Supporting Information for: Metallization and superconductivity of NBH_{12} compounds stabilized by dihydrogen bonds

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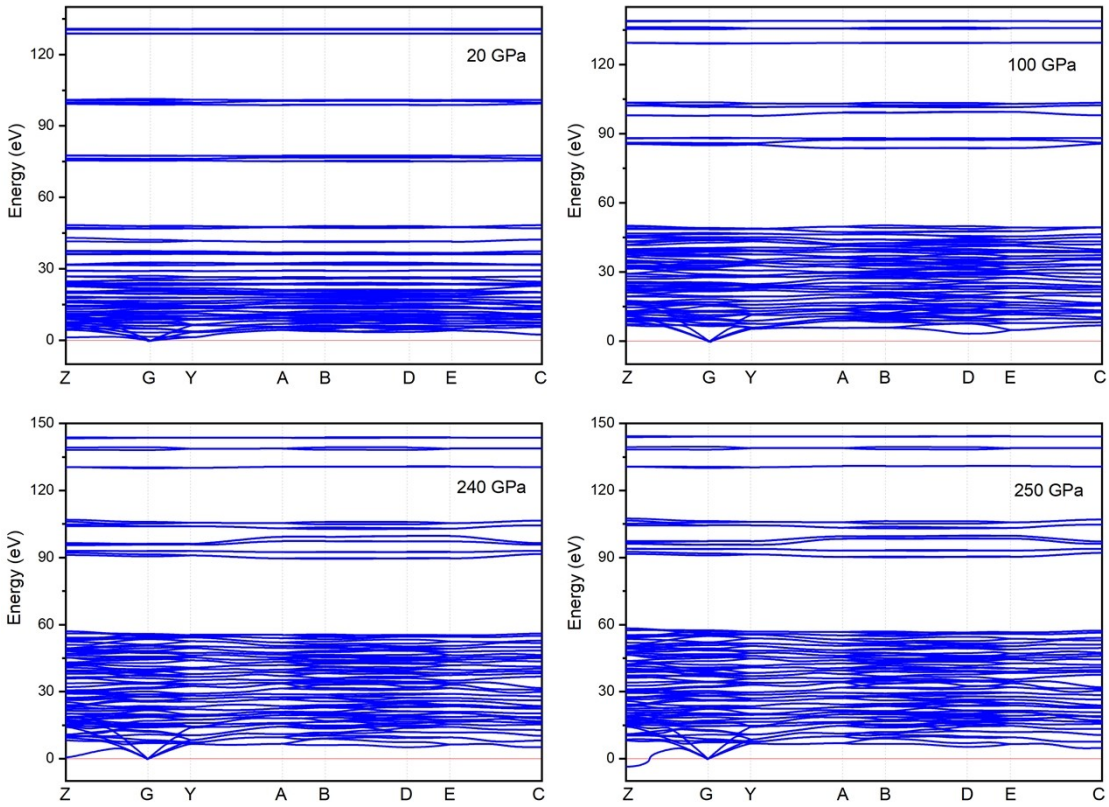

Figure S1. Phonon dispersions of $NH_3BH_3(H_2)_3$ at 20, 100, 240, 250 GPa.

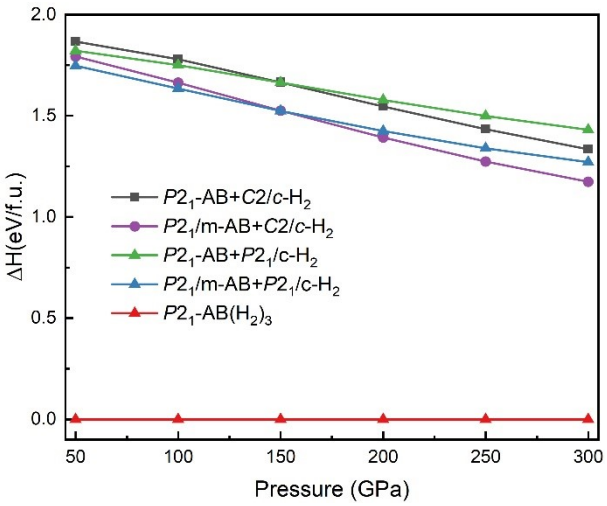

Figure S2. The enthalpy difference curves with respect to $AB(H_2)_3$ from divergent ideal routes as a function of pressure.

