Exploring Guest Inclusions and Interactions in a Binary Clathrate Hydrate of Cyclopentanemethanol and Methane

박기훈, 차민준†, 김동현
강원대학교
(minjun.cha@kangwon.ac.kr†)

In this study, cyclopentanemethanol (CPeM) was utilized as a new structure Ⅱ (sⅡ) hydrate former in the presence of methane (CH_4) gas. Guest inclusions of interactions in a (CPeM + CH_4) hydrate sample was identified with ^{13}C solid-state nuclear magnetic resonance (NMR) and powder X-ray diffraction (PXRD). In NMR spectra, it was identified that CPeM and CH_4 molecules were enclathrated in the large and small cages of sⅡ hydrate, respectively. Especially, a possible conformation of CPeM molecule in large cages of sⅡ hydrate was confirmed through conformational analysis of CPeM molecules. The crystal structure of the binary (CPeM + CH_4) hydrate was refined with Rietveld method, indicating that the formation of sⅡ hydrate with a lattice parameter of 17.28227 Å. In addition, the possible host-guest interactions in the binary (CPeM + CH_4) hydrate were discussed.

KEYWORD Clathrate Hydrate, NMR, PXRD, Cyclopentanemethanol