Spectroscopic identification of multiple hydrogen occupancy in binary clathrate hydrate

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Hydrogen clathrate hydrates receive attention due to their advantages of environmentally friendly feature, low cost and comparatively high storage efficiency. To form pure hydrogen hydrates typically requires very high pressure (~2000 bar) and low temperature conditions. The loading of multiple H2 molecules into both small and large cage under mild conditions is the key factor to utilize clathrate hydrates for hydrogen storage media. To explore the potential realization of H2 multiple cage occupancy under moderate conditions, reaction product of binary (LGM+ N2) hydrates with H2 molecules was synthesized and a series of microscopic analyses (Raman spectroscopy and high resolution powder diffraction) was conducted. Reaction product suggests possibility of multiple H2 occupancy in each cage at relatively low pressure. The idea was to substitute the large N2 molecule in N2 hydrate with the smaller H2 molecule. We acquired microscopic spectrum showing cage occupancy according to increase of H2 pressure, as well as cage occupancy comparison between reaction product and nonreaction product. Also, we obtained their lattice parameter for each sample to analyze correlation of lattice constant with cage occupancy.