

INFRARED SPECTROSCOPY OF $[\text{H}_2\text{O}-(\text{Kr})_n]^+$ ($n=1-3$): HEMIBOND FORMATION WITH WATER

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Spatial overlap of two non-bonding orbitals of ionized and neutral molecules can result in formation of a hemibond (two-center three-electron (2c3e) bond). Though hemibond formation between water and rare gas atom has been theoretically predicted, no definite experimental evidence has been reported. In the present study, we perform infrared spectroscopy of $[\text{H}_2\text{O}-(\text{Kr})_n]^+$ ($n=1-3$) clusters in the gas phase. Comparison of the observed spectral features in the OH stretch region with the ab initio anharmonic vibrational simulations demonstrates the hemibond formation between water and Kr in all the observed cluster sizes.