Abstract Submitted
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Theoretical determination of anisotropic thermal conductivity for crystalline 1,3,5-triamino-2,4,6-trinitrobenzene (TATB)[1] MATTHEW P. KROONBLAWD, THOMAS D. SEWELL, Department of Chemistry, University of MIssouri-Columbia — Bond stretching and three-center angle bending potentials have been developed to extend an existing rigid-bond TATB molecular dynamics (MD) force field (FF) for simulations requiring fully flexible molecules. The FF potentials were fit to experimental vibrational spectra and electronic structure predictions of vibrational normal modes and frequencies using a combination of zero Kelvin eigenmode analysis for the isolated molecule and finite-temperature power spectra for the isolated molecule and bulk crystal. Crystal structures computed using the revised FF are in good agreement with results from other computational models and experimental data. A non-equilibrium MD method was used to obtain the room temperature, atmospheric pressure thermal conductivity along three directions in a well-defined, non-orthogonal basis. The thermal conductivity was found to be significantly anisotropic with values of 1.13 ± 0.07, 1.07 ± 0.07 and 0.65 ± 0.03 W m-1 K-1 for directions nominally parallel to the a, b, and c crystal directions, respectively.

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