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Mechanism change in hot dense liquid nitromethane decomposition: ReaxFF molecular dynamics simulations NAOMI ROM, Fritz Haber Institute for Molecular Dynamics, Hebrew University, Jerusalem 91904, Israel, SERGEY ZYBIN, Materials and Process Simulation Center, 139-74, California Institute of Technology, Pasadena, CA 91125, USA, ADRI VAN DUIN, Department of Mechanical and Nuclear Engineering, Pennsylvania State University, University Park, PA 16802, USA, WILLIAM GODDARD, Materials and Process Simulation Center, 139-74, California Institute of Technology, Pasadena, CA 91125, USA, YEHUDA ZEIRI, Bio-medical Engineering, Ben Gurion University, Beer-Sheva 84105, Israel, GIL KATZ, RONNIE KOSLOFF, Fritz Haber Institute for Molecular Dynamics, Hebrew University, Jerusalem 91904, Israel — The decomposition mechanism of hot liquid nitromethane (NM) at various compressions and temperatures was studied using reactive force field (ReaxFF) molecular dynamics simulations. A competition between two initial thermal decomposition schemes is observed, depending on compression. At low densities unimolecular C-N bond cleavage is the dominant route, whereas when approaching Chapman-Jouget detonation conditions the dominant mechanism switches to the formation of CH_3NO fragment. The change in decomposition mechanism of hot liquid NM leads to different kinetic and energetic behavior and products distribution.

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