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Physicochemical and detonation properties of powerful explosive nitrates and their exploding action upon various barriers VLADIMIR GOLUBEV, THOMAS KLAPÖTKE, Ludwig-Maximilian University of Munich — The results on physicochemical and detonation properties for six powerful explosive nitrates such as aminotetrazolium nitrate (AT-NO_3), diaminotetrazolium nitrate (DAT-NO_3), diaminouronium nitrate (DAU-NO_3), 1-amino-3-nitro-guanidinium nitrate (ANQ-NO_3), oxalylhydrazinium nitrate (OHN) and oxalylhydrazinium dinitrate (OHDN) are presented in the paper. Physicochemical properties of these nitrates were determined with the use of methods of X-ray diffraction, nuclear magnetic resonance, mass spectrometry, infrared spectroscopy, differential scanning calorimetry. Sensitivities to impact, friction and electrostatic discharge were determined too. All possible quantum-chemical properties of molecules and mechanisms of their decomposition were calculated using the Gaussian 09 program. Detonation properties of explosive nitrates and equations of state of detonation products in the form of Jones-Wilkins-Lee were calculated using the EXPLO5 V.6.02 program. Calculations were fulfilled for explosive materials having the maximum crystalline density and for porous and having small additions of a polymeric binder ones. Comparative calculations on determination of exploding action of examined nitrates upon barriers, plates and shells of various materials were conducted using the ANSYS Autodyn 15.0 program in plain, cylindrical and spherical statements. For comparison all similar results were obtained also for such well-known explosives as RDX and HMX.

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