

Supplementary Information for:

**Structure and unconventional dihydrogen bonding of a pressure-stabilized hydrogen-rich
(NH₃BH₃)(H₂)_x (x = 1.5) compound**

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Figures S1–S4

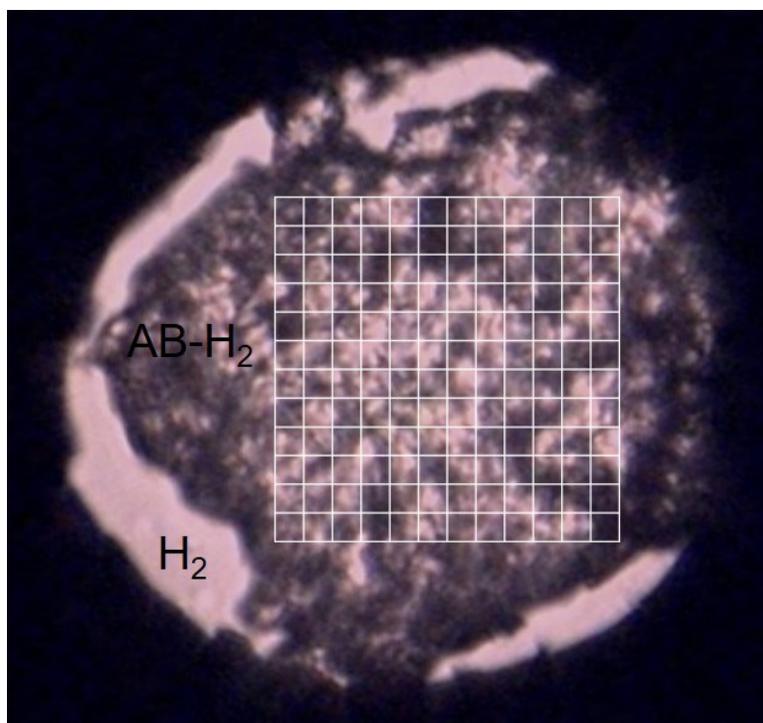


Fig. S1 A photomicrograph showing the reacted AB-H₂ phase surrounded by excess H₂ in a Be-Cu gasket hole. The square grid box with 5 μm grid spacing is the 60 x 60 μm² sample box through which X-rays scanned for collecting diffraction patterns.

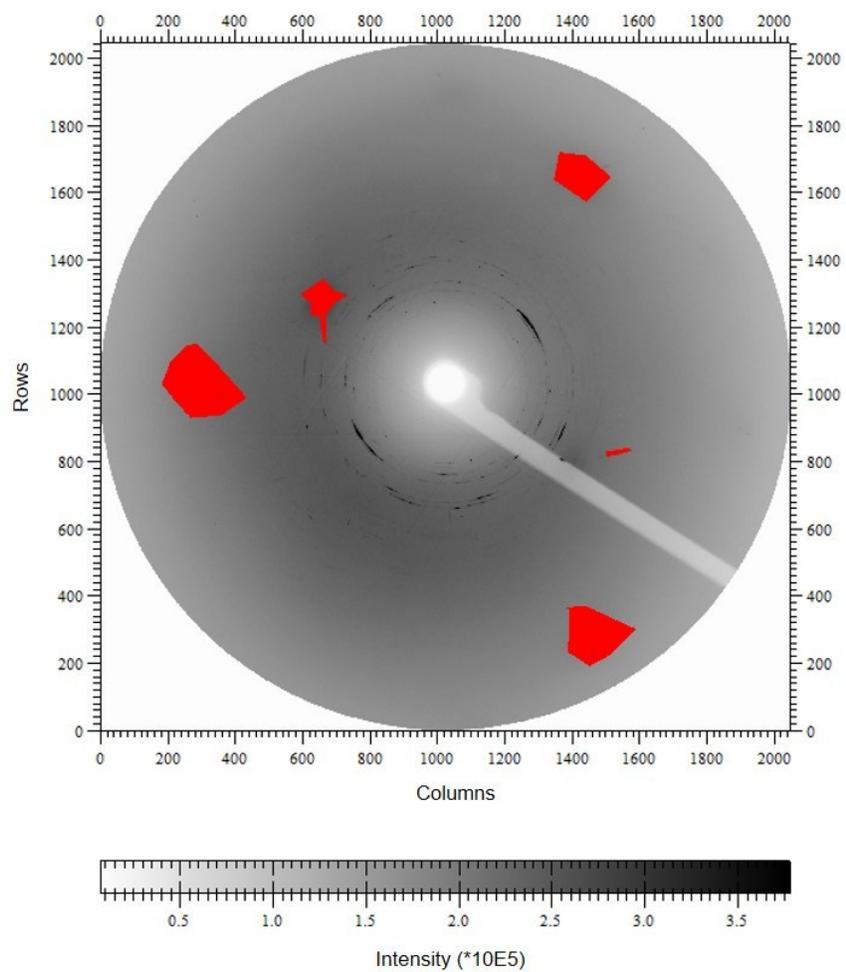


Fig. S2 A 2D Debye-Scherrer pattern obtained through summing up a total of 300 high-quality diffraction images. The red patches are masks for single crystal diamond reflections.

