

NORMAL MODE ANALYSIS ON THE RELAXATION OF AN EXCITED NITROMETHANE MOLECULE IN ARGON BATH

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In our previous work [Rivera-Rivera *et al.* *J. Chem. Phys.* 142, 014303 (2015).] classical molecular dynamics simulations followed, in an Ar bath, the relaxation of nitromethane (CH_3NO_2) instantaneously excited by statistically distributing 50 kcal/mol among all its internal degrees of freedom. The 300 K Ar bath was at pressures of 10 to 400 atm. Both rotational and vibrational energies exhibited multi-exponential decay. This study explores mode-specific mechanisms at work in the decay process. With the separation of rotation and vibration developed by Rhee and Kim [*J. Chem. Phys.* 107, 1394 (1997).], one can show that the vibrational kinetic energy decomposes only into vibrational normal modes while the rotational and Coriolis energies decompose into both vibrational and rotational normal modes. Then the saved CH_3NO_2 positions and momenta can be converted into mode-specific energies whose decay over 1000 ps can be monitored. The results identify vibrational and rotational modes that promote/resist energy lost and drive multi-exponential behavior. In addition to mode-specificity, the results show disruption of IVR with increasing pressure.

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