

THE MULTIMODE APPROACH TO CHALLENGING PROBLEMS IN VIBRATION SPECTROSCOPY

JOEL M. BOWMAN, STUART CARTER, and XINCHUAN HUANG, *Department of Chemistry and Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, GA 30322*; NICHOLAS HANDY, *Dept. of Chemistry, University of Cambridge, Cambridge, UK*.

I will briefly describe the code "MULTIMODE", developed in collaboration with Stuart Carter and Nicholas Handy, and then present applications to the series of molecules H_3O^+ , H_3O_2^- and H_5O_2^+ . I will also describe recent collateral work on developing full dimensional *ab initio*-based potential energy surfaces for these molecules. Some comparisons with Diffusion Monte Carlo calculations done by Anne McCoy on these molecules will also be presented.