

Supplementary Information for the paper entitled
“Pressure-induced superconductivity of the Ac-B-H hydrides”

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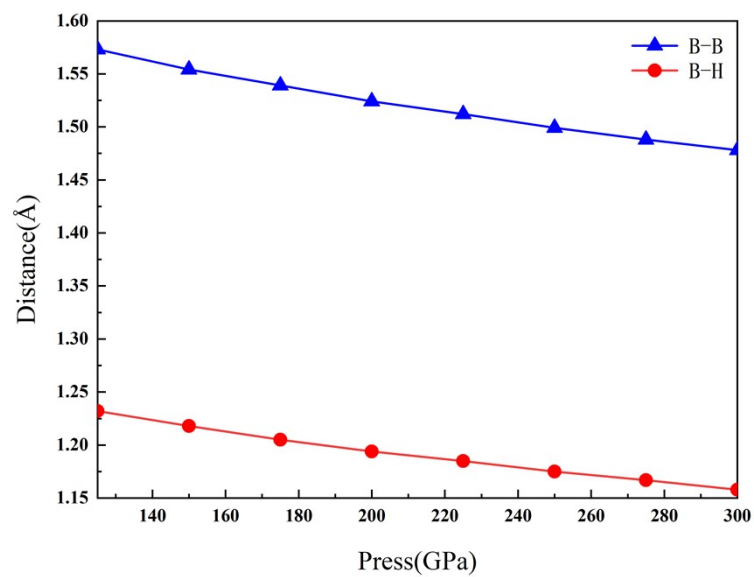


Fig. S1. The distance between B-B and B-H at different pressures for the predicted structure $I4/mmm$ -AcB₂H₈.

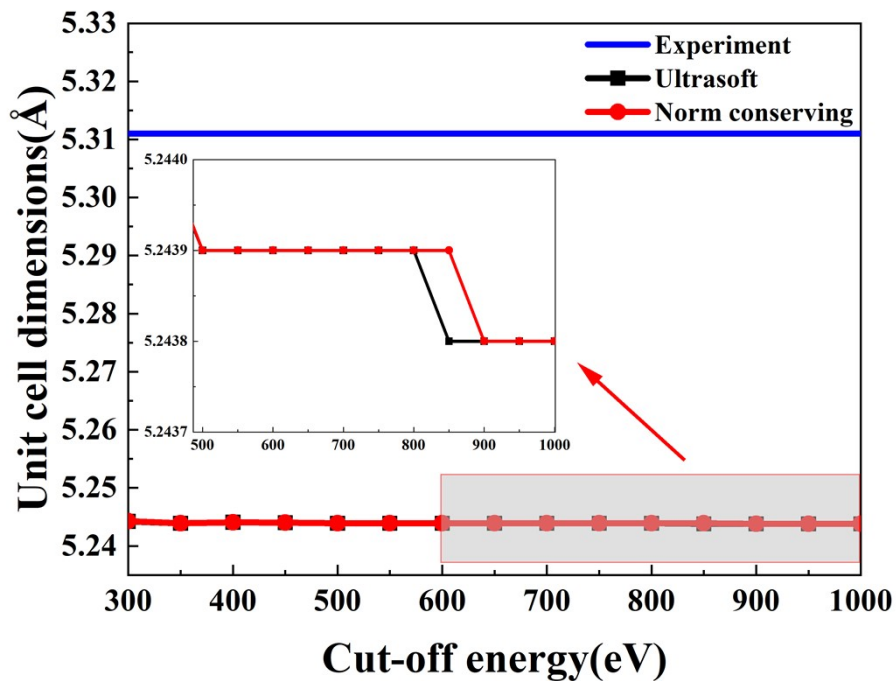


Fig. S2. Calculated lattice parameter of bulk Ac at 0 K and ambient pressure using ultrasoft pseudopotential (black line) and norm-conserving pseudopotential (red line), which were compared with the experimental data of bulk Ac (blue line).

