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Evolution of molecular crystal optical phonons near structural phase transitions NIGEL MICHKI, KATHERINE NIESSEN, MENGYANG XU, ANDREA MARKELZ, SUNY at Buffalo — Molecular crystals are increasingly important photonic and electronic materials. For example organic semiconductors are lightweight compared to inorganic semiconductors and have inexpensive scale up processing with roll to roll printing[1]. However their implementation is limited by their environmental sensitivity, in part arising from the weak intermolecular interactions of the crystal. These weak interactions result in optical phonons in the terahertz frequency range. We examine the evolution of intermolecular interactions near structural phase transitions by measuring the optical phonons as a function of temperature and crystal orientation using terahertz time-domain spectroscopy. The measured orientation dependence of the resonances provides an additional constraint for comparison of the observed spectra with the density functional calculations [2], enabling us to follow specific phonon modes. We observe crystal reorganization near 350 K for oxalic acid as it transforms from dihydrate to anhydrous form. We also report the first THz spectra for the molecular crystal fructose through its melting point.

1. Krebs, FC., et al. J.Materials Chem., 2009, 19(30): p. 5442-5451
2. Singh, R., et al. J. Phys. Chem. C, 2012. 116(42): p. 1035910364.

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