INFRARED PHOTODISSOCIATION SPECTROSCOPY OF COBALT CATION ACETYLENE COMPLEXES

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Cobalt cation-acetylene complexes are size-selected and studied with infrared laser photodissociation spectroscopy. $Co^+(C_2H_2)_n$ complexes are produced via laser vaporization in a pulsed supersonic expansion of argon seeded with acetylene. These complexes are mass-selected in a reflectron time-of-flight mass spectrometer, and their infrared spectra are measured in the C–H stretching region (2800 - 3400 cm⁻¹) with photodissociation spectroscopy. A coordination number of three is found for cobalt cation. Density functional theory calculations are performed with the B3LYP functional with the Def2TZVP basis set to support experimental spectra. Bands are observed for both the asymmetric and symmetric stretch of acetylene and are red-shifted from those of free acetylene. The presence of reacted and cation- π structures is investigated by comparing experiment to theory.