MICROSOLVATION OF PARTIALLY BOUND NITRILE - SO_3 COMPLEXES

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The rotational spectrum of HCN–HCN-SO_3 and its deuterated isotopomers have been observed by pulsed nozzle Fourier transform microwave spectroscopy. The complex is a symmetric rotor with the atomic ordering indicated and preliminary analysis yields an S-N bond length of 2.43 Å. This distance is approximately 0.15 Å shorter than the corresponding distance in HCN-SO_3, indicating that the remote HCN has a large effect on the nitrogen - sulfur bond. This result represents the first direct probe of the effect of a nearest neighbor on the structure of a partially bonded adduct. We also present measurements of the dipole moments of HCN-SO_3 and CH_3CN-SO_3 (4.416 $\pm$ 0.029 D and 6.06 $\pm$ 0.18 D, respectively). Examination of a series of SO_3 complexes indicates a substantial increase in polarity in these systems as dative bond formation proceeds. These results will be discussed in connection with the origins of the large gas-to- solid structure changes normally observed for partially bound species.