

MICROWAVE SPECTROSCOPY OF FLUOROSULFONIC ACID (FSO₂OH) AND ITS MONO- AND DIHYDRATES

AARON J REYNOLDS, *Chemistry Department, University of Minnesota, Minneapolis, MN, USA*; KARLA V. SALAZAR, WEI LIN, *Department of Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA*; KENNETH R. LEOPOLD, *Chemistry Department, University of Minnesota, Minneapolis, MN, USA*.

We report on the hydration of the superacid fluorosulfonic acid (FSO₂OH) as characterized by chirped-pulse and cavity microwave spectroscopy. Rotational transitions of the monomer in the 3-18 GHz region were readily observed. Each has a weaker partner arising from OH wagging, as previously observed in the spectra of triflic and methanesulfonic acids. Spectra for the monohydrate and dihydrate were collected using a chirped-pulse method, and rapidly assigned using the DAPPERS software. Cavity spectroscopy revealed two states for the monohydrate, presumably arising from an internal motion associated with the water moiety. Deuterium isotopologues of these complexes were collected by on-the-fly mixing using D₂O in place of H₂O. The computed structures (benchmarked against the observed rotational constants), involve hydrogen bonded rings analogous to those observed for many other hydrated oxyacids. Consistent with previously published theoretical work^a, acid dissociation is not predicted or observed for the mono- or dihydrates, although a correlation between degree of partial proton transfer and hydration is noted. The trihydrate is predicted to exist as a hydrated ion pair, but no such species has yet been identified in the observed spectrum.

^aLi, S.; Weber, K.H.; Tao, F.-M.; Gu, R. Theoretical Investigation of Ionic Dissociations of Fluorosulfonic Acid in Microsolvated Clusters, *Chem. Phys.* 2006, 323, 397-406.