

MICROWAVE SPECTRUM OF THE METHANESULFONIC ACID – WATER COMPLEX

ANNA HUFF, NATHAN LOVE, KENNETH R. LEOPOLD, *Chemistry Department, University of Minnesota, Minneapolis, MN, USA.*

The methanesulfonic acid water - complex ($\text{CH}_3\text{SO}_3\text{H}\cdot\text{H}_2\text{O}$) has been observed using pulse-nozzle Fourier transform microwave spectroscopy. The rotational spectra for the $\text{CH}_3\text{SO}_3\text{H}\cdot\text{D}_2\text{O}$ and $\text{CH}_3\text{SO}_3\text{D}\cdot\text{D}_2\text{O}$ isotopologues have also been obtained and analyzed. DFT calculations predict the two lowest energy conformers of $\text{CH}_3\text{SO}_3\text{H}\cdot\text{H}_2\text{O}$ to form a strong hydrogen bond between the water molecule and the acidic proton and a second, longer hydrogen bond with one of the S=O oxygens 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 $\text{CH}_3\text{SO}_3\text{H}\cdot\text{H}_2\text{O}$, where the unbound H_2O hydrogen atom is oriented away from the methyl group. In contrast to the triflic acid monohydrate ($\text{CF}_3\text{SO}_3\text{H}\cdot\text{H}_2\text{O}$) spectrum, there was no evidence of a pair of tunneling states arising from internal motion of the water. A and E internal rotor states were not resolvable in the observed spectrum, consistent with the predicted high barrier for methyl group internal rotation ($V_3=1000\text{ cm}^{-1}$).