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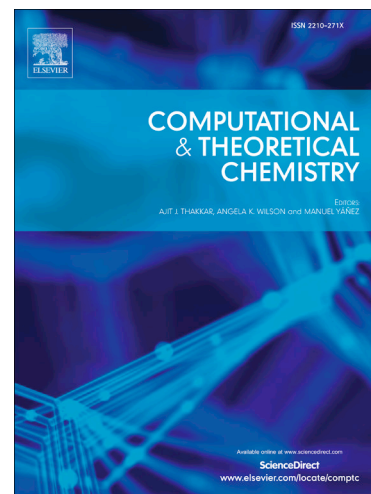
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Influence of CH₄ and C₃H₈ molecules on stability of double-cage of sI clathrate hydrate

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Abstract

Theoretical investigation on the stability of water cavities (5^{12} , $5^{12}6^2$, and $5^{12}/5^{12}6^2$) with the incorporation of a series of molecules (CH₄ and C₃H₈) is accomplished. Geometry optimization for the guest molecules, host cages, and their complexes was carried out at B3LYP/6-31+G(d) level, and on the basis of the optimized geometry, single-point energy calculation was performed at M06-2X/6-31++G(d) level to determine the interaction and stability energies. The relative energies of inclusion complexes were investigated to infer structural stability and occupancy of guest molecules. It is compared that the stabilization energy of double-cage encapsulated with CH₄/C₃H₈ guest molecule. It is found that fully occupied cages are more stable than partially occupied cages, and the stability of double-cage system in half full state gradually increases. For double-cage, CH₄@ 5^{12} /C₃H₈@ $5^{12}6^2$ cage is the most stable structure and the stability for the empty cage could be enhanced when water molecules number is increased. For CH₄@ 5^{12} /(guest)@ $5^{12}6^2$ and 5^{12} /(guest)@ $5^{12}6^2$, the interaction between guest molecule and host molecules enhances with the increase of molecular weight of the guest. Meanwhile, the formation of the CH₄@ 5^{12} cage is more favorable compared to the CH₄@ $5^{12}6^2$ cage.

Keywords: clathrate hydrate; double-cage; stability

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