MICROWAVE SPECTRA, STRUCTURES AND MODELING OF THE N_2O-SO_2 AND N_2O-N_2O-SO_2 COMPLEXES

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The microwave spectra of N_2O-SO_2 and N_2O-N_2O-SO_2 have been measured. The dimer lines are split due to a tunneling motion in the complex. The rotational constants of the higher frequency components of the doublets are A = 6126.9781(15) MHz, B = 1494.537(37) MHz and C = 1435.474(36) MHz, and those for the lower frequency components are A = 5500 MHz (fixed), B = 1463.484(23) MHz and C = 1420.953(23) MHz. The dipole moment has been measured, and the rotational constants for four isotopomers in addition to the normal species have allowed an inertial fit of the structure of the complex. The data indicate that the SO_2 straddles the N_2O asymmetrically (C_1 symmetry) with the sulfur closer to the oxygen end of N_2O. The trimer rotational constants are A = 1369.1014(11)

MHz, B = 1115.5816(11) MHz and C = 730.5790(4) MHz. The dipole moment and the spectra of four isotopomers in addition to the normal species have been measured. The N_2O molecules have a structure that is intermediate between crossed and T-shaped; the SO_2 straddles one N_2O and has one S-O bond aligned roughly parallel with the second N_2O. The structures of the dimer and trimer will be compared, and the success of semi-empirical and ab initio calculations at predicting the N_2O-SO_2 and N_2O-N_2O-SO_2 structures will also be explored.