INFRARED PHOTODISSOCIATION SPECTROSCOPY OF MASS-SELECTED METAL ION-BENZENE COMPLEXES

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Metal ion-benzene complexes of the form $M^+(\text{benzene})_{1,2}$ (M=V, Ti, Al) are produced by laser vaporization in a pulsed nozzle source, mass-selected in an ion-trap mass spectrometer and excited in the infrared with a free electron laser. Multiphoton dissociation occurs by the elimination of benzene molecules. The photofragment yield versus wavelength produces IR resonance-enhanced multiphoton photodissociation (IR-REMPD) spectroscopy for these complexes. Vibrational bands in the 600-1800cm^{-1}region are characteristic of the benzene molecular moiety perturbed by the metal bonding. Experimental data are compared to the IR spectra derived from density functional calculations. Vibrational patterns in $V^+(C_6H_6)$ indicate that the metal is bound in an η^6 π-bonding configuration, while $V^+(C_6H_6)_2$ is a sandwich. Trapped-ion IR-REMPD is a general method to access the vibrational spectra of novel organometallic complexes.