Simple Thermodynamic Equations for Cage Occupancy Ratio of Binary Clathrate Hydrate

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The competitive inclusion behavior of multi-guests in the cages of clathrate hydrates is not yet well understood in spite of its significant importance in both scientific and technological fields. Here, we derive simple and generalized expressions related to cage occupancy ratios of binary clathrate hydrates, measure the cage occupancy ratios and finally compare the proposed expressions with the experimental results. The present approaches cover three independent categories; the binary guests competitively occupy (1) both small and large cages, (2) only small cages and (3) only large cages. In addition, we demonstrate that cage occupancy ratio is a simple but powerful variable that indicate the guest behaviors. More importantly, the present approaches only need to have the precise composition measurements to reveal the general nature of guest popularity in cages, while the original van der Waals –Platteeuw model requires several complex variables such as Langmuir constants and fugacities as indispensable prerequisites. The present outcomes might play a significant role in understanding guest occupancy details and, furthermore, provide clues for designing and synthesizing the most efficient hydrate structures to store gaseous molecules for a specific purpose.