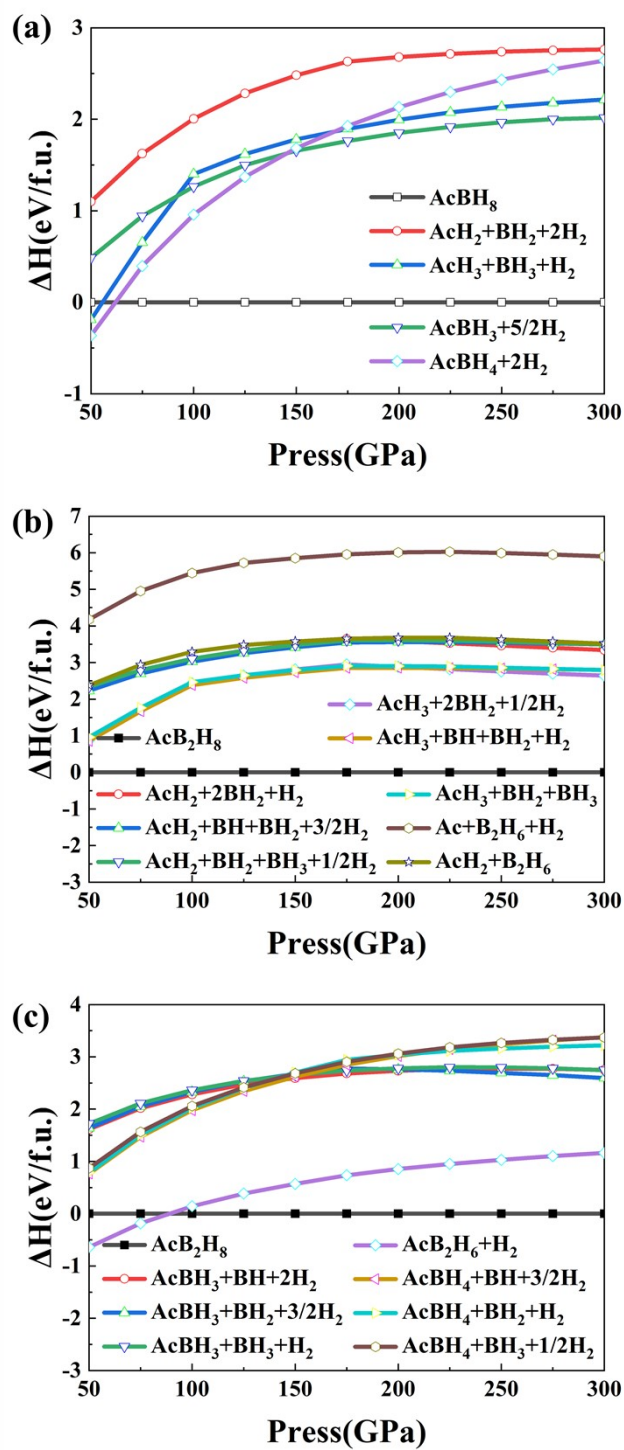


Fig. S3. (a) Enthalpy difference curves of R^3m - AcBH_8 at different pressures, (b) and (c) Enthalpy difference curves of $I4/mmm$ - AcB_2H_8 at different pressures.

Table S1. Lattice parameters and atomic fractional coordinates of the AcB_mH_n ($m = 1-3$ and $n = 3-12$) structures.

Space group Press	Lattice parameters	Atomic coordinates (fractional)				Sites
<i>R3m</i> AcBH_3 100GPa	a = 4.5338	H	0.07484	-0.53742	-0.04419	9b
	b = 4.5338	B	-0.66667	-1.33333	0.16718	3a
	c = 5.5462	Ac	-1.33333	-1.66667	0.34860	3a
<i>R3m</i> AcBH_4 70GPa	a = 3.6645	H	-0.31982	-0.15991	-0.09259	9b
	b = 3.6645	H	-0.33333	0.33333	-0.19568	3a
	c = 10.4031	B	0.33333	0.66667	-0.13817	3a
		Ac	0.00000	1.00000	-0.29275	3a
<i>R3m</i> AcBH_5 150GPa	a = 3.8705	H	0.01513	-0.49244	-0.06932	9b
	b = 3.8705	H	0.00000	0.00000	-0.08649	3a
	c = 7.9815	H	0.33333	-0.33333	0.13771	3a
		B	0.33333	-0.33333	-0.00966	3a
		Ac	0.00000	0.00000	-0.18217	3a
<i>R$\bar{3}$m</i> AcBH_8 70GPa	a = 4.1663	H	-0.17102	0.65796	-0.23366	18h
	b = 4.1663	H	-0.66667	0.66667	-0.07348	6c
	c = 9.2796	B	-0.33333	0.33333	-0.16667	3b
		Ac	0.00000	0.00000	0.00000	3a
<i>Imm2</i> AcB_2H_6 125GPa	a = 6.7790	H	0.30427	0.23353	0.16849	8e
	b = 3.8116	H	0.35409	0.50000	0.75217	4c
	c = 3.3085	B	0.61529	0.50000	0.12304	4c
		Ac	0.50000	0.00000	0.63276	2b
<i>I4/mmm</i> AcB_2H_8 125GPa	a = 3.6792	H	-0.50000	0.17851	0.33210	16n
	b = 3.6792	B	-0.50000	0.50000	0.38314	4e
	c = 6.7313	Ac	0.00000	1.00000	0.50000	2b