 into radical $N_3^{\bullet}$.

Keywords: enthalpies of formation and vaporization; "double difference" calculation method; radical; reorganization energy; bond energy

References

1. Inozemtsev, Ya. O., A. B. Vorobjov, A. V. Inozemtsev, and Yu. N. Matyushin. 2014. Calorimetriya enrgoemkikh soedineniy [Calorimetry of energetic materials]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 7:260–270.
2. Kon'kova, T. S., E. A. Miroshnichenko, Yu. N. Matyushin, A. B. Vorob'ev, J. O. Inozemtsev, I. L. Dalinger, T. K. Shkineva, and S. A. Shevelev. 2015. Energii soleobrazovaniya geterotsiklicheskikh soedineniy [Energies of salt formation for heterocycles]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 8(2):175–185.
3. Kon'kova, T. S., Yu. N. Matyushin, E. A. Miroshnichenko, and A. B. Vorob'ev. 2016. Termokhimicheskie svoystva soley shchelochnykh metallov trinitrofloroglyutsina. [Thermochemical properties of alkaline salts of 2.4.6-trinitrophloroglucinol]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 9(2):136–145.
4. 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.
5. Semenov, N. N. 1958. *O nekotorykh problemakh khimicheskoy kinetiki i reaktsionnoy sposobnosti* [On some problems of chemical rinetics and reactiviti]. Moscow: Izd-vo AN SSSR. 686 p.
6. Miroshnichenko, E. A., L. L. Pashchenko, T. S. Kon'kova, Yu. N. Matyushin, and A. A. Berlin. 2016. The enthalpies of formation and reorganization of aromatic radicals]. *Russ. Chem. Bull.* 65(8):1977–1980.
7. Pedley, J. B., R. D. Nailor, and C. P. Kirby. 1986. Termochemical data of organic compounds. London – New York: Chapman and Hall. 792 p.
8. Orlov, Y. D., Y. A. Lebedev, and I. S. Saifullin. 2001. *Termokhimiya organicheskikh svobodnykh radikalov* [Thermochemistry of organic free radicals]. Moscow: Nauka. 304 p.
9. Luo, Y. 2007. *Comprehensive handbook of chemical bond energies*. Boca Raton – London – New York: CRC Press. 1655 p.

Received January 10, 2017

Contributors

Miroshnichenko Eugeny A. (b. 1938) — 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; eamir02@mail.ru

Matyushin Yury N. (b. 1940) — Doctor of Science in technology, head of laboratory, N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; professor, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; ynm@polymer.chph.ras.ru

Kon'kova Tatiana S. (b. 1941) — 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; taskon@mail.ru

Orlov Yury D. (b. 1953) — Doctor of Sciense in chemistry, professor, head of department, Department of General Physics, Tver State University, 33 Zhelyabova Str., Tver 170100, Russian Federation; yurij.orlov@tversu.ru

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

Vorobeva Vera P. (b. 1946) — Candidate of Science in chemistry, senior research scientist, N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

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