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

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The complexes of $Sc_n(C_6H_6)_m$ (n =1, 2; m =1-3, n$\leq m$) and $Sc(C_{12}H_{10})$ 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 $^4A_1$ (C_{6v}) for the half-sandwich $Sc(C_6H_6)$, $^2B_{3g}(D_{2h})$ for the sandwich $Sc(C_6H_6)_2$, $^1A(D_2)$ for the double sandwich $Sc_2(C_6H_6)_3$ and $^2B_1(C_{2v})$ for the clamshell $Sc(C_{12}H_{10})$. The conclusions from this work are in consistent with the previous ZEKE spectroscopic studies.[a,b]

[a] B. R. Sohnlein, S. Li, and D.-S. Yang, J. Chem. Phys. 123 (21), 214306 (2005).
[b] B. R. Sohnlein, J. F. Fuller, and D.-S. Yang, J. Am. Chem. Soc. 128 (33), 10692 (2006).