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Theoretical studies of anisotropic energy transport in TATB crystals MATTHEW KROONBLAWD, THOMAS SEWELL, Univ of Missouri - Columbia — Anisotropic thermal transport properties were determined theoretically for single crystals of the insensitive explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) using molecular dynamics. TATB exhibits a graphitic-like layered packing structure with a two-dimensional hydrogen-bonding network within, but not between, the molecule-thick layers that comprise the crystal. Anisotropic thermal conductivity coefficients were determined for initially defect-free and defective TATB crystals at various temperatures and pressures, and direction-dependent relaxation of idealized hot spots was studied. The room temperature, atmospheric pressure thermal conductivity for TATB is predicted to be generally greater and more anisotropic than the thermal conductivities of other molecular explosives; conduction within the layers is at least 68% greater than conduction between them. The phonon mean free path length is predicted to be less than 1 nm. Decreases in thermal conductivity induced by molecular vacancy defects are also anisotropic and exhibit a linear dependence on defect density. Results from the hot-spot relaxation simulations were compared with and fit to an analytical solution for the one-dimensional continuum heat equation by treating the thermal diffusivity as a parameter. Validity of the continuum heat equation predictions for TATB is assessed for length scales below 20 nm.

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