$CLAM$ STRUCTURES OF METAL-BIPHENYL COMPLEXES: M-$C_{12}H_{10}$ (M = Sc, La, Ti)

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In the gas phase, the two phenyl rings of biphenyl ($C_{12}H_{10}$) are twisted with respect to each other by about 45^0. This rotation of the phenyl rings about the bridging C-C bond is driven by π-conjugation of the phenyl rings and steric repulsions between the ortho hydrogen atoms. We have discovered that metal coordination induces phenyl ring rotation and bending to form a $clam$ structure, where a metal atom is clamped by the two phenyl rings. In this talk, we will present examples of how this clam-type structure was identified using pulsed field ionization zero electron kinetic energy photoelectron spectroscopy and density functional theory calculations. The examples include the biphenyl complexes of scandium (Sc), lanthanum (La), and titanium (Ti), which are synthesized by laser vaporization molecular beam techniques. All these complexes are determined to have C_{2v} symmetry. The ground electronic states are $^2B_1$ for the neutral Sc- and La-$C_{12}H_{10}$ complexes and $^1A_1$ for the corresponding ions. The ground electronic states of Ti- and Ti^+-$C_{12}H_{10}$ are $^1A_1$ and $^2B_1$, respectively. In addition, we will discuss the binding effects of metal atomic size and electron configuration in these molecular systems.