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Hydrogen clathrate hydrate - novel hydrogen storage material: crystal structure, kinetics, and phase diagram KONSTANTIN LOKSHIN, YUSHENG ZHAO, Los Alamos National Laboratory — The detailed crystal structure information for the hydrogen clathrate hydrate was determined by neutron diffraction as a function of temperature (10-300 K) and pressure (1-2000 bar) for the first time. We found that hydrogen occupancy in the $(32+X)H_2*136H_2O$, x=0-16 clathrate can be reversibly varied by changing the large (hexakaidecahedral) cage occupancy between 2 and 4 molecules, but keeping single occupancy of the small (dodecahedral) cage in the sII structure. Above 130-160K the guest hydrogen molecules were found in the delocalized state, rotating around the centres of the cages. Decrease of temperature results in the rotation freezing followed by a complete localization below 50 K. We have discovered an extremely fast method of the clathrate synthesis, which allows the complete hydrogen hydrate formation in minutes. The influence of substitutions of different entities for hydrogen on the clathrate structure and stability was studied. High hydrogen capacity (up to 3.77 mass % at ambient pressure), fast kinetics, and readily accessible $P-T$ range are the features that make hydrogen clathrate an excellent candidate for a hydrogen storage material.

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