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Decomposition reactions in RDX at elevated temperatures and pressures[1] IGOR SCHWEIGERT, US Naval Research Laboratory — Mechanisms and rates of elementary reactions controlling condensed-phase decomposition of RDX under elevated temperatures (up to 2000 K) and pressures (up to a few GPa) are not known. Global decomposition kinetics in RDX below 700 K has been measured; however, the observed global pathways result from complex manifolds of elementary reactions and are likely to be altered by elevated temperatures. Elevated pressures can further affect the condensed-phase kinetics and compete with elevated temperatures in promoting some elementary reactions and suppressing others. This presentation will describe density functional theory (DFT) based molecular dynamics simulations of crystalline and molten RDX aimed to delineate the effects of elevated temperatures and pressures on the mechanism of initial dissociation and the resulting secondary reactions.

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