PFI-ZEKE SPECTROSCOPY OF METAL-POLYCYCLIC AROMATIC HYDROCARBONS: Sc-PYRENE and Sc-NAPHTHALENE

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Gas-phase complexes of scandium with pyrene ($C_{16}H_{20}$) and naphthalene ($C_{10}H_8$) are produced by using laser ablation and a polycyclic aromatic hydrocarbon (PAH) oven in a pulsed molecular beam source. The resulting Sc-PAH complexes are characterized with pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) photoelectron spectroscopy. The PFI-ZEKE spectrum of Sc-Pyrene exhibits vibrational progressions of 361 and 154 $\mathrm{cm}^{-1}$and a vibrational spacing of 144 $\mathrm{cm}^{-1}$, with the band origin at 40937 $\mathrm{cm}^{-1}$. Through comparison with *ab initio* and Franck-Condon factor calculations, it is determined that this spectral profile arises from a Sc-pyrene complex in which the scandium atom is bound to the "outer" ring in an $\eta^4$- configuration. The 361 $\mathrm{cm}^{-1}$progression is assigned to the $Sc^+$-ring stretch and 154 and 144 $\mathrm{cm}^{-1}$features are assigned to pyrene "flying" modes in the cation and neutral, respectively. For Sc-naphthalene, the spectrum shows four vibrational intervals of 389, 347, 298 and 112 $\mathrm{cm}^{-1}$, with the adiabatic ionization energy of 41192 $\mathrm{cm}^{-1}$. A preliminary analysis indicated the Sc atom is in an $\eta^2$ bonding mode in this complex. However, a detailed analysis is still in progress.