

ZEKE SPECTROSCOPY OF $\text{Al}(\text{C}_5\text{H}_5\text{N})$: A STUDY OF METAL- σ INTERACTION WITH A HETEROCYCLIC AROMATIC LIGAND

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A few years ago, a computational study was reported on cation- π interactions in Al^+ complexes with a series of aromatic compounds^a. However, for $\text{Al}^+(\text{C}_5\text{H}_5\text{N})$, the calculations indicated that Al^+ was σ -bound to the nitrogen in the ground electronic state. If Al^+ was π -bound to the ring, the potential energy surface was very flat and no minimum was located. Our photoelectron measurements on Al/Al^+ -pyridine vibrations agree with the theoretical predictions. The ground electronic states of $\text{Al}^+(\text{C}_5\text{H}_5\text{N})$ and its neutral species were determined to be $^1\text{A}_1$ and $^2\text{B}_1$ in C_{2v} symmetry. The aluminum-pyridine stretching frequencies were measured to be 278 cm^{-1} in the ionic $^1\text{A}_1$ state and 366 cm^{-1} in the neutral $^2\text{B}_1$ state. It is unusual that the metal-ligand stretching frequency of a cation complex is much smaller than that of the corresponding neutral species. This anomaly will be discussed in terms of orbital and electrostatic interactions.

^aD. Stöckigt, *J. Phys. Chem. A* **101**, 3800 (1997)