COMPUTATION OF INFRARED SPECTROSCOPIC FEATURES USING SYMMETRY

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

An efficient algorithm for the prediction of anharmonic infrared features of symmetric top molecules in the framework of second-order vibrational perturbation theory is presented. Higher-order derivatives of the energies are obtained by numerical differentiation of analytic second derivatives in conjuction with symmetry projection which leads to a major reduction of the computational demand. The performance of the implementation is illustrated by several exemples.