

MICROWAVE SPECTRUM OF TRIFLIC ACID DIHYDRATE AND TRIHYDRATE: EVIDENCE FOR COMPLETE PROTON TRANSFER IN A MICROSOLVATED SUPERACID

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

Microwave spectra have been observed for the dihydrate and trihydrate of triflic acid ($\text{CF}_3\text{SO}_3\text{H}-(\text{H}_2\text{O})_2$ and $\text{CF}_3\text{SO}_3\text{H}-(\text{H}_2\text{O})_3$). For the dihydrate, spectra for $\text{CF}_3^{34}\text{SO}_3\text{H}-(\text{H}_2\text{O})_2$ and $\text{CF}_3\text{SO}_3\text{H}-(\text{D}_2\text{O})_2$ were also identified. The fitted rotational constants for both the triflic acid dihydrate and trihydrate are in good agreement with those predicted from their respective global minimum structures at the M06-2X/6-311++G(3df,3pd) level of theory. The two water molecules in the dihydrate bind to triflic acid in a cyclic arrangement to form an 8-membered ring, resembling an insertion of a second water molecule into the weak hydrogen bond of the triflic acid monohydrate. For the triflic acid trihydrate, however, rather than forming a 10-membered ring from the insertion of a third water molecule into the dihydrate geometry, the global minimum structure represents a hydronium triflate ion pair solvated by two water molecules ($(\text{CF}_3\text{SO}_3^-\text{H}_3\text{O}^+)-(\text{H}_2\text{O})_2$). A summary of the sequential hydration of triflic acid leading to complete proton transfer will be discussed.