

Structural analysis of neutron powder diffraction pattern of clathrate hydrates

신규철[†], 차민준¹, 이원희², 이 혼³

경북대학교; ¹강원대학교; ²한국에너지기술연구원; ³KAIST

(kyuchul.shin@knu.ac.kr[†])

Clathrate hydrate is a sort of nonstoichiometric crystalline solids which are stabilized by various interactions between the hydrophobic guest molecules and the hydrogen-bonded water cluster. The crystal structures of a DClO₄ hydrate depending on temperature were identified by the direct space method and Rietveld refinement of the neutron powder diffraction patterns. A phase transition causing a position change of vacancy sites in host framework was observed at about 180 K and this transition is considered to result in weakened host proton-anion interactions and to induce a change of proton conduction behavior of the DClO₄ hydrate. The present findings provide a good explanation of the proton dynamics in the host framework of the hydrogen fluoride-free acid clathrate hydrates.