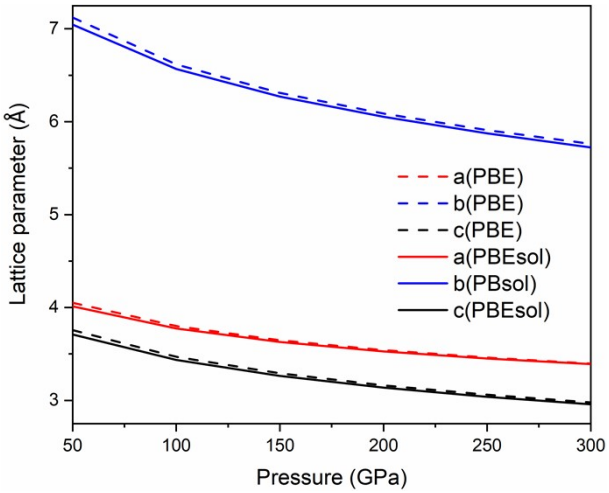

Figure S3. The lattice constants of $P2_1$-$NH_3BH_3(H_2)_3$ as a function of pressure.

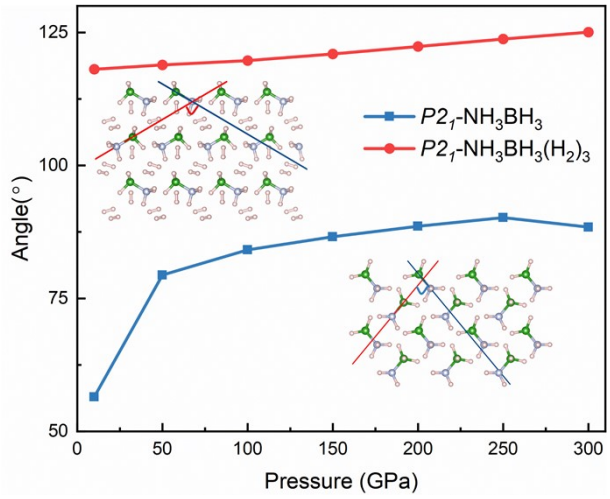

Figure S4. The tilt angle of the NH_3BH_3 molecular layers in $P2_1$-$NH_3BH_3(H_2)_3$ and pure NH_3BH_3 as a function of pressure.

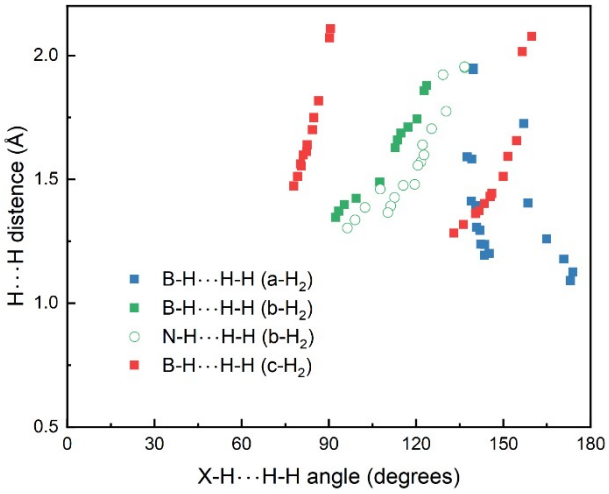

Figure S5. The dihydrogen bond length as a function of bond angle between AB and H_2 molecules.

