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Reaction Analysis of Shocked Nitromethane using Extended Lagrangian Born-Oppenheimer Molecular Dynamics ROMAIN PERRIOT, ED KOBER, SUE MNISZEWSKI, ENRIQUE MARTINEZ, ANDERS NIKLASSON, PING YANG, SHAWN MCGRANE, MARC CAWKWELL, Los Alamos National Laboratory — Characterizing the complex, rapid reactions of energetic materials under conditions of high temperatures and pressures presents strong experimental and computational challenges. The recently developed extended Lagrangian Born-Oppenheimer molecular dynamics formalism enables the long-term conservation of the total energy in microcanonical trajectories, and using a density functional tight binding formulation provides good chemical accuracy. We use this combined approach to study the evolution of temperature, pressure, and chemical species in shock-compressed liquid nitromethane over hundreds of picoseconds. The chemical species seen in nitromethane under shock compression are compared with those seen under static high temperature conditions. A reduced-order representation of the complex sequence of chemical reactions that characterize this system has been developed from the molecular dynamics simulations by focusing on classes of chemical reactions rather than specific molecular species. Time-resolved infra-red vibrational spectra were also computed from the molecular trajectories and compared to the chemical analysis. These spectra provide a time history of the species present in the system that can be compared directly with recent experiments at LANL.

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