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Simulations of Chemical Reactivity of Insensitive Energetic Materials Under Thermal and Shock Conditions[1] RIAD MANAA, LLNL, EVAN REED, Stanford University, LAURENCE FRIED, NIR GOLDMAN, LLNL — Results of quantum based simulations of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) crystals under thermal decomposition (high density and temperature) and shock compression conditions are presented. We conducted constant volume-temperature simulations, ranging from 0.35 to 2 nanoseconds, at ρ= 2.87 g/cm^{3}atT= 3500, 3000, 2500, and 1500 K, and ρ= 2.9 g/cm^{3}and 2.72 g/cm^3, at T = 3000 K. We also simulated crystal TATB's reactivity under steady overdriven shock compression at shock speeds of 8, 9, and 10 km/s for up to 0.43 ns duration. These simulations have enabled us to track the reactivity of TATB well into the formation of several stable gas products, such as H_2O, N_2, and CO_2. Our simulations revealed a hitherto unidentified region of high concentrations of nitrogen-rich heterocyclic clusters in reacting TATB, whose persistence impede further reactivity towards final products of fluid N_2 and solid carbon. Our simulations also predict significant populations of charged species such as NCO^-, H^+, OH-, H_3O^+, and O^{-2}, the first such observation in a reacting explosive. A reduced four steps, global reaction mechanism with Arrhenius kinetic rates for the decomposition of TATB, along with comparative thermo-chemical decomposition kinetics has been constructed and will be discussed.

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