Abstract Submitted
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Potential and kinetic energetic analysis of phonon modes in varied molecular solids BRENT KRACZEK, US Army Research Laboratory — We calculate partitioned kinetic and potential energies of the phonon modes in molecular solids to illuminate the dynamical behavior of the constituent molecules. This enables analysis of the relationship between the characteristics of sets of phonon modes, molecular structure and chemical reactivity by partitioning the kinetic energy into the translational, rotational and vibrational motions of groups of atoms (including molecules), and the potential energy into the energy contained within interatomic interactions[1]. We consider three solids of differing size and rigidity: naphthalene (C_10 H_6), nitromethane (CH_3NO_2) and α-HMX ($C_4H_8N_8O_8$). Naphthalene and nitromethane mostly act in the semi-rigid manner often expected in molecular solids. HMX exhibits behavior that is significantly less-rigid. While there are definite correlations between the kinetic and potential energetic analyses, there are also differences, particularly in the excitation of chemical bonds by low-frequency lattice modes. This suggests that in many cases computational and experimental methods dependent on atomic displacements may not identify phonon modes active in chemical reactivity. 1. Kraczek, Chung, *J. Chem. Phys.* 138:074505 (2013).

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