MOLECULAR STRUCTURES AND ELECTRONIC STATES OF SC-TERPHENYL COMPLEXES DETERMINED BY PULSED FIELD IONIZATION-ZERO ELECTRON KINETIC ENERGY PHOTOELECTRON SPECTROSCOPY

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Scandium complexes of p- and m-terphenyls were prepared in laser-vaporization supersonic molecular beams and studied by pulsed field ionization-zero electron kinetic energy photoelectron spectroscopy and density functional theory calculations. Several initial structures with Sc binding at different phenyl rings and bridging carbon bonds were considered in the calculations. A structure with the six-fold Sc binding at the terminal ring of these terphenyls was identified in our experiments. In both complexes, the ground electronic state of the neutral complexes was determined to be ^{4}A, and that of the corresponding ion was ^{3}A. For Sc-(p-terphenyl), the adiabatic ionization energy of 38838(6) cm^{-1} and a ring bending frequency of 49 cm^{-1} was measured for the quartet neutral molecule, and four vibrational frequencies of 354, 309, 77, and 44 cm^{-1} were identified for the triplet ion. These ion frequencies were assigned to two metal-ligand stretches, a ring torsion, and a ring bend, respectively. For Sc-(m-terphenyl), the adiabatic ionization energy was measured to be 38290(6) cm^{-1}, and seven ion vibrational frequencies were determined to be 436, 377, 355, 330, 303, 279, and 46 cm^{-1}. Similar to the p-terphenyl complex, these ion frequencies were assigned to metal-ligand stretches and ring deformations.