

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Normal mode analysis on the relaxation of an excited nitromethane molecule in argon bath¹ LUIS RIVERA-RIVERA, Department of Chemistry, Texas AM University, College Station, TX77843, ALBERT WAGNER, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL 60439 — In our previous work [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, a range spanning the breakdown of the isolated binary collision approximation. Both rotational and vibrational energies exhibit 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. Increasing pressure can be shown to increasingly interfere with post-collision IVR.

¹The work was supported by the U.S. Department of Energy, Office of Science, Chemical Sciences, Geosciences, and Biosciences Division

Albert Wagner
Argonne National Laboratory

Date submitted: 11 Nov 2016

Electronic form version 1.4