

## 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.