Multiple Occupancy of Hydrogen in Clathrate Hydrate Driven by Molecular Exchange

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Hydrogen clathrate hydrates receive attention due to their advantages of environmentally friendly feature, low cost and comparatively high storage efficiency. The loading of multiple H_2 molecules into both small (5^{12}) and large ($5^{12}6^4$) cage under mild conditions is the most important factor to utilize clathrate hydrates for hydrogen storage media. Furthermore, balancing the formation pressure with high storage capacity is one of the most significant factors. In this study, we introduced a new concept that uses (LGM+N_2) hydrates to capture hydrogen clusters under relatively mild conditions, even observing double H_2 occupancy in 5^{12}-cages. The cage occupancy and structures of hydrates were identified by the Raman spectroscopic analysis and the high resolution powder diffraction. Reaction product suggests possibility of multiple H_2 occupancy in both 5^{12} and $5^{12}6^4$-cage at relatively low pressure. The unique and abnormal role of N_2 as a preoccupied co-guest significantly affects the H_2 population in a crystalline hydrate matrix and further lowers pressure for structure stabilization.