MICROWAVE SPECTRUM OF THE METHANESULFONIC ACID – WATER COMPLEX

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The methanesulfonic acid water - complex (CH_3SO_3H-H_2O) has been observed using pulse-nozzle Fourier transform microwave spectroscopy. The rotational spectra for the CH_3SO_3H-D_2O and CH_3SO_3D-D_2O isotopologues have also been obtained and analyzed. DFT calculations predict the two lowest energy conformers of CH_3SO_3H-H_2O to form a strong hydrogen bond between the water molecule with the acidic proton and a second, longer hydrogen bond with one of the S=O bonds to form the 6-membered ring-like structure that is typical of oxyacid monohydrates. The observed rotational constants and isotope shifts are in best agreement with those predicted for the global minimum structure of CH_3SO_3H-H_2O, where the unbound H_2O hydrogen atom is oriented away from the methyl group. In contrast to the triflic acid monohydrate (CF_3SO_3H-H_2O) spectrum, there was no evidence of a pair of tunneling states arising from internal motion of the water. Additionally, A and E internal rotor states were not resolvable in the observed spectrum, consistent with the predicted high barrier for methyl group internal rotation (V_3=1000 cm^{-1}).