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Thermal Decomposition of TATB at Extreme Conditions RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — Detailed description of chemical reaction mechanisms of solid energetic materials at high-pressure and temperatures is essential for understanding events that occur at the reactive front of these materials and the subsequent building of predictive models of materials properties. We report the results of two ab initio based molecular dynamic simulation of the chemistry of TATB, at density of 2.9 g/cm^3 and temperature of 1500K, and at density of 2.87 g/cm^3 and temperature of 2500 K. The molecular forces are determined using the self-consistent-charge, density-functional - based tight-binding method. Following the dynamics for a time scale of up to forty picoseconds allows the construction of approximate rate laws for typical products such as H_2O, N_2, CO, and CO_2. The reaction rates of these products will be compared to those obtained previously for HMX at similar conditions. This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

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