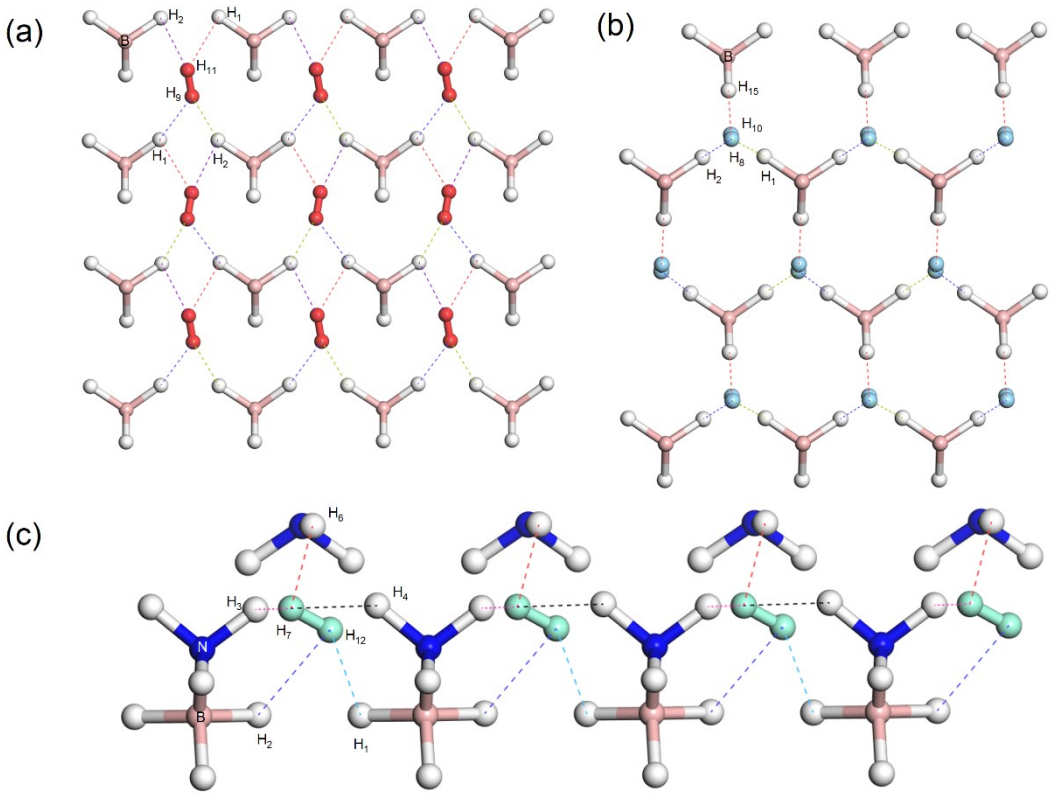

Figure S6. The dihydrogen bonding between AB and H_2 molecules

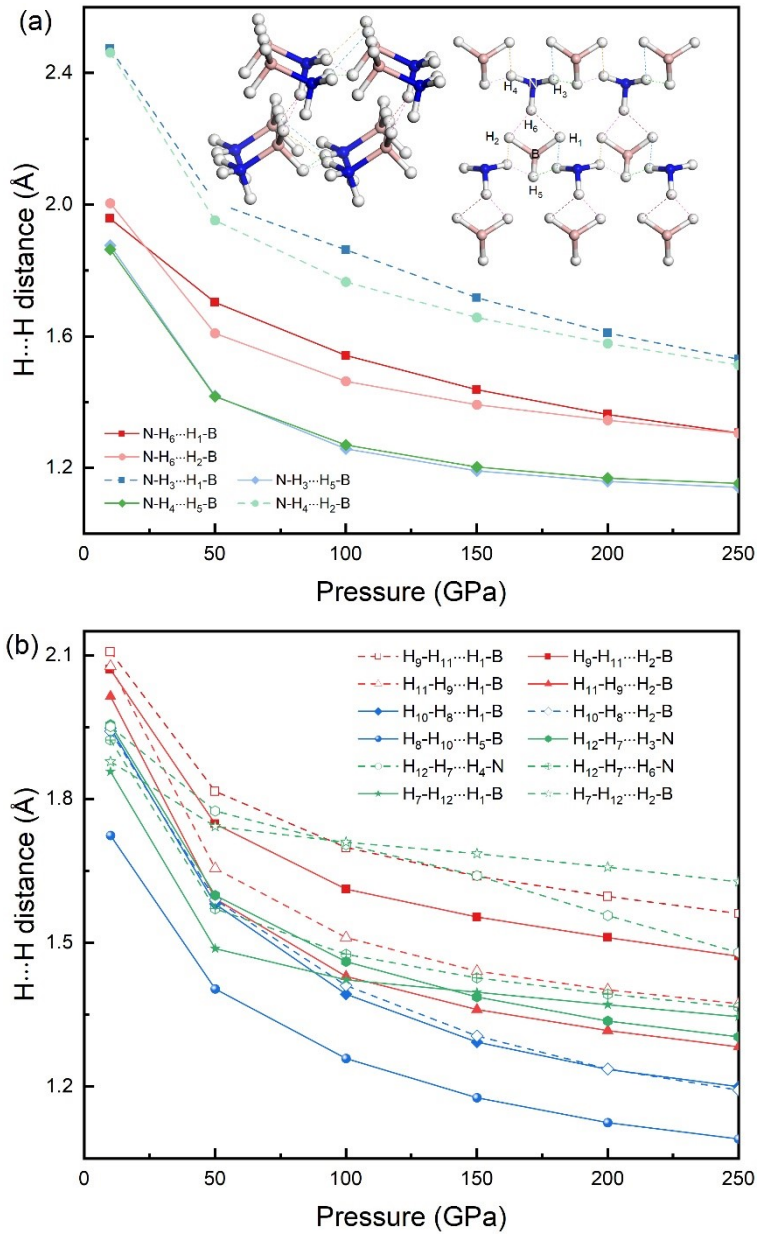

Figure S7. The dihydrogen bonding distance as a function of pressure. (a) The dihydrogen bond between AB in $AB(H_2)_3$. The dihydrogen bond between AB and H_2 in $AB(H_2)_3$.

