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Ab Initio MD Computation of the Vibrational Relaxation Time in HE Molecules. ALEXANDER SELEZENEV, ALEXEI ALEINIKOV, RFNC - VNIIEF — Ab Initio MD simulation has been used to compute equilibrium time for the intramolecular vibrational degrees of freedom in molecules of TNT, RDX, HMX and PETN. Computation of intramolecular forces field was done utilizing the code "Gaussian" with HF/STO-3G method. Ab Initio MD simulations have been carried out for the decomposition of TNT and RDX molecules as they collide. For the kinetic energy of molecular collisions, its threshold values have been found where decomposition of the molecules should occur before the equilibrium distribution of collision energy into vibrational degrees of freedom.

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