FT MICROWAVE SPECTROSCOPY AND *AB INITIO* INVESTIGATION OF N_2-SO_3, OC-SO_3, and OC-SO_3-Ar

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The weakly bound complexes N_2-SO_3, OC-SO_3, and OC-SO_3-Ar have been studied using Fourier Transform Microwave Spectroscopy. Four isotopomers have been observed for each species, and the systems have been determined to be symmetric tops, with the atomic arrangements indicated. Rotational constants for the parent isotopomers are 1628.61130(51), 1614.71706(83), and 591.10961(46) MHz for N_2-SO_3, OC-SO_3, and OC-SO_3-Ar, respectively. The N-S distance in N_2-SO_3 is 2.936(14) $\AA$ and preliminary analysis gives a C-S distance of 2.865 $\AA$ in OC-SO_3. Structural analysis of the trimer is underway, as are Stark effect measurements for OC-SO_3 and OC-SO_3-Ar.

Ab initio results for all three complexes are also reported. Geometry optimizations for OC-SO_3-Ar indicate an increase of 0.03 $\AA$ and 0.04 $\AA$ in the C-S and Ar-S distances, respectively, relative to the corresponding dimer species. Calculations at the MP2 level give a binding energy of -6.03 kcal/mol for OC-SO_3-Ar, which is only about 0.2 kcal/mol larger than the sum of the binding energies for OC-SO_3 and Ar-SO_3.

This study was undertaken as a prelude to studies probing the microsolvating effect of non-polar or slightly polar species (Ar, N_2, and CO) on partially bonded complexes such as HCN-SO_3.