Guest-Host Hydrogen Bonding Effect on Thermodynamic stabilities in the binary Clathrate Hydrate with isomeric guest molecules

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Clathrate hydrates are commonly known for a kind of guest-host compound stabilized by physically stable interaction between guest and host water molecules. A conventional model for predicting hydrate phase equilibrium only concerns physical interactions. However, guest-host interactions need to be more investigated to help understanding their influence on the physicochemical and thermodynamic nature of clathrate hydrate. In the present work, the relation between thermodynamic stability and the guest-host interaction has been studied with isomeric guest molecules, which have similar van der Waals interaction and different probability of hydrogen bond, to investigate the quantitative effect of guest-host hydrogen bond.