

General relationship of Cage occupancy ratio of clathrate hydrates

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This study focuses on the cage occupancy of guest molecules at infinitely dilute state. At extreme conditions of highly diluted guest concentrations the direct measurements of cage occupancy ratio representing the competitive inclusion of multi-guest species appear to be so difficult because of spectroscopic intensity limitation, but its thermodynamic significance might be considerable due to the fact that the infinite-dilution value of cage occupancy ratio can provide the valuable thermodynamic information as the very unique and guest-specific parameter. In order to experimentally identify gaseous guest popularity in sI and sII cages we used the solid-state NMR, Gas Chromatography, and direct gas measurements. Further, we derived the simple and generalized thermodynamic equation related to cage occupancies at infinite dilution starting from van der Waals-Platteeu model. Both experimental and predicted values agree well within experimental error range. Moreover, we derived the general relationship between cage occupancies in the full range of guest concentration. In this research, we revealed that the cage occupancy ratio is a key value to explain the thermodynamic behaviors of enclathrated guest molecules.