DETERMINATION OF THE DIPOLE MOMENT OF H_3N-SO_3

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The dipole moment of H_3N-SO_3 has been determined using pulsed nozzle Fourier transform microwave spectroscopy. The value obtained, 6.204(12) D, is in reasonable agreement with published ab initio estimates [a]. These measurements follow our previously reported [b] structural work on this complex in which the intermolecular N-S bond was shown to be significantly longer in the gas phase than in the solid state. Presumably, the mechanism for the contraction of the N-S bond upon crystallization involves a sharply rising dipole moment function at shorter distances. Thus, the present result is especially interesting in connection with the observed gas-solid structure changes. The complex has also been postulated as a potential seed molecule for the nucleation of atmospheric aerosols, and we comment on possible implications of its phase-dependent structure and bonding on the kinetics and thermodynamics of the nucleation process.

[a] M. W. Wong, K. B. Wiberg, and M. J. Frisch, J. Am Chem. Soc. 114, 523 (1992).
[b] M. Canagaratna, J. A. Phillips, H. Goodfriend, and K. R. Leopold, J. Am. Chem. Soc., 118, 5290 (1996).