

Asymmetric Structure Induced Thermal Expansion Behavior Occurring in Tetrahydrofuran + Diatomic Hydrogen Clathrate Hydrates

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Clathrate hydrates are a type of inclusion compounds stabilized by van der waals interaction between guest molecules and host lattice (water). In this study, we investigated the asymmetric structure induced thermal expansion behavior occurring in tetrahydrofuran (THF) + diatomic hydrogen clathrate hydrates by high-resolution neutron powder diffraction. In the binary (THF + X) clathrate hydrate system (X = HD, D₂, and H₂) known to cubic Fd3m structure, lattice parameters of (THF + X) clathrate hydrates are refined by Fullprof software. Comparing to the results from H₂ and D₂ in (THF + X) clathrate hydrate system, lattice parameter of THF + HD system exhibits larger than that of THF + H₂ and D₂. Because HD has much lower molecular weight than D₂, we conclude that thermal behavior of THF + HD clathrate hydrate is induced by asymmetric structure of HD guest. This abnormal expansion of clathrate hydrates clearly due to asymmetric van der waals radii of HD guest might be one of important physical properties to understand the physico-chemical properties of clathrate hydrates.