EVIDENCE OF PROTON TUNNELING IN THE ROTATIONAL SPECTRUM OF THE PROPIOLIC ACID-FORMIC ACID HYDROGEN BONDED COMPLEX

KEVIN O. DOUGLASS, PAM L. CRUM, RICHARD D. SUENRAM, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*.

We have measured the rotational spectrum of the hydrogen bonded system of propiolic acid and formic acid. The spectral fitting was aided by density functional calculations and FTMW-MW double resonance spectroscopy. The structure is predicted to be an 8 member ring system where the hydrogen bonding takes place between the acid functionalities of the monomers. The spectra were obtained using a neat 4:1 mixture of propiolic - formic acid while heating the nozzle to 50°C. The spectrum was measured from 10 to 22 GHz. Each a-type rotational transition consists of a doublet with an intensity ratio that alternates with even and odd K_a and are suggestive of 3:1 hydrogen spin statistics. These doublets result from proton tunneling splitting. The results of the proton tunneling splitting will be presented.