Phase Equilibria and Spectroscopic Identification of Binary (Allyl alcohol + Methane) Hydrates

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Herein, allyl alcohol (AA) was discovered to form structure Ⅱ (sⅡ) hydrate in the presence of methane (CH_4) as a help gas. For understanding the guest inclusion behaviors and crystal structure of the binary (AA + CH_4) hydrate, spectroscopic tools, such as solid-state nuclear magnetic resonance (NMR), Raman and powder X-Ray diffraction (PXRD), were used in this study. NMR results showed that the crystal structure of the binary (AA + CH_4) hydrate was structure Ⅱ. In addition, the conformation of the AA molecule in the hydrate cages were also determined from NMR spectra. The guest inclusion behavior and crystal structure of the binary (AA + CH_4) hydrate were also confirmed in the Raman pattern. The PXRD pattern of the binary (AA + CH_4) hydrate was refined by the Rietveld analysis with direct space method. As a result, AA (guest) and water-based frame (host) may interact via strong hydrogen bonding. Finally, the phase equilibrium conditions of the binary (AA + CH_4) hydrate was also measured and the results showed that the equilibrium temperatures of the binary (AA + CH_4) hydrate is slightly lower than those of the pure methane hydrate at the same pressure conditions.