INFRARED RESONANCE ENHANCED PHOTODISSOCIATION SPECTROSCOPY OF GAS PHASE Ni^+ (Benzene)_n and Ni^+ (Benzene)_n Ar COMPLEXES

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Ni⁺(Benzene)_n and Ni⁺(Benzene)_nAr complexes are produced by laser vaporization in a pulsed supersonic expansion. Ions of interest are mass selected in a reflectron time-of-flight mass spectrometer where they photodissociate after excitation from a tunable infrared OPO/OPA laser system. Photodissociation of Ni⁺(benzene)_n complexes occurs by the elimination of whole neutral benzene molecules while the argon tagged species lose argon. Infrared Resonance Enhanced Photodissociation (IR-REPD) spectra are obtained by monitoring the fragment ion intensity while scanning the infrared laser system in the region from 2700-3300 cm⁻¹. Vibrational bands in this region lie near to, but shifted from, the ν_{12} free benzene C-H stretching mode due to the perturbation from the metal cation. A significant change in the spectrum occurs after the addition of the third benzene molecule to the complex indicating solvation. Interpretation of the observed infrared spectra and density functional theory obtained for these prototypical π -bonded organometallic complexes will be discussed.