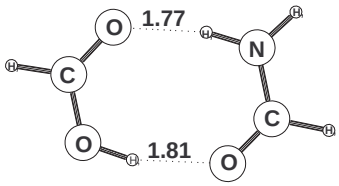
MICROWAVE SPECTRUM AND PARTIAL GAS PHASE STRUCTURE OF A FORMIC ACID-FORMAMIDE COMPLEX [a]

ADAM M. DALY, STEPHEN G. KUKOLICH, *Department of Chemistry and Biochemistry, 1306 E. University, Tucson, Arizona 85721*; BRYAN SARGUS, *Catalina Foothills High School Teacher, Tucson, Arizona 85718.*

The rotational spectrum of 5 isotopomers of the complex formed between formic acid and formamide have been measured and analyzed using a pulsed beam fourier transform microwave spectrometer. The rotational constants and nitrogen's quadrupole coupling strength for $HC^{12}OOH - H_2N^{14}COH$ are A=5889.51(9), B=2148.734(2), 1575.127(1), $eQq_{aa} = 1.020(8)$, $eQq_{bb} = 1.98(1)$ and $eQq_{cc} = -2.998(9)$ MHz. Using the 15 rotational constants obtained with $HC^{13}OOH$, HCOOD, DCOOH and $H_2N^{15}CHO$ isotopologes, key structural information was obtained from a least squares fit. R(CO-HN) distance of 1.77$\AA$ and R(OH-OC) distance of 1.81$\AA$ and an (COH) angle of formic acid of 121° was obtained that was very different from the monomer value of 106.9°. Density functional theory using B3PW91, HCTH407 and TPSS and MP2 calculations were performed using 6-311++G(d,p) and compared to experimentally determined values.



[a] Supported by THE NATIONAL SCIENCE FOUNDATION