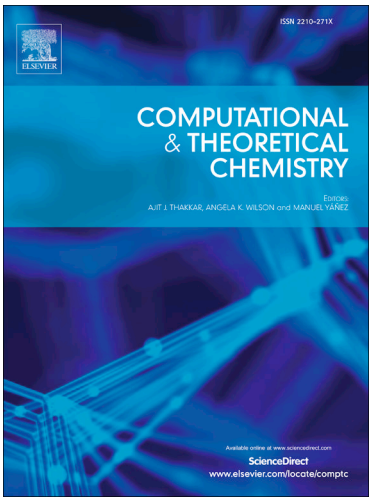

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PII: S2210-271X(17)30496-6
DOI: https://doi.org/10.1016/j.comptc.2017.11.019
Reference: COMPTC 2676

To appear in: *Computational & Theoretical Chemistry*

Received Date: 2 October 2017
Revised Date: 27 November 2017
Accepted Date: 27 November 2017

Please cite this article as: T. An, H. Zhang, Q. Zhang, Y. Wang, P. Shi, Influence of CH_4 and C_3H_8 molecules on stability of double-cage of sI clathrate hydrate, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.11.019

Influence of CH_4 and C_3H_8 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 (CH_4 and C_3H_8) 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 CH_4/C_3H_8 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, $CH_4@5^{12}/C_3H_8@5^{12}6^2$ cage is the most stable structure and the stability for the empty cage could be enhanced when water molecules number is increased. For $CH_4@5^{12}$/(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 $CH_4@5^{12}$ cage is more favorable compared to the $CH_4@5^{12}6^2$ cage.

Keywords: clathrate hydrate; double-cage; stability

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