HOW DOES SCANDIUM ATOM BIND TO 1-PHENYL NAPHTHALENE?

BRADFORD R. SOHNLEIN, JASON F. FULLER, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

The complex of scandium with 1-phenyl naphthalene ($C_{16}H_{12}$) is produced by the reaction of laser-ablated scandium atoms with the vapor of the ligand introduced from a container outside the source chamber. The resulting scandium complex is characterized with pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) electron spectroscopy. The PFI-ZEKE spectrum begins at 37594(5) cm^{-1} and exhibits vibrational intervals of 81, 162, 287, 340, 362, and 398 cm^{-1} in the scandium monocation complex. Through comparison with ab initio and Franck-Condon factor calculations, it is determined that this spectrum arises from a rice-ball like structure. The scandium atom is centered over the bridging carbons between the naphthalene and phenyl group. The phenyl group is rotated about 50° by scandium coordination and bends towards the metal. The 340 cm^{-1} spacing is assigned to the metal-(bridging carbons) symmetric stretch and the other observed intervals to ligand-based vibrations.