Spectroscopic and crystallographic analyses of the binary HPF_6 and CH_4 clathrate hydrate

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The HPF_6 clathrate hydrates possess two intrinsic crystalline structures with the variation of H_2O concentration. The HPF_6•$6H_2O$ hydrate has been found to have the type VII structure, which is composed of $4^6 6^8$ cages fully occupied by $PF6^-$. On the other hand, HPF_6•$7.67H_2O$ hydrate with sI structure is built by vacant 5^{12} cages and PF_6^- filled $5^{12}6^2$ cages. However, at lower concentration of PF_6^-, the HPF_6•$17H_2O$ hydrate, type VII structure does not appear and the hydrate phase maintains sI structure as PF_6^- anion is partially filled with large $5^{12}6^2$ cages of sI hydrate. When CH_4 gas molecules are introduced, their structure is also maintained with sI structure. It seems that at high pressure, CH_4 gas molecules penetrate to pure hydrate phase and occupy vacant cages without any structural transition. To characterize the hydrates, Raman spectroscopy and X-ray diffractometer are used.