Thermodynamic stability and structural characteristics of clathrate hydrate incorporated with ammonium fluoride

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Hydrate frameworks stability is influenced by guest molecules capable of hydrogen bonding with surrounding water molecules. Thermodynamic stability of co-host clathrate hydrate incorporated with ammonium fluoride (NH4F) was inhibited by interaction between two ions (NH4+ and F-) and water molecules by hydrogen bonding. In addition, structural characteristics and molecular behavior were identified by using a high resolution powder diffraction (HRPD) analysis, solid-state 13C NMR, and Raman spectroscopy. The hydrate samples of NH4F + CH4 were confirmed to be structure I cubic Pm3n, whereas lattice constants of clathrate hydrate tend to decrease in proportion to the NH4F concentration. Furthermore, NH4F incorporation into framework promotes the conversion rate from ice to hydrate owing to rearrangement processes of randomly distributed ions. The present findings on the co-host role in thermodynamic stability and lattice shrinkage via restructuring the host water framework might provide important information on guest-host interactions of clathrate hydrates.