MICROWAVE INVESTIGATIONS OF C_5H_5N-SO_3 AND HCCCN-SO_3: THE PRINCIPLE OF HARD AND SOFT ACIDS AND BASES APPLIED TO PARTIALLY BONDED SYSTEMS

S. W. HUNT, D. L. FIACCO, M. CRADDOCK, and K. R. LEOPOLD , *Department of Chemistry, University of Minnesota, Minneapolis, MN 55455*.

The Lewis acid-base adducts C_5H_5N-SO_3 and HCCCN-SO_3 have been studied by Fourier transform microwave spectroscopy. The spectrum of C_5H_5N-SO_3 indicates a short N-S bond length of 1.91540(66) Å and free rotation of the SO_3 unit. In contrast, HCCCN-SO_3 is more weakly bound with an N-S distance of 2.5676(76) Å, only slightly less than the expected van der Waals interaction distance. The NSO angles are $98.9212(45)^o$ and $91.89(36)^o$ for C_5H_5N-SO_3 and HCCCN-SO_3 respectively. A Townes and Dailey analysis of the ^{14}N quadrupole coupling constant of C_5H_5N-SO_3 indicates a transfer of 0.54 electrons upon formation of the dative bond. This is a physical measurement of the "soft" portion of the chemical interaction and comparisons are made with other adducts of SO_3. Bonding is considered in light of Pearson's concept of Hard and Soft Acids and Bases, [a] noting the correlation of adduct properties, such as electron transfer and bond length, with the energy gap between the donor and acceptor orbital.

[a] R. G. Pearson J. Am. Chem. Soc. 85, 3533 (1963).