Temperature-Dependent Release of Guest Molecules and Structral Transformation of Hydroquinone Clathrate

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The structural transformations and guest dynamics of guest-loaded compounds(CO2-, CH4-, and CO2/CH4-loaded β -form hydroquinone (HQ) clathrates) in which gases were encapsulated and guest-free compounds(although there were no gases encapsulated in the host framework, the compound was characterized by a specific space) were evaluated using X-ray diffraction and Raman spectroscopy. In addition, temperature-dependent Raman spectra were measured in the temperature range 300-385 K at increments of 5 K. The CH4 molecules rapidly escaped from the β -form HQ clathrate in the temperature range 360 to 380 K, whereas the CO2 molecules were gradually released from the β -form HQ clathrate framework in the wide temperature range 300 to 380 K. It was also found that both CO2 and CH4 molecules were rapidly released from the CO2/CH4-loaded β -form HQ clathrate framework in the temperature range 360 to 380 K. However, all of the guest-free and guest-loaded β -form HQ clathrates revealed fully converted to the α -form HQ clathrate temperature at 385 K. These results demonstrate the strong effect of temperature on both guest-host interactions and the stability of the framework structure.