

# ENERGIES OF CHEMICAL BONDS AND REORGANIZATION OF FREE RADICALS

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**Abstract:** Based on fundamental definitions of chemical physics, the design procedure of energies of chemical bonds and energies of reorganization of fragments of molecules into radicals after unimolecular radical reaction of molecules decomposition has been suggested. Energies of reorganization and energies of chemical bonds for different compounds of composition CaHbOcNd, including polyyradicals, have been determined.

**Keywords:** energy of bond; radical; energy of radical reorganization

## References

1. Semenov, N. N. 1958. *O nekotorykh problemakh khimicheskoy kinetiki i reaktsionnoy sposobnosti* [On some problems of chemical kinetics and reactivity]. Moscow: Izd-vo AN SSSR. 686 p. (In Russian.)
2. Miroshnichenko, E. A., T. S. Kon'kova, Yu. N. Matyushin, and A. A. Berlin. 2014. Entalpiya obrazovaniya 3-metilfurazanila-4 radikala [Formation enthalpy of 3-methylfurazane-4 radical]. *Dokl. Akad. Nauk* 456(6):673–675. (In Russian.)
3. Cox, J. D., D. D. Wagman, and V. A. Medvedev, eds. 1989. CODATA key values for Values for Thermodynamics. New York, Washington, Philadelphia, London.
4. Pedley, J. B. 1994. *Thermochemical data and structures of organic compounds*. Vol. 1. Texas, USA: Thermodynamic Research Center. College Station. 209 p.
5. Orlov, Y. D., Y. A. Lebedev, and I. S. Saifullin. 2001. *Termokhimiya organicheskikh svobodnykh radikalov* [Thermochemistry of organic free radicals]. Moscow: Nauka. 304 p. (In Russian.)
6. Luo, Y. 2007. *Comprehensive handbook of chemical bond energies*. Boca Raton – London – New York: CRC Press. 1655 p.
7. Nazin, G. M., and G. B. Manelis. 1994. Termicheskoe razlozhenie aliphaticeskikh nitrosoedineniy [Thermal decomposition of alifatic nitrocompounds]. *Uspekhi Khimii* 63(4):327–337. (In Russian.)

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