GAS PHASE MEASUREMENTS OF MONO-FLUORO-BENZOIC ACIDS AND THE DIMER OF 3-FLUORO-BENZOIC ACID[a]

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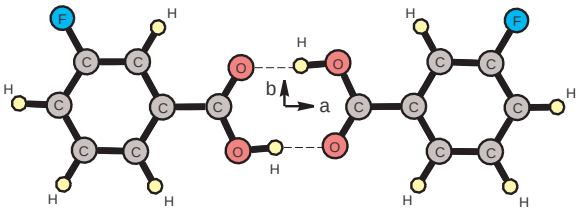

The gas phase homodimer of 3-fluorobenzoic acid was detected and the spectra showed evidence of proton tunneling. Experimental rotational constants are A(0^+)= 1151.8(5), B(0^+)=100.3(5), C(0^+)= 87.64(3) MHz and A(0^-)=1152.2(5), B(0^-)= 100.7(5), C(0^-)=88.85(3) MHz for the two ground vibrational states split by the proton tunneling motion. The tunneling splitting (ΔE) is approximately 560 MHz. This homodimer appears to be the largest carboxylic acid dimer observed with F-T microwave spectroscopy. Additionally, the microwave spectra of the mono-fluoro-benozic acids, (2-fluoro, 3-floro and 4-fluoro) benzoic acid have been measured in the frequency range of 4-14 GHz using a pulsed beam Fourier Transform microwave spectrometer. Measured rotational transition lines were assigned and fit using a rigid rotor Hamiltonian. Assignments were made for 3 conformers of 2-fluorobenzoic acid, 2 conformers of 3-fluorobenzoic acid and 1 conformer of 4-fluorobenzoic acid.

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