

## 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  $cm^{-1}$  and a vibrational spacing of 144  $cm^{-1}$ , with the band origin at 40937  $cm^{-1}$ . 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  $cm^{-1}$  progression is assigned to the  $Sc^+$ -ring stretch and 154 and 144  $cm^{-1}$  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  $cm^{-1}$ , with the adiabatic ionization energy of 41192  $cm^{-1}$ . 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.