PFI-ZEKE SPECTROSCOPY OF Sc-C_6H_5X (X=F, OH, and CH_3) COMPLEXES

CHANGHUA ZHANG, *Department of Chemistry, University of Kentucky, Lexington, Kentucky 40506-0055. State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, P. R. China*; SERGE KRASNOKUTSKI and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, Kentucky 40506-0055*.

Scandium complexes of fluorobenzene, toluene and phenol are produced in laser-vaporization supersonic molecular beams and studied with pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) spectroscopy. The PFI-ZEKE experiment measures precise ionization energies and Sc-C_6H_5X(X=F, OH, and CH_3) stretching and other low-frequency vibrations. The combination of these spectroscopic data with density functional theory and multidimensional Franck-Condon factor calculations determines the preferred Sc binding sites and ground electronic states of the neutral and ionized complexes. For all three complexes, the ground electronic states of the neutral and ionized forms are ^{2}A and ^{1}A, respectively. Although Sc binds with all ring carbon atoms, the binding is not equal among these carbons. This differential binding leads to a non-planar ring structure with two carbon atoms bending toward the metal center.