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Characterization of Fast Energy Transport Mechanisms in PEG Oligomers[1] LAYLA QASIM, ARKADY KURNOSOV, YUANKAI YUE, ALEXANDER BURIN, IGOR RUBTSOV, Tulane Univ — Vibrational energy transfer in molecules can be ballistic, which is fast and efficient, or diffusive which is governed by random-walk IVR steps. Different regimes of intramolecular vibrational energy transport were studied in a series of terminally-functionalized PEG oligomers of various length by relaxation-assisted two-dimensional infrared spectroscopy. Energy transport was initiated through short mid-IR excitation on the localized end groups and the speed of vibrational transport in PEGs was measured to be 5.5 Å/ps. The total through-chain transport time was detected up to 9.8 ps through 12 PEG units. To gain insight into the mechanism of energy transport, the dispersion relations of the PEG chain bands were calculated and indicated that although many bands are participate in energy transport, most of them do not have sufficient lifetimes to support ballistic transport for PEG oligomers exceeding 8 units. Theoretical modeling was performed and indicated that the transport is initially ballistic and then switches to a directed diffusive regime without abrupt changes of the transport speed. The approaches developed in this study are applicable to other chain types, particularly those involving heteroatoms in the backbone.

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