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Thermal decomposition of condensed nitromethane from molecular dynamics using the ReaxFF Reactive force field SI-PING HAN, Theoretical Division, Los Alamos National Laboratory and MSC, Caltech, ADRI VAN DUIN, WILLIAM A. GODDARD, III, MSC, Caltech, ALEJANDRO STRACHAN, Theoretical Division, Los Alamos National Laboratory — We study the thermal decomposition and subsequent reaction of the energetic material nitromethane (CH_3NO_2) using molecular dynamics (MD) with the ReaxFF first principles-based reactive force field. We characterize the chemistry of liquid and solid nitromethane at high temperatures (2000-3000 K) and density 1.97 g/cm^3 for times up to 200 picosec. At $T=3000 \text{ K}$ the first reaction in the decomposition of nitromethane is an inter-molecular proton transfer leading to CH_3NOOH and CH_2NO_2 . For lower temperatures ($T=2500$ and 2000 K) the first reaction during decomposition is often an isomerization reaction involving the scission of the C-N bond the formation of a C-O bond to form methyl nitrate (CH_3ONO) . Also at very early times we observe intra-molecular proton transfer events. The main product of these reactions is H_2O , which starts forming following the initiation steps. The appearance of H_2O marks the beginning of the exothermic chemistry. Recent quantum mechanics-based MD simulations on the chemical reactions for a crystalline sample heated to $T=3000 \text{ K}$ for 10 ps are in excellent agreement our ReaxFF MD, providing a direct validation of ReaxFF.

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