THE RATE OF EXPANSION AND THE CHEMICAL COMPOSITION OF THE DECOMPOSITION PRODUCTS OF HETEROCYCLIC COMPOUNDS BASED ON 1,2,4,5-TETRAZINES

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To evaluate the properties of energy materials, it is customary to focus on a set of data on thermal stability, friction and impact sensitivity, caloric content of chemical reactions in various reaction modes, and calculated characteristics obtained by classical thermodynamic methods. This approach has proven to be relatively safe and does not require a large amount of resources during screening, both for synthesizing large amounts of a substance and for performing complex calculations. However, in most cases, these data are not sufficient to select a particular material, for example, for use in vehicle airbags. Therefore, there is a need to develop and develop additional experimental methods that make it possible to determine the average mass characteristics of the gas phase of the decomposition products and the velocity of movement of the gas phase using as little substance as possible.

This paper shows the application of the methodology developed at RFNC – VNIITF for determining the mass expansion rate of gaseous products of chemical reactions [1, 2] when screening the properties of polyazot compounds based on the heterocyclic base 1,2,4,5-tetrazine. Gaseous products were formed as a result of the decomposition of energy materials at high-intensity impacts from 0.2 to 2000 K/s. The weight of the sample varied from 2 to 5 mg. In addition, chemical composition analysis was performed simultaneously, as well as energy diagrams of processes and diagrams of particle movement after decomposition of 1,2,4,5-tetrazine derivatives.

The conducted studies show a direct relationship between the rate of expansion of chemical reaction products and the molecular structure of the compounds under study, which indicates a significant contribution of catalytic effects that accelerate the processes of chemical interaction between components, both in the solid and in the gas phase. It was found that the content of nitro groups leads to a decrease in the formation of dicyanate (C_2N_2) and hydrocyanic acid (HCN) [3], increases the average mass velocity of the products of decomposition reactions and the role of the chemical potential in the general thermodynamic equation [4].

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