MICROWAVE SPECTRUM AND LARGE AMPLITUDE MOTION OF METHANESULFONIC ACID

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

Microwave spectra have been recorded for methanesulfonic acid (CH_3SO_3H) and its –OD isotopologue. No internal rotation of the methyl group was observed, consistent with the calculated high barrier of 2.7 kcal/mol. A pair of tunneling states has been observed for both species, however, and is attributed to large amplitude wagging of the hydroxyl hydrogen from one side of the molecule to the other. The predicted barrier to this motion, obtained from M06-2X/6-311++G(3df,3pd) calculations, is 0.7 kcal/mol. For CH_3SO_3D, the tunneling energy was directly determined to be $\Delta E = 6471.9269(17)$ MHz from the measurement of *c*-type spectra. In the case of the parent species, however, transitions displaced by the tunneling energy have not been located and are likely above the maximum frequency accessible by the spectrometer (20 GHz). Thus, the value of ΔE could not be experimentally determined. Nonetheless, a satisfactory fit was obtained for transitions involving J"= 0 and J" = 1 (nine frequencies for each state). Suggestions for further work at higher frequencies will be presented.