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Bonding changes in compressed $NaBH_4$ probed by inelastic X-ray scattering[1] ANDREW CORNELIUS, RAVHI KUMAR, MALCOLM NICOL, University of Nevada, Las Vegas, MICHAEL HU, HPCAT and Carnegie Institution of Washington, PAUL CHOW, Argonne National Laboratory — Hydrogen storage for commercial applications is an ongoing challenge in materials science research in recent years. Complex borohydrides are technologically promising materials due to their light weight and high gravimetric and volumetric hydrogen density. So far knowledge of the structural and bonding changes in these systems is elusive due to low z elements and lack of in-situ experimental probes. Here we present the first experimental results of boron K-edge inelastic X-ray scattering performed on $NaBH_4$ revealing the nature of bonding changes during compression up to 12 GPa. $NaBH_4$ undergoes structural phase transition from cubic (Fm-3m) to tetragonal (P421/c) above 6 GPa and to orthorhombic (Pnma) above 8.3 GPa. The high pressure tetragonal and orthorhombic phases show weakening of B-H bonding during phase transition. Further, $NaBH_4$ may be considered as a representative example for isostructural systems since a similar structural sequence is also observed in KBH_4 on compression. The experimental details and the inelastic x-ray scattering results will be presented.

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