Rotational isomers of isopentane appearing in the large cages of structure-H clathrate hydrates

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Hi-power decoupling (HPDEC) ^{13}C NMR spectra were obtained for sH (isopentane + CH_4) hydrate and (MCH + CH_4) hydrate and compared with liquid isopentane and MCH spectra in order to analyze the conformation of acyclic large guest molecules. For (isopentane + CH_4) hydrate, the resonance line shifting was detected between isopentane in hydrate and liquid isopentane, in the other hand, any shifting was not detected between MCH in hydrate and liquid MCH. The differences in the chemical shifts between sH hydrate and liquid isopentane was checked through the use of a hydrogen-hydrogen steric perturbation model. From the overall results, we concluded that one of the smallest acyclic guest molecules, isopentane, participating in the formation of a structure-H clathrate hydrate is encaged, confirming the gauche conformation in large cavities.