INFRARED PHOTODISSOCIATION SPECTROSCOPY OF TRANSITION METAL-ACETYLENE COMPLEXES AS A STUDY OF METAL Π -BONDING

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 $M^+(C_2H_2)_nAr_m$ (M = V, Fe, Co, Ni) complexes are produced, isolated and studied by infrared photodissociation spectroscopy near the region of the asymmetric and symmetric C-H stretches of acetylene (3289 cm⁻¹, 3374 cm⁻¹). The acetylene symmetric C-H stretch is infrared inactive but gains IR intensity upon metal ion complexation. Experimental spectra are compared to B3LYP predicted frequencies. The combined spectra and theory of the monoacetylene complexes reveal that iron, cobalt, and nickel form π -complexes, whereas $V^+(C_2H_2)$ is a three-membered ring metallacycle with vibrations similar to cyclopropene. The structures of Ni⁺(C₂H₂)₁₋₄ are also revealed by comparing experimental spectra to theory.