

STRUCTURAL ANALYSIS AND DIPOLE MOMENT DETERMINATION OF THE GAS-PHASE TRIMETHYLAMINE SULFUR TRIOXIDE COMPLEX

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The structure and dipole moment of the Lewis acid-base adduct $(\text{CH}_3)_3\text{N-SO}_3$ have been determined by microwave spectroscopy. Analysis yields an N-S bond length of $1.914(33) \text{ \AA}$ and an NSO angle of $100.0(4)^\circ$. These data indicate that the formation of the N-S dative bond is nearly (but not entirely) complete in the gas phase. Comparison with previous work on the closely related system $\text{H}_3\text{N-SO}_3$ indicates that the increased basicity of the $(\text{CH}_3)_3\text{N}$ relative to that of H_3N is effective at driving the dative bond further towards completion. Analysis of nuclear hyperfine structure indicates that about 0.6 electrons are transferred from the nitrogen to the SO_3 upon formation of the complex. This is significantly larger than that observed in $\text{H}_3\text{N-SO}_3$. The dipole moment, obtained from Stark effect measurements, of $7.111(7) \text{ D}$, arises from a combination of charge transfer, out-of-plane distortion of the SO_3 and the intrinsic moment of $(\text{CH}_3)_3\text{N}$.