

Tuning Phenomenon Appearing in CH₄ + THF Double Clathrate Hydrates and Analysis by Using ¹³C NMR Spectroscopy

박제성, 이 혼*
한국과학기술원
(h_lee@kaist.ac.kr*)

The concept of tuning phenomenon in double hydrate systems has been suggested to enhance the gas storage capacity through molecular interactions. In this report, the existence of critical guest concentration (CGC) is investigated by using ¹³C NMR spectroscopy in CH₄ + THF (tetrahydrofuran) double clathrate hydrate. The temperature and pressure conditions were kept constant at 268 K and 20 bar to avoid any possible appearance of pure CH₄ hydrate. The hydrate samples for NMR spectra were prepared from 5.6 to 0.05 mol% at the stoichiometric THF concentration. The cage occupancy ratio could be obtained from experimental NMR peak areas in combination with the thermodynamic equation of van der Waals and Platteeuw. The value increases continuously until it reaches a maximum, CGC, at a specific THF concentration of 0.2 mol%. We confirmed that the general tuning patterns at two different pressures of 20 and 100 bars are found to be essentially the same.