Multiple hydrogen molecular loading into sII hydrate induced by water-soluble sH former

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Hydrogen storage in clathrate hydrate imposes various important physical processes occurring in the inclusion compounds. Multiple H2 occupation in the nano-sized cage formed by hydrogen-bonded water framework shows the possibility of clathrate hydrate as future hydrogen storage materials. We present here, for the first time, H2 molecular loading into structure II (sII) hydrate induced by water-soluble sH former (1-methylpiperidine) as evidenced by PXRD and Raman spectroscopic measurements. Structural change is accompanied by reducing the concentration of 1-methylpiperidine, as the concentration decreased below 2.8 mol% and structure transition from structure H to the favorable structure II proceeds. In the course of structural transition, hydrate structure is fully tuned to adopt hydrogen clusters (2-4 H2 molecules) in 51264 cages and single occupancy in 512 cages which significantly increase hydrogen storage wt% by 40-60% compared to sH hydrate.