

Examining a Complex Tuning Mechanism Occurring in Mixed Hydrates

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The guest molecule dynamics occurring in hydrate cages appears to be very complex and, therefore, for its complete understanding at the molecular level, more sophisticated approaches which use various types of spectroscopic tools must be adopted. Solid ^{13}C MAS NMR is used to obtain fundamental information regarding the distribution of the guests over the cage sites. Additionally, PXRD, Raman, and other spectroscopic data, whenever necessary, are measured in order to determine the overall pattern of structure transformation and cage creation variables. First of all, one of the unique inclusion phenomena that can be observed in the host-guest networks of hydrates, a tuning concept, is proposed and proven via both the macroscopic and microscopic identification of target hydrates. For this investigation, two different mixed hydrate systems are specially chosen and closely examined, by altering the water-soluble large guest concentration. The experimental results confirm that the gaseous guest-molecule distributions, as well as the hydrate compositions, determined by adjusting the concentration of the liquid guest, are found to differ completely from those simply predicted or measured by classical and macroscopic means. This ‘tuning mechanism’ plays an important role in understanding hydrate cage dynamics, and, further, must be one of the strategies used to enhance the gas storage capacity of mixed hydrate systems, including a water-soluble liquid hydrate promoter, for application to gas storage and transportation.