ZEKE SPECTROSCOPY OF GROUP VIB $M(C_6H_6)_2$ (M = Cr, Mo, W) SANDWICH COMPLEXES

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Dibenzene complexes of chromium, molybdenum, and tungsten, $M(C_6H_6)_2$ (M = Cr, Mo, W), were produced by laser ablation in a supersonic jet and probed by pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) electron spectroscopy. The adiabatic ionization potentials were measured to be 44081(6), 44581(11), and 43635(6) cm^{-1} for $Cr(C_6H_6)_2$, $Mo(C_6H_6)_2$, and $W(C_6H_6)_2$, respectively. The chromium-dibenzene spectrum displays three quanta excitations of the 265 cm^{-1} metal-benzene symmetric stretch mode in the cation, whereas the molybdenum and tungsten complexes show only one excitation of the metal-ligand stretch of 277 and 370 cm^{-1}, respectively. The shift in the ionization energy from the bare metal atom to the complex (10494, 12623 and 19792 cm^{-1}) and metal-ligand stretch frequencies increase, as the group is descended. These observations indicate a stronger metal-benzene interaction for the heavier atoms, especially tungsten. The ground states of the neutral and ionic complexes appear to be in D_{6h} symmetry with the hydrogen atoms slightly bent towards the metal center, as suggested by the good agreement between experiment and theory.