The Phase Transition of Hydrogen–bonded Ferroelectric PbHPO₄ under High Pressure

<u>Yuki Nakamoto</u>^a, Tomoko Kagayama^a, Katsuya Shimizu^a, Kiyoshi Deguchi^b, Takamitsu Yamanaka^c, ^aKYOKUGEN, Osaka Univ., Osaka. ^bDept. Mat. Sci. Inst. Sci. and Tech. Shizuoka. ^cDept. Earth and Space Science, Grad. School Sci. Osaka Univ. Osaka, Japan. E-mail: nakamoto@rcem.osaka-u.ac.jp

PbHPO₄ (LHP), undergoes a phase transition from Phase I to Phase II at $T_{\rm C}$ =310 K under ambient pressure. The lower-temperature ferroelectric phase (Phase II) with pseudo-one dimensional hydrogen bonded structure has a space group of Pc. The paraelectric phase (Phase I) has been assumed to have P2/c. The Tc is gradually lowed with increasing pressure and then Tc goes down to room temperature, The transition pressure has been determined to be 0.15 GPa [1]. But the phase transition was no more found over 3 GPa. In this present work, x-ray powder diffraction study of LHP was carried out using synchrotron radiation with diamond anvil pressure cell under hydrostatic conditions at room temperature on BL-18C (KEK), Tsukuba. We could not detect any differences in the diffraction patterns of Phase II and Phase I with increasing pressure up to 5 GPa. By further compression a new pressure-induced phase (Phase III) appears at about 6.5 GPa. We have determined that the structure of Phase III has a possible space group of *Pmmm*, which is stable up to 17 GPa. During decompression cycle, phase III is covered back to the original phase I at 0.7 GPa.

[1] Mylov V. P., et al., *Sov. Phys. –Crystallogr.*, 1979, **24**, 738. Keywords: ferroelectrics, high pressure, phase transition