

Conformational change of  $\alpha,\beta$ -unsaturated carbonyl compound in clathrate hydrate and its phase equilibria

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Clathrate hydrates, one of inclusion compounds, are composed of host water molecules and small gaseous or organic guest molecules. Clathrate hydrates have been researched extensively due to their potential of engineering applications such as gas storage and separation. The most well-known three structures (sI, sII and sH) of clathrate hydrates are determined by the characteristics of guest molecules such as size and shape. Like 3-methyl-1-butanol and 2-methylpropane-2-peroxol, methyl vinyl ketone is regarded as one of sII hydrate formers and investigated in this study. Since methyl vinyl ketone is an  $\alpha,\beta$ -unsaturated carbonyl compound, both s-cis and s-trans conformers exist in nature. However, by Raman spectroscopy, we observed that only s-trans form of methyl vinyl ketone is thermodynamically preferred in solution phase, and only s-cis form is enclathrated with methane in sII hydrate. Moreover, conformational change occurs inside the cavities with gamma-ray radiation. By the way, we measured phase equilibria of methyl vinyl ketone + methane hydrate with various concentrations, and methyl vinyl ketone shows a little bit thermodynamic inhibition effect.