THEORETICAL MODELING OF ANHARMONICITIES

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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.