Hydrogen multiple occupancy in tuned cages of clathrate hydrates

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Clathrate hydrates are composed of both small and large cages made by host water frameworks. Small cage called as dodecahedral cavity is too small to accommodate multiple hydrogen molecules. The possibility of double hydrogen occupancy in dodecahedral cavity has been suggested, but it is still controversial issue. Here we discover the unique phenomenon of multiple hydrogen occupancy in dodecahedral cavities by tuning the cage dimensions. The degree of molecular hydrogen storage depends on the concentration of guest promoter in the hydrate matrix through tuning cage dimensions. The discovery in this study provides the strategy for increasing hydrogen storage capacity in clathrate hydrates.