MICROWAVE INVESTIGATION OF SULFURIC ACID MONOHYDRATE

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We report the first microwave spectroscopic investigation of the 1:1 complex of H\textsubscript{2}O-H\textsubscript{2}SO\textsubscript{4} and several of its deuterated and \textsuperscript{18}O containing isotopomers. The complex is prepared in situ via reaction of water and SO\textsubscript{3} using a co-injection source in which H\textsubscript{2}O vapor is introduced into the early stages of an Ar + SO\textsubscript{3} expansion. Both a- and c- type spectra for fourteen isotopomers have been measured and are consistent in all cases with that of a near-prolate rotor with appreciable dipole moment components along the a- and c- inertial axes. The spectra of the isotopomers containing H\textsubscript{2}\textsuperscript{18}O are complicated by internal motion of the water unit affecting both the a-type K\textsubscript{a-1} = 0 and several of the c-type transitions. The possible internal motions giving rise to the observed spectral splittings as well as the ground state structural parameters of the H\textsubscript{2}O-H\textsubscript{2}SO\textsubscript{4} complex will be discussed and compared to recent DFT calculations.\textsuperscript{a,b}