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Hexanitrohexaazaisowurtzitane – sorption of solvent vapors. Comparison with crystalline energy components-cyclic nitramines, benzotrifuroxane, ammonium perchlorate

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Abstract

The article presents experimental results of determining the sorption characteristics of hexanitrohexa-azaisowurtzitane and other crystalline energy components of vapors of a number of solvents of different classes. The following cyclic nitramines were used as sorbents: hexanitrohexaazaisowurtzitane (HNIW), octogen (NMX), gexogen (RDX), bicycle-octogen (BCO), as well as benzotrifuroxane (BTF) and ammonium perchlorate (PA). Most of the solvents form stable or unstable co-crystallisates with HNIW and contain complexing groups: carbonyl, ether, sulfoxide, nitrile, etc. The list of solvents includes a number of compounds used as solvents and precipitators in the crystallization of HNIW and other nitramines, BTF and PA: acetone, dimethylacetamide, dimethylsulfoxide, dimethylformamide, 1,4-dioxane, tetrahydrofuran, cyclohexanone, ethyl acetate, *N*-methylpyrrolidone, acetonitrile, ethyl alcohol, water, hexane, *o*-, *p*-, *m*-xylenes, toluene. Experimental conditions: a closed volume that ensures the realization of the pressure of saturated solvent vapors at a temperature of 23-25 °C.

Three types of sorption kinetics have been established for the sorbents and solvents under consideration (monotonically increasing dependences over the sorption time from 500 to 5000 hours): with saturation and formation of co-crystallites HNIW/solvent; without saturation and with formation of the liquid phase – a solution of crystalline components with their partial or complete dissolution; without saturation and formation of the liquid phase.

It is shown (with some exceptions that require additional research) that the necessary conditions for the sorption of the considered crystalline components of solvent

vapors are nominal signs – the formation of sorbent/solvent co-crystallites (for HNIW, NMX, RDX, BCO, BTF) or molecular complexes in solutions (for BTF and PA). In the preliminary grouping of solvents by the type of complexing groups, a linear relationship between the rate of sorption of solvent vapors by nitramines and the pressure of saturated solvent vapors is shown. There is no correlation of the sorption capacity and sorption rate of HNIW, HMX, RDX, BCO, BTF solvent vapors with their other properties: permittivity, dipole moment, relative donor and acceptor numbers, solubility, etc. The results of IR spectroscopy and thermal analysis of the obtained samples of materials are discussed, and the results of electron scanning microscopy of changes in the structure of the surface and in the volume of crystals of energy components during the sorption of solvent vapors are presented. Two new BCO co-crystallites with solvents were obtained.

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