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Molecular Dynamics Simulations of the First Reactions in Nitrate Ester-based Explosives MARC CAWKWELL, ED KOBER, THOMAS MYERS, VIRGINIA MANNER, Los Alamos National Laboratory — In order to better understand and manipulate explosive sensitivity, we have prepared and analyzed a series of pentaerythritol tetranitrate-based explosives with systematic changes to the molecular structure. Reactive, extended Lagrangian Born-Oppenheimer molecular dynamics simulations have been performed on this series of molecules in the condensed phase to understand how the reactivity changes with the molecular modifications. The net reactions occurring over the first few hundred picoseconds under conditions of static high temperature and shock compression have been identified by an innovative analysis of coordination geometry changes and reaction types rather than attempting to detail each individual reaction. The evolution of temperature and pressure owing to evolving chemistry in the shock compressed materials were also captured accurately. Changes in exothermicity and the populations of intermediate and product moieties are connected to the systematic changes in stoichiometry. The results of the simulations are compared to preliminary estimates of sensitivity derived from small scale impact tests on materials synthesized recently at LANL.

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