

Spectroscopic Observation of Structural Transition in Trimethylamine Semi-Hydrate

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In recent study, several alkylamine hydrates have been studied in an effort to reveal the structural transitions from semi- to 'canonical' clathrate hydrate in the presence of secondary guest molecules. Trimethylamine (TMA) is known to form the semi-clathrate hydrate, and it has been reported that the structural transition of the TMA semi-clathrate hydrate may not occur in the presence of hydrogen gas. In this study, we investigate the structural transition of TMA hydrate by CH₄. Powder X-ray diffraction was used to analyze the crystal structure of a binary (TMA + CH₄) clathrate hydrate, and the results showed that the structural transition from semi- to cubic structure II hydrate can occur in the presence of methane gas. ¹³C solid-state NMR and Raman spectroscopy were used to confirm the distribution of guest molecules. Finally, we measured the phase equilibrium conditions of a binary (TMA + CH₄) clathrate hydrate. The guest-induced structural transformation in amine semi-clathrate hydrates can provide useful insight into the complex nature of the host-guest inclusion system, and these results can be applied to research on potential gas storage and transportation areas.