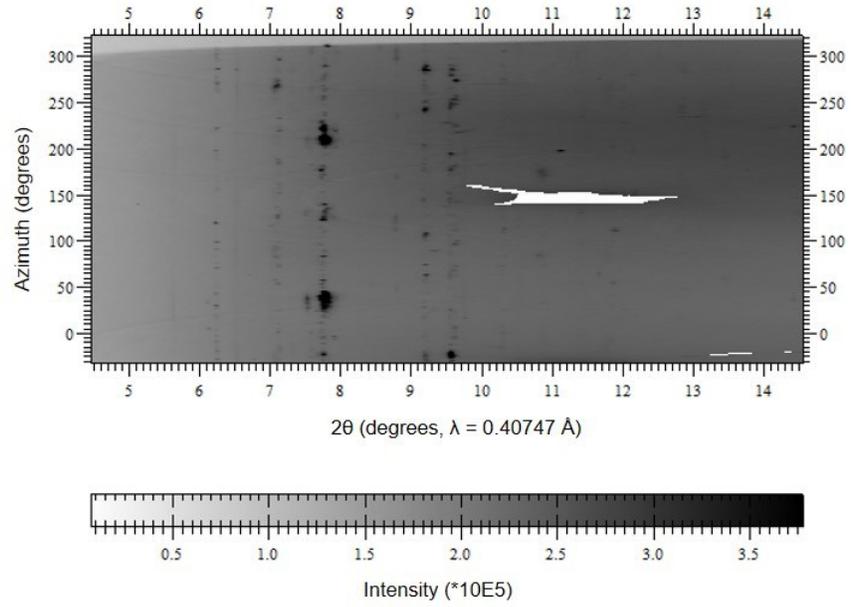


Fig. S3 The caked XRD pattern of AB-H₂ at 6.2 GPa showing detector azimuth (degrees) versus 2θ. The texture is clearer in this caked pattern.

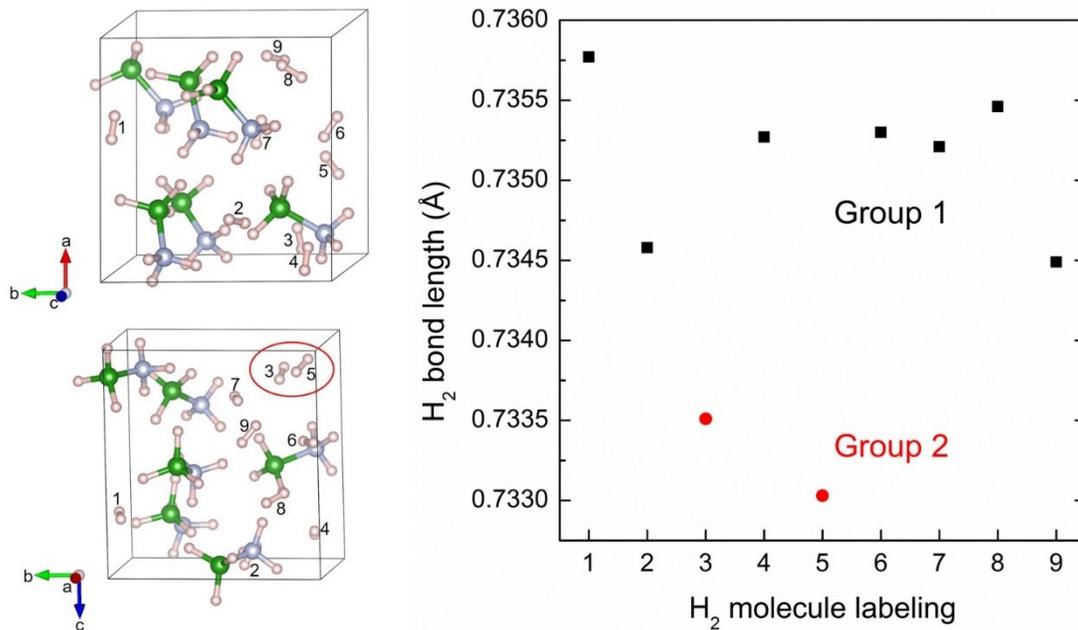


Fig. S4 The intramolecular H-H bond length of the nine H₂ molecules in the unit cell of the new AB-H₂ phase. The H₂ molecules are labeled from 1 to 9 in the left panel, and the corresponding bond length of each molecule is plotted in the right panel. The nine molecules can be easily divided into two groups based on the bond length difference. Group 1 that contains seven H₂ molecules shows an average of 0.3% bond length elongation compared to group 2 molecules.