# $HALF-SANDWICH$ STRUCTURES OF SCANDIUM AND TITANIUM CYCLOOCTATETRAENE COMPLEXES

JUNG SUP LEE, YUXIU LEI, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

Unlike benzene, 1,3,5,7-cyclooctatetraene (COT) is not an aromatic molecule and has a tub-like structure in its ground electronic state. However, coordination of Sc or Ti converts the tub-like structure into a planar ring structure. The M-COT (M = Sc, Ti) complexes formed by interactions of laser-vaporized metal atoms and the organic ligand are studied by pulsed field ionization-zero electron kinetic energy photoelectron spectroscopy and density functional theory calculations. The theoretical calculations predict that both Sc/$Sc^+$ and Ti/$Ti^+$ prefer the $\eta^8$ binding with slightly different M-C distances. The resulting Sc/$Sc^+$ and $Ti^+$ complexes have $C_{4v}$ molecular symmetry, whereas Ti-COT has $C_{2v}$ symmetry, due to Jahn-Teller distortion. By comparing the experimental measurements and theoretical calculations, the photoelectron spectrum of the Sc complex is assigned to the $^1A_1 \leftarrow {}^2A_1$ transition with a strong 0-0 transition at 42261(5) $cm^{-1}$. On the other hand, the spectrum of the Ti complex is due to the transitions from two neutral states with similar energies, $^3B_1$ and $^3B_2$, to ionic $^2A_1$ electronic state. These transitions display strong 0-0 transitions at 40887(5) and 40863(5) $cm^{-1}$, respectively. In addition, a major vibrational progression (338 and 330 $cm^{-1}$ for the $Sc^+$- and $Ti^+$-COT stretch frequencies, respectively) and a number of vibrational hot bands are observed for the two complexes.