ZEKE SPECTROSCOPY OF Al(C_5H_5N): 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 $Al^+(C_5H_5N)$, 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 $Al^+(C_5H_5N)$ and its neutral species were determined to be $^1A_1$ and $^2B_1$ in C_{2v} symmetry. The aluminum-pyridine stretching frequencies were measured to be 278 cm^{-1}in the ionic $^1A_1$ state and 366 cm^{-1}in the neutral $^2B_1$ 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.

[a]D. Stöckigt, *J. Phys. Chem. A* **101**, 3800 (1997)