THEORETICAL STUDY ON FERMI RESONANCE OF THE EXCESS PROTON VIBRATION IN BINARY CLUSTERS

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In protonated binary clusters, location and magnitude of delocalization of the excess proton is shown to correlate to the difference of the proton affinities of the two components[a]. Theoretical calculations on a series of protonated binary clusters have shown that Fermi resonance can occur in clusters containing amines. For examples, in $(CH_3)_3N\text{-}H^+\text{-}X$, the $N\text{-}H^+$ stretching frequency is high than the first overtone of $N\text{-}H^+$ bending modes. As the $N\text{-}H^+$ stretching frequency decreases by increasing the proton affinity of X, Fermi resonance inevitably shall occur. At least both $N\text{-}H^+$ bending modes seem to couple with the $N\text{-}H^+$ stretching mode; we performed multi-dimensional mode analyses to understand this coupling.

[a] J. R. Roscioli, L. R. McCunn, M. A. Johnson *Science* **316**, 249 (2007).