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Structural transitions in NaBH4 under pressure¹ RAVHI KUMAR,

ANDREW CORNELIUS, University of Nevada, Las Vegas — The structure of the technologically important hydrogen storage compound NaBH₄ has been investigated under pressures up to 30 GPa by in situ angle dispersive high pressure x-ray diffraction using synchrotron x-rays and a diamond anvil cell. Our experimental results show pressure-induced structural transitions of α -NaBH₄ (cubic – Fm3m) to β – NaBH₄ (tetragonal – $P42_1c$) at 6.3 GPa and further to orthorhombic phase (Pnma) at 8.9 GPa. The high pressure orthorhombic phase is found to be stable up to 30 GPa. The cubic phase is completely recovered on releasing the pressure to the ambient.

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Ravhi Kumar University of Nevada, Las Vegas

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