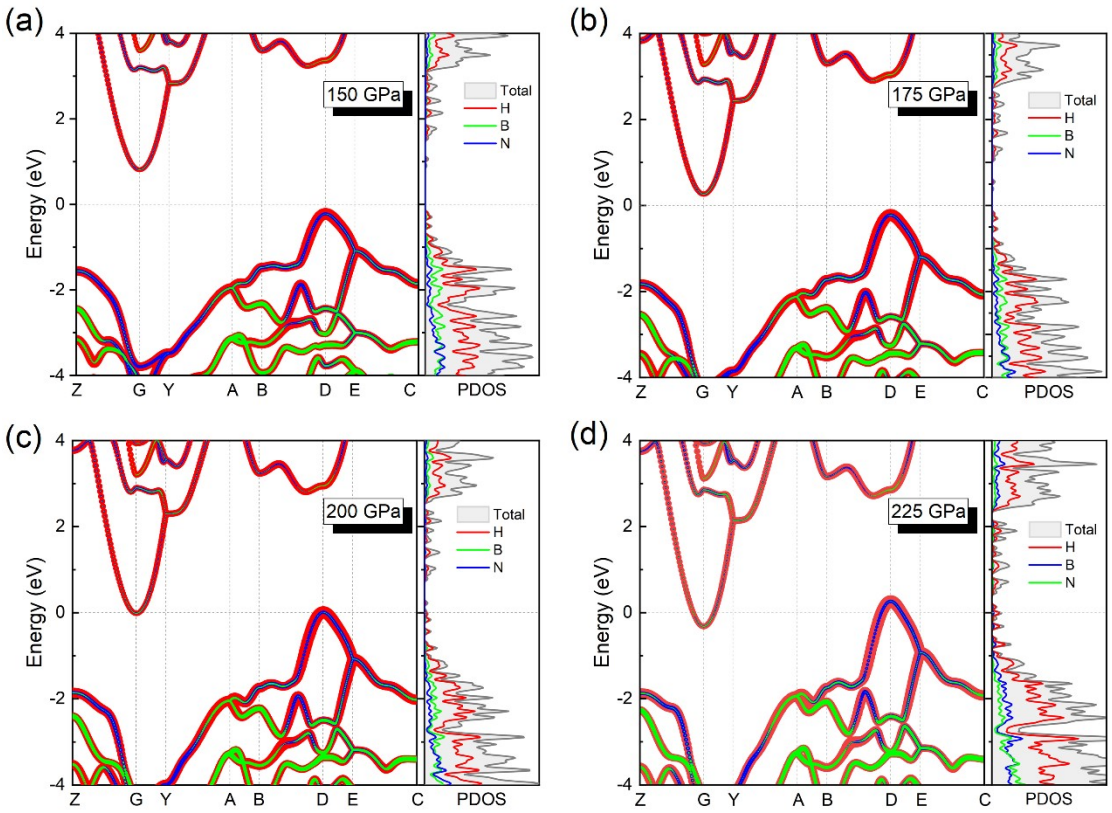

Figure S8. The atom-projected electron band structure and density of states (PDOS) of $P2_1$-$NH_3BH_3(H_2)_3$ at 150 GPa, 175 GPa, 200 GPa and 225 GPa are spectively shown in (a), (b), (c) and (d). The Fermi level is set to zero and depicted as the gray line. The red, blue, and green dots respectively represent the contributions of H, B, and N atoms to the electron band structure.

Table S1 Calculated structural parameters of the predicted phase of $NH_3BH_3(H_2)_3$ at 100 GPa.

Compound	Space group	Lattice parameters (Å)	Atomic coordinates (fractional)			
			atoms	X	Y	Z
$NH_3BH_3(H_2)_3$	$P2_1$	**a**=3.7998 **b**=6.618 **c**=3.4681 $\alpha=\gamma=90^\circ$ $\beta=62.866$	H1(2a)	1.07438	0.58226	-0.37043
			H2(2a)	0.57949	0.58556	-0.30810
			H3(2a)	0.42703	0.08214	-0.24234
			H4(2a)	1.11350	0.15920	-0.31033
			H5(2a)	0.97738	0.39077	-0.50924
			H6(2a)	0.53444	0.26260	-0.49728
			H7(2a)	1.02686	0.91098	-0.03396
			H8(2a)	0.74368	0.35328	-0.11938
			H9(2a)	0.89938	0.18044	-0.20690
			H10(2a)	0.51233	0.86844	-0.49233
			H11(2a)	1.23237	0.22976	-0.89500
			H12(2a)	0.18445	0.59830	-0.24966
			B(2a)	0.47333	0.98709	0.01060
			N(2a)	0.84543	0.87670	-0.16776