MOLECULAR DYNAMICS SIMULATION OF THERMAL DECOMPOSITION OF ORGANIC SUBSTANCES

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Abstract: Molecular dynamics simulation of the thermal decomposition of organic compound was performed using the example of a molecule containing a triazine ring under constant volume conditions with an instantaneous rise in temperature up to 4000 K. Possible decomposition mechanisms described in the literature and the results of simulation were compared with the available data on the growth and decrease of molecules from experimental and theoretical studies. The combination of decomposition products has been studied to determine the kinetic mechanism of fast-flowing reactions based on existing decomposition models. The relative content of molecules that make up the main share in the system after reaching equilibrium of the main decomposition products of the investigated organic substances is presented.

Keywords: molecular dynamics simulation; thermal decomposition; decomposition products; 1,3,5-trinitro-1,3,5-triazacyclohexane

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