

AN INFRARED SPECTROSCOPIC STUDY ON THE FORMATION OF THE HYDROGEN BONDED INCLUSION-STRUCTURES IN THE PROTONATED METHANOL WATER CLUSTERS

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We measured IR spectra of the protonated methanol–water mixed clusters ($\text{H}^+(\text{CH}_3\text{OH})_n(\text{H}_2\text{O})_1$, $n = 6 - 10$) in the OH stretching vibrational region. Spectra of their Ar tagged clusters were also measured to explore hydrogen-bonded structure changes by the vibrational cooling. The temperature dependence of the isomer distribution was also examined by the harmonic superposition approximation (HSA) simulation. No essential change of the structures with the Ar tagging (lowering of temperature) was concluded in the size range of $n = 8 - 10$, indicating the remarkable stability of the inclusion structures in this size range. On the other hand, at $n = 7$, the large isomer distribution change with the Ar tagging is suggested. Moreover, at $n = 6$, the IR spectrum showed dramatic changes upon the Ar tagging. The protonated site switching from water to methanol well explained these observed changes.