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Melt-Curve and Liquid-State Transport Properties of TATB: A Molecular Dynamics Study NITHIN MATHEW, Los Alamos National Laboratory, MATTHEW KROONBLAWD, Lawrence Livermore National Laboratory, THOMAS SEWELL, University of Missouri-Columbia, DONALD THOMPSON, University of Missouri-Columbia (Emeritus) — Phase boundaries and pressure/temperature-dependent properties of reactants are critical inputs for predictive modeling of high-explosives at the meso/macro scales. The pressure-dependent melting of TATB (1,3,5-Triamino-2,4,6-trinitrobenzene) and pressure/temperature-dependent transport properties of liquid TATB are predicted using classical, non-reactive molecular dynamics simulations for pressures up to P= 20 kbar. The melt-curve, obtained using solid-liquid coexistence simulations, is well represented by the Simon-Glatzel equation. The shear viscosity and self-diffusion coefficient of liquid TATB are predicted to have an Arrhenius temperature dependence at all pressures. A linear temperature dependence (P <15 kbar) and a linear density dependence (>1200 kgm-3) is predicted for thermal conductivity. At similar densities: (1) the shear viscosity of liquid TATB is close to liquid Nitromethane (NM) but lower than liquid HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) and RDX (hexahydro-1,3,5-trinitro-s-triazine) and (2) the self-diffusion coefficient is higher than that of liquid nitromethane, HMX, and RDX. These differences could be attributed to the lower conformational flexibility of TATB and NM molecules compared to HMX and RDX. The thermal conductivity of TATB is predicted to be 20% greater than the conductivity of liquid HMX at a given density.

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