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Far-infrared phonon behavior in the undersconstrained negative thermal expansion system $Zr(WO_4)_2$ ZACK SCHLESINGER, University of California Santa Cruz, CHANDRA TURPEN, University of California Santa Cruz, JASON HANCOCK, University of California Santa Cruz, GLEN KOWACH, City College of New York, ART RAMIREZ, Lucent/Bell Labs — $Zr(WO_4)_2$ is an unusual material in that it contracts isotropically as it is heated over a very broad temperature range from about 10 to 1000 K. Temperature dependence of the lattice volume and specific heat indicate that the important energy range for the mechanism of this negative thermal expansion (NTE) phenomenon is about 2 to 12 meV. Using infrared spectroscopy, we have studied[1] the optic phonons as a function of temperature. Comparison of energy levels to the measured specific heat and neutron density-of-states indicates that anomalous features arise in precisely the spectral region where NTE phonons are believed to exist. In addition, lattice-dynamical modeling suggests that most of the low-energy modes involve a combination of twisting and translational motion of WO_4 tetrahedra. We will discuss the relationship of these data to the origins of negative thermal expansion and the possible role of geometrical frustration in sustaining the unusual environment that supports NTE in this under-constrained open-structured system. [1] J. N. Hancock et al, Phys. Rev. Lett. 93, 225501 (2004), cond-mat/ 0409533.

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