

## RELAXATION OF VIBRATIONAL, ROTATIONAL, AND CORIOLIS ENERGIES OF AN EXCITED NITROMETHANE MOLECULE IN ARGON BATH

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Our previous work [Rivera-Rivera *et al.* *J. Chem. Phys.* 142, 014303 (2015)] used classical molecular dynamics simulations to study the pressure effects on the relaxation of a nitromethane ( $\text{CH}_3\text{NO}_2$ ) molecule in an argon bath at 300 K and pressure ranging from 10 to 400 atm. The molecule was instantaneously excited by statistically distributing 50 kcal/mol among all its internal degrees of freedom. The saved  $\text{CH}_3\text{NO}_2$  positions and momenta are then used to separate the vibrational and rotational energy of the molecule following the methodology developed by Rhee and Kim [*J. Chem. Phys.* 107, 1394 (1997)]. The vibrational, rotational, and Coriolis energies exhibited multi-exponential decay. It is also found, that at later times the three energies decay approximately exponentially with similar decay rates. The mode-specific decomposition of these three energies produces, for each of the eight studied pressures, approximately 30 separate decay curves whose signal rises above statistical noise. Which vibrational and rotational modes these decay curves represent, and how their pressure dependence varies, gives insight into how excess energy equilibrates in  $\text{CH}_3\text{NO}_2$ .