INFRARED PHOTODISSOCIATION SPECTROSCOPY OF CATION-MOLECULAR COMPLEXES

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Transition metal cation-molecular complexes are produced in pulsed supersonic molecular beams by laser vaporization. These ions are mass-selected in a specially designed reflectron time-of-flight mass spectrometer and studied with infrared laser photodissociation spectroscopy. Infrared spectra are compared to the predictions of theory (DFT and/or MP2) to elucidate the structures of these ions and their electronic states. Transition metal (Co, V, Nb) carbonyls are studied in the C-O stretching region and transition metal-water complexes are studied in the O-H stretching region. In both cases, the spectra reveal coordination numbers and ligand or solvent molecular vibrational shifts as a function of cluster size.