THEORETICAL MODELING OF ANHARMONICITIES

LUCAS KOZIOL, ANNA I. KRYLOV, Department of Chemistry, University of Southern California, Los Angeles, CA 90089.

Anharmonicities in molecular vibrations are highly sensitive to the potential energy surface. Variational methods can reach quantitative accuracy in modeling anharmonic spectra; however, their effectiveness is limited by the quality of the PES. A form is discussed which contains full nuclear permutational symmetry; this both reduces the number of data points required for fitting, and avoids artifactual errors from an unsymmetrized PES. Preliminary results for the diazomethane molecule will also be discussed.