

## CALCULATION OF VIBRATIONAL ENERGY LEVELS: VPT2 VS. A VARIATIONAL APPROACH

M. E. HARDING, J. VÁZQUEZ, J. F. STANTON, *Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712, USA.*

For several potentials a detailed comparison of vibrational energy levels obtained via variational calculations employing the complete vibrational Hamiltonian<sup>a</sup> and second-order vibrational perturbation theory (VPT2) is carried out.

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<sup>a</sup>J. K. G. Watson, *Mol. Phys.*, 15, 479 (1968);19, 465 (1970).