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Single Molecule Relaxation in Crystalline Nitromethane LUIS RIVERA-RIVERA, University of Missouri-Columbia, ALI SIAVOSH-HAGHIGHI, University of North Texas, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Classical molecular dynamics simulation results for the relaxation of a single molecule in perfect crystalline nitromethane (CH_3NO_2) at 250 K and 1 atm hydrostatic pressure will be presented. The molecule was instantaneously excited by statistically distributing excitation energy between 25.0 kcal/mol and 125.0 kcal/mol, initially all in the form of kinetic energy, among the 21 degrees of freedom. Following a subpicosecond interval dominated by intramolecular reequilibration of kinetic and potential energy, loss of kinetic energy from the excited molecule is approximately exponential, with time constants between 11.7 ps and 13.7 ps. A non-linear and non-monotonic correlation between the exponential relaxation time constant and excitation energy is predicted. Energy transfer from the excited molecule to surrounding quasi-spherical shells of molecules occurs concurrently to the first and second shells, but with more energy per molecule transferred more rapidly to the first shell.

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