

## HALF-SANDWICH COMPLEXES OF GROUP III (Sc, Y, and La) METALS WITH CYCLOOCTATERAENE

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1,3,5,7 – Cyclooctatetraene (COT, C<sub>8</sub>H<sub>8</sub>) is one of the most versatile ligands used in organometallic chemistry, with coordination modes of  $\eta^2$ ,  $\eta^4$ ,  $\eta^6$ , and  $\eta^8$ . COT is non-aromatic with a tub conformation; however, its dianion (C<sub>8</sub>H<sub>8</sub>)<sup>2-</sup> is aromatic and planar. In this work, we have studied group III M-COT (M = Sc, Y, and La) 1:1 complexes using pulsed field ionization - zero electron kinetic energy (ZEKE) photoelectron spectroscopy and density functional theory. The ZEKE spectra of these complexes show a strong 0-0 transition and a major metal-ligand stretching progression. The ionization energies are measured to be 42261(5), 40747(5), and 36641(5) cm<sup>-1</sup>; and the M<sup>+</sup>-COT stretching frequencies are 338, 300, and 278 cm<sup>-1</sup> for the triad. The ionization energies of the metal complexes decrease down the group as expected from those of the bare metal atoms. The metal-ligand stretching frequencies decrease with increasing the mass of the metal atoms. In coordination with theory, the neutral and ionized complexes are determined to be in C<sub>4v</sub> point group, with M/M<sup>+</sup> in  $\eta^8$  binding to the planar COT; the observed transition is assigned to <sup>1</sup>A<sub>1</sub> ← <sup>2</sup>A<sub>1</sub>. The conformation change of the COT molecule upon metal coordination is associated with the metal to ligand electron transfer and metal-ligand orbital interaction.