

VIBRATIONAL SPECTRA OF $\text{H}_3\text{O}^+\cdots\text{X}_n$: INTERPLAY BETWEEN FERMI RESONANCE AND COMBINATION BAND

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Solvation of H_3O^+ is an interesting and important problem in Chemical Physics. To gain a better understanding of the vibrational coupling in solvated H_3O^+ , many studies using gas-phase Infra-Red Pre-Dissociation (IRPD) spectroscopy have been attempted. In experimental spectra of $\text{H}_3\text{O}^+\cdots\text{Ar}_3$, a pronounced splitting of O-H stretching near 3300 cm^{-1} is attributed to Fermi Resonance with overtone of bending. But a peculiar band at similar frequency observed in $\text{H}_3\text{O}^+\cdots(\text{N}_2)_3$ has been assigned to be a combination band with hydrogen-bonded stretching modes. To gain further insight into the mechanism of these two types of anharmonic coupling, we have measured IRPD spectra of $\text{H}_3\text{O}^+\cdots\text{Kr}_3$, and $\text{H}_3\text{O}^+\cdots(\text{CO})_3$. Ab Initio Anharmonic Algorithms have been applied to $\text{H}_3\text{O}^+\cdots\text{X}_3$, ($\text{X}=\text{Ne}$, Ar , Kr , N_2 , CO and H_2O) to examine the interplay between Fermi resonance and combination band.