INFRARED PHOTODISSOCIATION SPECTROSCOPY OF FIRST ROW TRANSITION METAL-CARBONYL CATIONS

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Transition metal-carbonyl cations are generated in a laser vaporization/supersonic expansion cluster source, mass selected and studied using infrared laser photodissociation spectroscopy. The carbonyl stretching region (2050-2350 cm^{-1}) is probed using a tunable infrared OPO/OPA system. Several cluster sizes are investigated and insight into their stability and geometry is obtained. $Cu(CO)_4^+$ has a complete coordination sphere, consistent with 18-electron stability and a tetrahedral structure similar to that of isovalent $Ni(CO)_4$. $Ti(CO)_6^+$ has a complete coordination sphere and does not satisfy the 18-electron rule. DFT calculations are performed and reported to corroborate the experimental data.