THERMODYNAMIC STUDY OF SOME AZIDONITROCOMPOUNDS. ENERGIES OF REORGANIZATION OF RADICALS

Pashchenko L.L.,[1] ***Miroshnichenko E.A.****[2]

[1]*MSU, Moscow, Russia,* [2]*ICP RAS, Moscow, Russia*

**eamir02@mail.ru*

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Pashchenko L.L., Miroshnichenko E.A. Lomonosov Moscow State University, Leninskie Gory 1-3, 119991, Russia Semenov Institute of Chemical Physics RAS, Kosygin str. 4, Moscow, 119991, Russia

Azidonitro containing compounds are important industrial chemicals with a broad range of applications. This class of compounds is widely used in the synthesis of many diverse products. Some compounds are highly explosive. To investigate the stability and performance of these chemicals, knowledge of the enthalpy of formation is an essential requirement. Other thermo chemical properties, such as enthalpies of vaporization and energies of reorganization of azido-radicals are needed for the characterization of the chemical degradation pathways of their compounds. Despite the extensive studies of azidonitro containing compounds, available thermo chemical experimental information is often scarce and frequently shows significant discrepancy among published results. In this work the enthalpies of formation and vaporization of five azidonitro containing compounds are determined, Using experimentally obtained values, the standard enthalpies of formation in gas phase are calculated. The bond dissociation energies are calculated. Using fundamental equations of the chemical physics, the calculation scheme of the energies of reorganization of molecules fragments into radicals is offered. The new calculation method is offered to determine the energies of reorganization of molecule fragment into radical and the energies of reorganization of nitroazidoaromatic radicals. Reorganization energies of azido radicals and bond dissociation energies are calculated. The new calculation method for determination of the energy of reorganization of azido radical gives a way to calculate (kJ mol-1): the enthalpy of formation of radicals, bond dissociation energy median thermo chemical bond energies. Reorganization energies of radicals are calculated, which is near to energy of reorganization of acetylene radicals. Bond dissociation energies for calculation process of reorganization energy of azidonitro radicals are obtained from the enthalpies of formation of compounds and literature data. Obtained ours data of reorganization energies of azidonitroradicals and bond dissociation energies are needed for energy calculations of the kinetics of the reactions involving azidonitro containing compounds.