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Systematic study of the explosive chemical kinetics of derivatives of ETN and PETN at low pressure MARC CAWKWELL, ROMAIN PERRIOT, VIRGINIA MANNER, Los Alamos National Laboratory — The time-to-explosion of energetic materials as a function of temperature and pressure should follow Arrhenius kinetics. We have computed the activation energy and volume of a series of derivatives of erythritol tetranitrate (ETN) and pentaerythritol tetranitrate (PETN) to identify how modifications to the underlying chemistry affect sensitivity to explosion. The recently developed *lanl*31 DFTB parameterization for organic materials was used to perform long-duration reactive molecular dynamics simulations of the derivatives. The simulations were performed in the microcanonical ensemble, which allows the time at which exothermic runaway occurs to be identified clearly. Multiple simulations were performed for each initial temperature and pressure to obtain representative statistics of the time-to-explosion. The effective activation energies and volumes that are obtained from the temperature and pressure dependence of the time-to-explosion are not chemically specific but instead represent the full set of reaction paths that occur prior to exothermic runaway in hot, condensed phase explosives. We compare the computed activation enthalpies to the results of experimental measurements of the relative sensitivities of the derivatives.

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