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Thermodynamic properties of nitroalkanes and there radicals

© Eugeny A. Miroshnichenko,*+ **Tatiana S. Kon'kova**,
Yury N. Matyushin, **Yaroslav O. Inozemtsev** and **Vera P. Vorob'eva**
N.N. Semenov Institute of Chemical Physics. Russian Academy of Sciences.
Kosygin St., 4. Moscow, 119991. Russia. Fax: +7 (495) 137-82-97. E-mail: eamir02@mail.ru

*Supervising author; +Corresponding author

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Abstract

On the basis of experimental measurements and literature data, enthalpies of combustion and formation of a series of nitroalkanes in the standard state in the gas phase have been recommended. The technique of calculating the bond dissociation energies of nitroalkanes on the basis of the experimental values of enthalpies of atomization energies and non-valence interactions of nitro groups have been proposed. The calculated values of dissociation energies of C-NO_2 were compared with data on the kinetics of thermal decomposition. It is also proposed to calculate bond dissociation energies of C-NO_2 in nitroalkyl radicals on the basis of the enthalpies of atomization and non-valence interactions energies of nitro groups. Change patterns of the bond dissociation energies of C-NO_2, CC, and CH in nitroalkanes, and their radicals have been defined.