Structural Identification of Butanol Hydrates and Effects of Hydroxyl Group Positioning on Hydrate Stability

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In this study, we investigated the crystal structures and phase equilibria of butanols + CH_4 + H_2O systems to reveal the hydroxyl group positioning and its effects on hydrate stability. Four butanol isomers are used as clathrate hydrate formers, and the structure of these hydrates was identified with powder X-ray diffraction (PXRD). In addition, Raman spectroscopy was used to analyze the guest distributions and inclusion behaviors of large alcohol molecules in these hydrate systems. We also revealed that guest molecules can be captured in the large cages of structure II hydrates without any hydrogen bonding interaction between the hydroxyl group of the guests and the water-host framework by finding the existence of a free OH bonding. However, Raman spectra of the binary (1-butanol + CH_4) hydrate did not show the free OH signal, indicating that there could be possible hydrogen bonding interactions between the guests and hosts. We also measured the four-phase equilibrium conditions of the butanols + CH_4 + H_2O systems.