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Structural changes in borohydride hydrogen storage materials[1]
RAVHI KUMAR, HiPSEC, Dep.Physics, University of Nevada Las Vegas, NV 89154, ANDREW CORNELIUS, HiPSEC, Department fo Physics and Astronomy, University of Nevada Las Vegas, NV 89154, MALCOLM NICOL, HiPSEC, Department of Physics and Astronomy, University of Nevada Las Vegas, NV 89154 — Angle dispersive powder x-ray diffraction and Raman experiments were performed on ABH_4 (A = K, Rb) at high pressures up to 27 GPa. We demonstrate that KBH_4 exhibits structural phase transitions from the ambient α-KBH4 phase (cubic Fm-3m) to β-KBH_4 (tetragonal-P421c) at 3.8 GPa and to γ-KBH_4 phase (orthorhombic-Pnma) at 6.8 GPa which is similar to the phase transition sequence observed for NaBH4 earlier [1]. However, $RbBH_4$ undergoes two successive pressure induced structural transitions from the ambient cubic Fm-3m phase to an orthorhombic Pnma phase around 2.9 GPa and then to a monoclinic phase above 8 GPa. The high pressure monoclinic phase is found to be stable up to 27 GPa. The experimental results reveal the phase transition sequence exhibited by $RbBH_4$ is different from the pressure induced changes observed in similar cubic compounds $NaBH_4$ and KBH_4. The results further show that both the transition pressure and the structural ordering at high pressures are influenced by the atomic size of the alkali cation in these compounds.
[1]. R.S. Kumar and Andrew L. Cornelius, App.Phys.Lett., 2005, 87, 261916.

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