# A DIABATIC BASIS APPROACH TO THE DETERMINATION OF TUNNELING SPLITTINGS IN FORMIC ACID DIMER

GEORGE L. BARNES and EDWIN L. SIBERT III, *University of Wisconsin-Madison, Madison, Wisconsin 53706*.

Formic Acid Dimer (FAD) is the smallest molecule which is held together through a double hydrogen bond. This type of hydrogen bonding structure is found in many large biological systems, however, high level theoretical treatment of such systems is currently intractable. By studying the FAD system in detail insights into other larger systems may be possible. Tunneling splitting of FAD for the ground state and with one quantum of CO stretch have recently been measured by Madeja and Havenith (J. Chem. Phys. **117**, 7162 (2002)). We have calculated a three dimensional reaction surface potential for FAD while treating all other degrees of freedom as a set of coupled harmonic oscillators. This problem provides a challenging case of coupling between the degrees of freedom. Great care must be taken between adiabatic and diabatic representations. By making use of a diabatic representation for the reaction surface potential a small and efficient basis set is defined. Our goal is to investigate the effects of vibrational excitation on the calculated tunneling splittings.