MICROSCOPIC COMPATIBILITY BETWEEN METHANOL AND WATER IN HYDROGEN BOND NETWORK DEVELOPMENT IN PROTONATED CLUSTERS

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Infrared spectroscopy was applied to $H^+(MeOH)_m(H_2O)_n$ (m=1-4, n=6-21) protonated mixed clusters, and its size-dependent hydrogen bond network development was probed by the spectral signature of the dangling OH stretch bands. It was found that the mixed clusters form the 3-D cage structure at the same total cluster size as $H^+(H_2O)_n$, indicating the microscopic compatibility between methanol and water in the hydrogen bond network development. DFT calculations also supported such compatibility. The migration of the excess proton and the location of the protonated site are also discussed on the basis of the DFT calculations.