

## MICROWAVE INVESTIGATION OF SULFURIC ACID MONOHYDRATE

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We report the first microwave spectroscopic investigation of the 1:1 complex of H<sub>2</sub>O-H<sub>2</sub>SO<sub>4</sub> and several of its deuterated and <sup>18</sup>O containing isotopomers. The complex is prepared in situ via reaction of water and SO<sub>3</sub> using a co-injection source in which H<sub>2</sub>O vapor is introduced into the early stages of an Ar + SO<sub>3</sub> 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<sub>2</sub><sup>16</sup>O are complicated by internal motion of the water unit affecting both the a-type K<sub>-1</sub> = 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<sub>2</sub>O-H<sub>2</sub>SO<sub>4</sub> complex will be discussed and compared to recent DFT calculations.<sup>a,b</sup>

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<sup>a</sup>S. Re, Y. Osamura, K. Morokuma, J. Phys. Chem. A 103, 3535 (1999).

<sup>b</sup>H. Arstila, K. Laasonen, A. Laaksonen, J. Chem. Phys. 108, 1031 (1998).