PFI-ZEKE STUDY OF METAL-π INTERACTION IN TRANSITION METAL-BENZENE COMPLEXES: M(C_6H_6) (M = Sc, Y, La)

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Metal interactions with aromatics are of fundamental importance in organometallic chemistry and catalytic processes. Metal-benzene complexes provide a prototype to investigate such metal-π interactions. We have produced M(C_6H_6) (M = Sc, Y, La) complexes in supersonic molecular beams and obtained their electronic spectra using pulsed-field-ionization ZEKE (zero-electron-kinetic-enery) spectroscopy. From the ZEKE spectra, we have measured adiabatic ionization potentials (AIPs) and intermolecular stretching frequencies. The spectra also allowed for the determination of the molecular conformation of these species. The AIPs of M(C_6H_6) are 41600, 41060, and 36821 cm^{-1}, and the M/M^+-C_6H_6 stretching frequencies are 324/375, 288/328, and 246/292 cm^{-1}, in the order of M = Sc, Y, and La. Both the neutral and ionic complexes are in C_{6v} symmetry.