AN ADIABATIC MODEL OF THE BENDING DYNAMICS OF ACETYLENE

ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210.*

The dynamics and spectroscopy of ($J = 0$) acetylene bending degrees of freedom are investigated using a reduced dimensional Hamiltonian, derived using an adiabatic separation of slow bending motions from fast stretching motions.[a] The seven adjustable parameters in this model are the force constants of a restricted sextic expansion of an effective potential, which have been fit to five experimentally determined transition energies and the two harmonic frequencies. We find that the eigenvalues of this model Hamiltonian reproduce the observed transition energies for states with up to 10 600 cm^{-1} of vibrational excitation. A dispersed fluorescence spectrum out of the excited $\tilde{A}$ state, calculated from this model, will be compared to the experimental spectrum obtained by Solina, *et al.*[b] Pathways for energy flow out of the experimental zero-order bright state will also be discussed. With minor modification, a global bend force field is determined that qualitatively describes the vinylidene vibrations and quantitatively describes the acetylene vibrations, allowing for extensions of this effective force field to the development of a global potential for acetylene.

[a] A. B. McCoy and E. L. Sibert, *J. Chem. Phys.*, submitted

[b] S. A. Solina, J. P. O'Brien, R. W. Field and W. F. Polik, *Ber Bunsenges. Phys. Chem.*, **99**, 555 (1995).