PHOTOELECTRON AND PHOTOION SPECTROSCOPY OF SCANDIUM-METHYLBENZENE COMPLEXES

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We report here single UV photon pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) photoelectron spectra of jet-cooled Sc-[$C_6H_{6-n}(CH_3)_n$] (n = 2, 3, and 6) complexes and two-photon IR-UV photoionization spectra of Sc-[$C_6(CH_3)_6$]. Adiabatic ionization energies and low-frequency metal-ligand and ligand-based vibrational modes are measured from the single-photon PFI-ZEKE spectra, and C-H stretching frequencies are determined from the two-photon IR-UV spectra. The ionization energies of these Sc complexes decrease with increasing methyl substations of hydrogen in the benzene ring. The C-H frequencies of hexamethylbenzene are significantly shifted due to Sc coordination. The ZEKE transitions of the di- and tri-methyl substituted complexes are sharp, while those of the hexa-methyl species are rather broad. The observed electronic transitions are $^1A \leftarrow {}^2A$ for Sc-[1,4-$C_6H_4(CH_3)_2$] (C_2), $^1A' \leftarrow {}^2A'$ for Sc-[1,3,5-$C_6H_3(CH_3)_3$] (C_s), and $^1A_1 \leftarrow^2 A_1$ for Sc-[$C_6(CH_3)_6$] (C_{2v}).