

PHOTODISSOCIATION SPECTROSCOPY OF METAL ION-NEON COMPLEXES

JOHN E REDDIC, MICHEAL A DUNCAN, STEVE H PULLINS, *Department of Chemistry, University of Georgia, Athens, Ga 30602.*

The weakly bound complexes of the form M^+-Ne ($M = Mg, Ca$) are prepared in a pulsed nozzle/laser vaporization cluster source and the low lying electronic states are studied with mass-selected photodissociation spectroscopy. The M^+ ($^2P \leftarrow ^2S$) atomic resonance line is the chromophore giving rise to the molecular spectra for both Ca^+ and Mg^+ complexes. A $^2\Sigma^+$ ground state with $^2\Sigma^+$ and $^2\Pi$ excited states are derived from these atomic transitions. Electronic transitions to the red of the atomic resonance line assign to the $A \ ^2\Pi \leftarrow X \ ^2\Sigma^+$ system indicating that the complex is more strongly bound in the excited state than in the ground state. Unresolved dissociative states are observed the blue of the atomic transitions and assigned to the $B \ ^2\Sigma^+$ excited states. Extrapolation of the M^+-Ne stretch determines the excited state dissociation energy to be $D_0' = 1696 \text{ cm}^{-1}$, and an energetic cycle determines the ground state value to be $D_0'' = 112 \text{ cm}^{-1}$ for the Mg^+-Ne complex. Similar extrapolations for the Ca^+-Ne complex determine $D_0' = 857 \text{ cm}^{-1}$ and $D_0'' = 103 \text{ cm}^{-1}$. Analysis of rotationally resolved spectra determine bond lengths for the Mg^+-Ne complex of $r_0'' = 3.20 \text{ \AA}$ and $r_0' = 2.60 \text{ \AA}$. Analysis of rotationally resolved spectra for the Ca^+-Ne complex determine bond lengths of $r_0'' = 3.87 \text{ \AA}$ and $r_0' = 3.24 \text{ \AA}$. For the Ca^+-Ne complex, an additional electronic transition is observed to the red of the (forbidden) $^2D \leftarrow ^2S$ atomic resonance lines and is assigned to the $^2\Sigma^+ \leftarrow ^2\Sigma^+$ transition in the complex. Extrapolation of the Ca^+-Ne stretch determines the excited state dissociation energy to be $D_0' = 61 \text{ cm}^{-1}$. Rotationally resolved data determines the excited state bond length to be $r_1' = 4.27 \text{ \AA}$.