INFRARED PHOTODISSOCIATION SPECTROSCOPY OF CATIONIC TRANSITION METAL-NITROGEN COM-PLEXES

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Transition metal-nitrogen complexes of the form $TM^+(N_2)_n$ (TM=V, Fe, Nb) are produced in a laser vaporization pulsed nozzle cluster source, size selected with a time-of-flight mass spectrometer and excited in the infrared with an infrared OPO/OPA. Infrared photodissociation occurs by elimination of whole N₂ molecules and the photofragement yield versus wavelength produces IR resonance-enhanced photodissociation (REPD) spectra for the clusters. Vibrational bands seen in the 2100 - 2400 cm⁻¹ region correspond to the N-N stretch but are shifted from those of free N₂. Density functional theory calculations on the bond energeries, geometries and frequency shifts for the TM⁺(N₂)_n are also discussed in regard to periodic trends.