ROTATIONAL SPECTROSCOPY OF THE NH_3-SO_3-H_2O SYSTEM

S. W. HUNT, C. S. BRAUER, M. CRADDOCK, K. R. LEOPOLD, *Department of Chemistry, University of Minnesota, Minneapolis, MN 55455*.

Previous reports of atmospheric sulfate aerosol formation indicate significantly enhanced nucleation rates in the presence of elevated concentrations of ammonia.[a] Computational studies[b] predict the most stable structure for NH_3-SO_3- H_2O ternary system is the hydrogen bonded complex, H_2SO_4-NH_3, but a second minimum, only 0.4 kcal/mol higher in energy occurs for the hydrated form of sulfamic acid $(H_3N\text{-}SO_3)\cdot H_2O$. In this report, we present microwave spectroscopic results obtained in a supersonic jet seeded with H_2O, NH_3, and SO_3. A-type rotational spectra of a near-prolate asymmetric top requiring the simultaneous presence of NH_3, H_2O, and SO_3 in the jet have been observed. The transitions correlate with the intensity of known H_3N-SO_3 spectra, and spectroscopic constants are consistent with those predicted for $(H_3N\text{-}SO_3)\cdot H_2O$.[b] Assignment to H_2SO_4-NH_3, however, cannot be ruled out on the basis of data corresponding to the parent isotopic form alone. Isotopic work is in progress, and spectral results will be reported. A novel, dual-injection arrangement, in which two gases are independently admitted into the early phases of the supersonic expansion, has been developed and will be described as well.

[a] R. J. Werber; P. H. McMurry; L. Mauldin; D. J. Tanner; F. L. Eisle; F. J. Brechtel; S. M. Kreidenweis; G. L. Kok; R. D. Schillawski; D. Baumgardner *J. Geophys Res.* **103**, 16385 (1998).

[b] L. J. Larson; F-M. Tao, *J. Phys. Chem. A*, in press.