

SEQUENTIAL CLUSTERING OF HCl IN ARGON: NEAR INFRARED SPECTRA OF Ar₂HCl AND Ar₃HCl

DAVID T. ANDERSON, SCOTT DAVIS and DAVID J. NESBITT, *JILA, National Institute of Standards and Technology and Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado 80309-0440.*

High resolution near infrared spectra of the $\nu_{\text{HCl}}=1\leftarrow 0$ fundamental stretch in Ar₂HCl and Ar₃HCl have been characterized using a slit-jet infrared spectrometer. Analysis of the jet cooled, rotationally resolved spectra i) permit unambiguous identification of the cluster size, ii) provide vibrationally averaged geometries in the $\nu_{\text{HCl}}=1$ excited state, and iii) allow the vibrational shift of the HCl chromophore to be measured as a function of the number of Ar atoms in the complex. The equilibrium structures of the Ar_nHCl (n=1-3) clusters calculated using accurate Ar-Ar and Ar-HCl pair potentials are consistent with the vibrationally averaged structures inferred spectroscopically. The vibrational redshifts for the Ar_nHCl (n=1-3) reflect a near-linear dependence on the number of Ar atoms, which is qualitatively reproduced by simple classical calculations of the $\nu_{\text{HCl}}=0$ and 1 pairwise additive potential surfaces. Finally, predictions of the HCl matrix shifts in a relaxed fcc lattice of Ar atoms significantly overshoot the matrix value and indicate an appreciable sensitivity to non-nearest neighbors in 2nd, 3rd and higher order solvation shells.