DIPOLE MOMENT OF THE SULFURIC ACID MONOMER.

G. SEDO, J. CURTIS, and K. R. LEOPOLD, *Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455*.

The dipole moment of the sulfuric acid monomer, H_2SO_4, has been revisited using pulsed-nozzle Fourier transform microwave spectroscopy. A total of 91 Stark-shifted frequencies at a series of electric field strengths have been recorded for the known $1_{10} \leftarrow 0_{00}$ transition. The total molecular dipole moment ($\mu_{tot} = \mu_c$) was found to be 2.9643(67) D, which is approximately 0.24 D greater than the best value previously available. An extensive computational investigation has also been performed in order to determine the effect of theoretical method and basis set on the calculated dipole moment. Calculations using the PW91 density functional perform exceedingly well and result in calculated values that converge to good agreement with the current experimental value.