

## Thermodynamic and Spectroscopic Investigation of Binary 2,2-Dimethyl-1-Propanol+ CO<sub>2</sub> Gas Hydrates

**Authors :** Seokyeon Moon, Yun-Ho Ahn, Heejoong Kim, Sujin Hong, Yunseok Lee, Youngjune Park

**Abstract :** Gas hydrate is a non-stoichiometric crystalline compound consisting of host water-framework and low molecular weight guest molecules. Small gaseous molecules such as CH<sub>4</sub>, CO<sub>2</sub>, and N<sub>2</sub> can be captured in the host water framework lattices of the gas hydrate with specific temperature and pressure conditions. The three well-known crystal structures of structure I (sI), structure II (sII), and structure H (sH) are determined by the size and shape of guest molecules. In this study, we measured the phase equilibria of binary (2,2-dimethyl-1-propanol + CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>) hydrates to explore their fundamental thermodynamic characteristics. We identified the structure of the binary gas hydrate by employing synchrotron high-resolution powder diffraction (HRPD), and the guest distributions in the lattice of gas hydrate were investigated via dispersive Raman and <sup>13</sup>C solid-state nuclear magnetic resonance (NMR) spectroscopies. The end-to-end distance of 2,2-dimethyl-1-propanol was calculated to be 7.76 Å, which seems difficult to be enclathrated in large cages of sI or sII. However, due to the flexibility of the host water framework, binary hydrates of sI or sII types can be formed with the help of small gas molecule. Also, the synchrotron HRPD patterns revealed that the binary hydrate structure highly depends on the type of help gases; a cubic Fd3m sII hydrate was formed with CH<sub>4</sub> or N<sub>2</sub>, and a cubic Pm3n sI hydrate was formed with CO<sub>2</sub>. Interestingly, dispersive Raman and <sup>13</sup>C NMR spectra showed that the unique tuning phenomenon occurred in binary (2,2-dimethyl-1-propanol + CO<sub>2</sub>) hydrate. By optimizing the composition of NPA, we can achieve both thermodynamic stability and high CO<sub>2</sub> storage capacity for the practical application to CO<sub>2</sub> capture.

**Keywords :** clathrate, gas hydrate, neopentyl alcohol, CO<sub>2</sub>, tuning phenomenon

**Conference Title :** ICCDUSD 2018 : International Conference on Carbon Dioxide Utilization and Sustainable Development

**Conference Location :** London, United Kingdom

**Conference Dates :** January 18-19, 2018