

IR-UV RESONANT TWO-PHOTON IONIZATION SPECTROSCOPY OF $\text{Sc}_n(\text{BENZENE})_m$ ($n = 1, 2$; $m = 1-3$) AND $\text{Sc}(\text{BIPHENYL})$

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The complexes of $\text{Sc}_n(\text{C}_6\text{H}_6)_m$ ($n = 1, 2$; $m = 1-3$, $n \leq m$) and $\text{Sc}(\text{C}_{12}\text{H}_{10})$ were synthesized in a laser-vaporization metal cluster beam source. The C-H stretching frequencies of these complexes were measured with IR-UV resonant two-photon ionization spectroscopy. The experimental C-H stretching frequencies were compared with those of the free ligands and with the B3LYP/6-311+G(d,p) calculations. From these comparisons, the ground electronic states were determined to be $^4\text{A}_1(\text{C}_{6v})$ for the half-sandwich $\text{Sc}(\text{C}_6\text{H}_6)$, $^2\text{B}_{3g}(\text{D}_{2h})$ for the sandwich $\text{Sc}(\text{C}_6\text{H}_6)_2$, $^1\text{A}(\text{D}_2)$ for the double sandwich $\text{Sc}_2(\text{C}_6\text{H}_6)_3$ and $^2\text{B}_1(\text{C}_{2v})$ for the clamshell $\text{Sc}(\text{C}_{12}\text{H}_{10})$. The conclusions from this work are in consistent with the previous ZEKE spectroscopic studies.^{a,b}

^aB. R. Sohnlein, S. Li, and D.-S. Yang, *J. Chem. Phys.* 123 (21), 214306 (2005).

^bB. R. Sohnlein, J. F. Fuller, and D.-S. Yang, *J. Am. Chem. Soc.* 128 (33), 10692 (2006).