

Intracavity conformational change of enclathrated guest molecules and its secondary guest-dependent characteristics

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Numerous hydrocarbons in clathrate hydrates have been studied because of their ability to thermodynamically stabilize clathrate phases. A comprehensive understanding of the guest-host interactions is essential to use hydrate materials for practical applications. Many acyclic hydrocarbons favor the gauche- or cis- conformation, which is less stable in terms of molecular geometry, when these molecules are enclathrated in the hydrate cavities and no cases of intracavity changes of guest conformation have been reported to date. In this study, we present the first report of conformational changes of acyclic guest molecule occurring in the hydrate cavities induced by the intercavity electron transfer after γ -irradiation. Moreover, we demonstrate that thermodynamic stability of clathrate hydrate phases is also changed. Interestingly, these phenomena are highly dependent on the types of secondary guest molecules because of different electron affinities. The present results provide meaningful information to understand the physicochemical properties of clathrate hydrates.