

THEORETICAL STUDIES OF THE FUNDAMENTAL AND OVERTONE SPECTRUM OF OXALIC ACID

DA MATTHEWS, JF STANTON, *Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.*

The vibrational frequencies and intensities for all states up to two quanta are calculated for oxalic acid ($C_2H_2O_4$) at the CCSD(T) level. The effect of different internal hydrogen bonding configurations on the OH stretching level structures for the five conformers studied is discussed.