

Calculations of NMR parameters of methane clathrate hydrates

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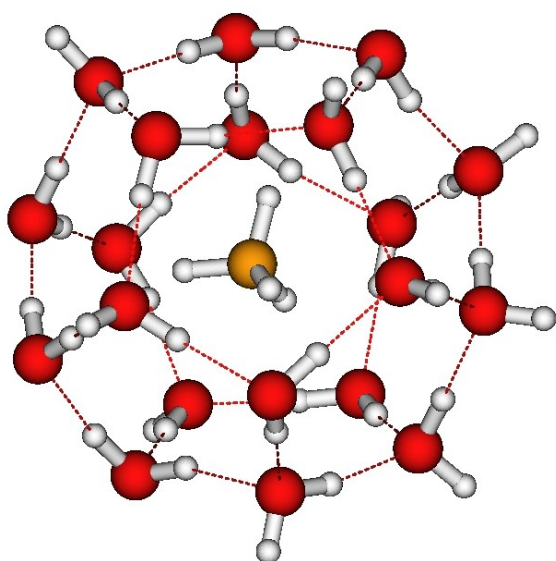
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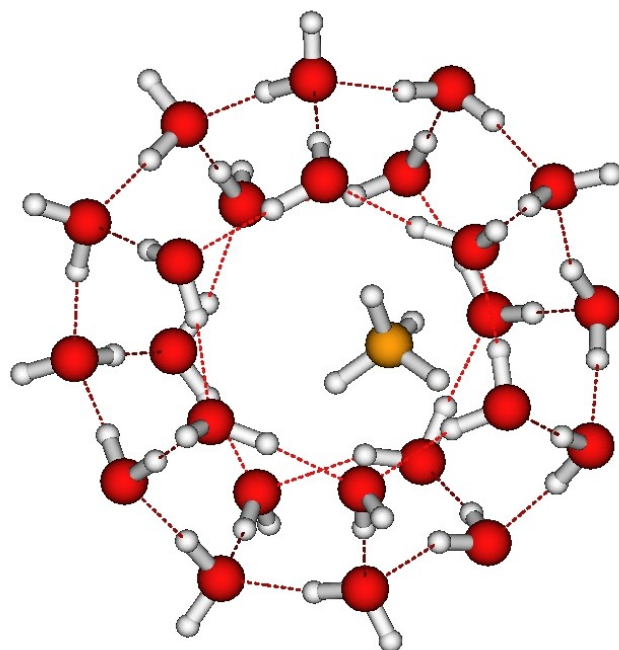
Abstract

Clathrate hydrates are solid compounds in which water encapsulates non-polar molecules. Such structures exist in huge amounts in nature, mostly with methane as a trapped guest. Methane clathrate hydrates are abundant on sea floor and in the regions of permafrost on land. The total amount of carbon in the form of methane clathrate hydrates is, according to most conservative estimates, equal to all the other carbon deposits (natural gas, crude oil, hard and brown coal etc.) combined. That is why methane clathrate hydrates can become a very important energy source in the future.

Here we present the results of DFT/B3LYP calculations of NMR parameters for methane molecule inside two cages that are forming the structure of methane clathrate hydrates (structure sI). Interactions between methane and water molecules of the cages are described. Stability of two types of cavities filled with methane molecules is also discussed and changes in the hydrogen bonding between water molecules are investigated.



Cage 5¹²



Cage 5¹²6²