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Infrared Spectroscopy of Metal Ion Complexes: Models for Metal Ligand Interactions and Solvation

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Weakly bound complexes of the form M^+L_x ($M=Fe, Ni, Co, etc.; L=CO_2, C_2H_2, H_2O, benzene, N_2$) are prepared in supersonic molecular beams by laser vaporization in a pulsed-nozzle cluster source. These species are mass analyzed and size-selected in a reflectron time-of-flight mass spectrometer. Clusters are photodissociated at infrared wavelengths with a Nd:YAG pumped infrared optical parametric oscillator/amplifier (OPO/OPA) laser or with a tunable infrared free-electron laser. $M^+(CO_2)_x$ complexes absorb near the free CO_2 asymmetric stretch near 2349 cm^{-1} but with an interesting size dependent variation in the resonances. Small clusters have blue-shifted resonances, while larger complexes have additional bands due to surface CO_2 molecules not attached to the metal. $M^+(C_2H_2)_n$ complexes absorb near the C-H stretches in acetylene, but resonances in metal complexes are red-shifted with respect to the isolated molecule. Ni^+ and Co^+ complexes with acetylene undergo intracluster cyclization reactions to form cyclobutadiene. Transition metal water complexes are studied in the O-H stretch region, and partial rotational structure can be measured. $M^+(benzene)$ and $M^+(benzene)_2$ ions ($M=V, Ti, Al$) represent half-sandwich and sandwich species, whose spectra are measured near the free benzene modes. These new IR spectra and their assignments will be discussed as well as other new IR spectra for similar complexes.