ZEKE SPECTROSCOPY AND ELECTRONIC STATES OF BIS(BENZENE) TITANIUM AND VANADIUM SANDWICH COMPLEXES

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Ti- and V-$(C_6H_6)_2$ sandwich complexes seeded in helium supersonic beams have been studied by pulsed field ionization zero electron kinetic energy photoelectron spectroscopy and theoretical calculations. The electronic states of the neutral and ionic complexes have been determined by comparison of experimental and simulated spectra. The ground electronic states of the neutral Ti- and V-$(C_6H_6)_2$ complexes are determined to be $^1A_{1g}$ and $^2A_{1g}$, respectively. In these states, the sandwich complexes have η^6-binding between the metal and each benzene ring and are in an eclipsed D_{6h} configuration. Ionization of these neutral states causes the benzene rings to pucker slightly and leads to Jahn-Teller distorted D_{2h} sandwich ions. The Ti^+- and V^+-$(C_6H_6)_2$ ions are in the $^2B_{3g}$ and $^3B_{3g}$ electronic states. The ionization energies of Ti- and V-$(C_6H_6)_2$ are measured to be 5.731(3) and 5.784(5) eV, and the symmetric metal-benzene stretching frequencies in these corresponding ions are 228 and 231 cm^{-1}.