Invited Lecture IL 08

Molecular Behavior of 1-Pentanol Guest in the NH_4F-doped Clathrate Hydrate

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Abstract (less than 300 words)

In pure water and even in the presence of help gases, 1-pentanol (1-PeOH) cannot form the clathrate hydrate structures both because of its size that is not appropriate for either the structure II $5^{12}6^4$ or structure H $5^{12}6^8$ cages and the presence of a hydrophilic OH group that tends to destabilize the clathrate hydrate framework. [1] Recently, the NH_4F doping in the clathrate framework was suggested to make the hydrate lattice more resistant to disruption by host-guest hydrogen bonding. [2.3] In this work, we report the synthesis of 1-pentanol + methanol binary structure II clathrate hydrate doped with NH_4F and demonstrate that the space filling of 1-pentanol as a guest molecule can be managed by the hydrogen bonding between doped NH_4F in the water framework and the hydroxyl group of 1-pentanol. The structural characterization of 1-PeOH + methanol hydrates was conducted by the powder X-ray diffraction (PXRD) pattern analysis and the solid state ^{13}C NMR spectroscopy. The 1-PeOH guest conformations and molecular interactions in the clathrate cages and the guest conformations was also investigated by the solid state ^{13}C NMR spectroscopy and molecular dynamics simulations. Additionally, the 1-PeOH hydroxyl group was observed to be incorporated in the clathrate hydrate water framework. The findings in this work show that doping the clathrate hydrate lattice with NH_4F and using methanol as a helper guest can be used for stabilizing heavier alcohol molecules which cannot be encaged in normal clathrate hydrates.

References

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