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Theoretical determination of anisotropic thermal conductivity for crystalline 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) MATTHEW KROONBLAWD, THOMAS SEWELL, University of Missouri-Columbia — Bond stretching and three-center angle bending potentials have been developed to extend an existing rigid-bond TATB molecular dynamics force field [D. Bedrov, O. Borodin, G. D. Smith, T. D. Sewell, D. M. Dattelbaum, and L. L. Stevens, J. Chem. Phys. **131**, 224703 (2009)] for simulations requiring fully-flexible molecules. The potentials were fit to experimental vibrational spectra and electronic structure predictions of vibrational normal modes using a combination of zero kelvin eigenmode analysis for the isolated molecule and power spectra for the isolated molecule and crystal. A reverse non-equilibrium molecular dynamics method [F. Müller-Plathe, J. Chem. Phys. **106**, 6082 (1997)] 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 1.13, 1.07, and 0.65 $\mathrm{W{\cdot}m^{-1}{\cdot}K^{-1}}$ for directions nominally parallel to the **a**, **b**, and **c** lattice vectors, respectively.

Matthew Kroonblawd
University of Missouri-Columbia

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