

INFRARED PHOTODISSOCIATION SPECTROSCOPY OF $\text{Co}^+(\text{H}_2\text{O})\text{RG}$ WITH He, Ne, AND Ar RARE GAS TAGGING.

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Complexes of $\text{Co}^+(\text{H}_2\text{O})$ and $\text{Co}^+(\text{D}_2\text{O})$ are produced via laser vaporization of cobalt metal in a supersonic expansion of rare gas seeded with water. Infrared photodissociation spectroscopy is accomplished with the aid of rare gas tagging by He, Ne, or Ar. The effect of Co^+ on the ortho-para nuclear spin statistics of H_2O and D_2O are investigated. The OH stretching frequencies of water were found to red shift by about 40 cm^{-1} , and the water bending mode was found to blue shift by 23 cm^{-1} . Rotational resolution was achieved for helium tagged water complex. The combined effect of spin-orbit coupling and spin-rotation coupling in these complexes is discussed and compared to the previously studied systems $\text{Sc}^+(\text{H}_2\text{O})$ and $\text{Ti}^+(\text{H}_2\text{O})$. Electronic structure calculations with CASSCF/cc-pVTZ were used to determine the single reference character of the ground electronic state. MN15/cc-pVTZ was used to compute vibrational frequencies.