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Energy Transfer Between Coherently Delocalized States in Thin Films of the Explosive Pentaerythritol Tetranitrate (PETN) Revealed by Two-Dimensional Infrared Spectroscopy. JOSHUA OSTRANDER, University of Wisconsin, Madision, ROBERT KNEPPER, ALEXANDER TAPPAN, JEFFERY KAY, Sandia Natl Labs, MARTIN ZANNI, University of Wisconsin, Madision, DARCIE FARROW, Sandia Natl Labs — Pentaerythritol tetranitrate (PETN) is a common secondary explosive and has been used extensively to study shock initiation and energy propagation in energetic materials. We report 2D IR measurements of PETN thin films that resolve vibrational energy transfer and relaxation mechanisms. Ultrafast anisotropy measurements reveal a sub-500 fs reorientation of transition dipoles in thin films of vapor-deposited PETN that is absent in solution measurements, consistent with intermolecular energy transfer. The anisotropy is frequency dependent, suggesting spectrally heterogeneous vibrational relaxation. Cross peaks are observed in 2D IR spectra that resolve a specific energy transfer pathway with a 2 ps time scale. Measurements of the transition dipole strength indicate that these vibrational modes are coherently delocalized over at least $15-30$ molecules. We discuss the implications of vibrational relaxation between coherently delocalized eigenstates for mechanisms relevant to explosives. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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