

COMPARISONS OF THE STRUCTURE AND SPECTROSCOPY OF THE $M \cdot XH(A^2\Sigma^+)$ ($M=Ne, Ar, Kr; X = O,S$) COMPLEXES.

CHRISTOPHER C. CARTER, TERRY A. MILLER, HEE-SEUNG LEE and ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH, 43210.*

Over the past several years we have performed high resolution spectroscopic experiments on the $M \cdot XH(A^2\Sigma^+)$ ($M=Ne, Ar, Kr; X = O,S$) family of complexes. Based on these studies, we have fit a set of empirical potential surfaces that reproduce the experimental band origins to within 1 cm^{-1} and the rotational constants to within 1%. In this talk, we will discuss these potentials and the experimental spectroscopic trends in this class of systems. In the case of $Ne \cdot SH$, the most weakly bound of these species with a D_0 of 41 cm^{-1} , only one quantum of excitation in either of the van der Waals modes is necessary to allow the complex to sample both the Ne-SH and the Ne-HS minima on the potential. In contrast, in the most strongly bonded case of the $Kr \cdot OH$ complex, D_0 is 1772 cm^{-1} , and all of the assigned states are found to be localized in the Kr-HO minimum of the potential. Manifestations of this range of bonding, from van der Waals to near covalent in strength, in the spectroscopic constants will also be discussed.