Supporting Information
Pressure induced superconductivity in ternary yttrium borohydride system

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Table S1. Detailed structural information and ΔH_c and ΔH_s of the predicted Y-B-H compounds at selected pressures. ΔH_c **(in meV/atom)**, the distance of the given stoichiometry from the convex hull in the triangular phase diagrams. ΔH_s **(in meV/atom)**, the distance of the given structure from the lowest enthalpy structure of the same stoichiometry.

Stoichiometry	**Space group**	**Pressure (GPa)**	ΔH_c **(meV/atom)**	ΔH_s	**Stoichiometry**	**Space group**	**Pressure (GPa)**	ΔH_c **(meV/atom)**	ΔH_s
YBH	R3m	50	13	0	YBH	P6/mmm	50	42	29
	R3m	100	63	63		P6/mmm	100	0	0
	R3m	150	142	142		P6/mmm	150	0	0
YBH_2	Cmcm	50	0	0	YBH_3	Ama2	50	74	0
	Cmcm	100	0	0		Ama2	100	43	0
	Cmcm	150	0	0		Ama2	150	20	0
YBH_4	P3	50	60	0	YBH_4	Amm2	50	56	116
	P3	100	115	70		Amm2	100	45	0
	P3	150	109	101		Amm2	150	8	0
YBH_5	P3m1	50	57	0	YBH_5	F-43m	50	71	14
	P3m1	100	36	0		F-43m	100	42	6
	P3m1	150	14	0		F-43m	150	29	15
YBH_6	Pmna	50	24	0	YBH_7	P1	50	17	0
	Pmna	100	20	0		P1	100	68	0
	Pmna	150	34	0		P1	150	56	0
YBH_8	P1	50	18	0	YBH_7	P-3m1	50	285	268
	P1	100	54	0		P-3m1	100	225	157
	P1	150	75	28		P-3m1	150	248	192
YBH_8	Fm-3m	50	511	493	YBH_8	Pm	50	59	41
	Fm-3m	100	418	364		Pm	100	56	2
	Fm-3m	150	294	247		Pm	150	47	0
YBH_9	Pm	50	94	0	YBH_9	Cm	50	180	86
	Pm	100	86	0		Cm	100	105	19
	Pm	150	101	17		Cm	150	84	0
YBH_{10}	P1	50	0	0	YBH_{12}	P1	50	37	0
	P1	100	0	0		P1	100	71	0
	P1	150	0	0		P1	150	72	0
YBH_{11}	P1a	50	74	0	YBH_{11}	P1b	50	100	26
	P1a	100	88	2		P1b	100	86	0
	P1a	150	92	32		P1b	150	60	0
YB_2H_2	P6mm	50	178	0	YB_2H_4	C2m	50	134	0
	P6mm	100	156	0		C2m	100	113	0
	P6mm	150	153	0		C2m P-	150	100	0
YB_2H_6	C2	50	6	0	YB_2H_{10}	3m1	50	0	0
	C2	100	0	0		P-3m1	100	21	0
	C2	150	0	0		P-3m1	150	39	0

YB_2H_8	C2m	50	40	0	YB_2H_8	P2	50	69	29
	C2m	100	94	73		P2	100	21	0
	C2m	150	143	104		P2	150	39	0
YB_2H_{12}	P1	50	26	0	YB_2H_{12}	Cm	50	189	163
	P1	100	179	131		Cm	100	47	0
	P1	150	491	431		Cm	150	60	0

Table S2**.** Detailed structural information of the predicted Y-B-H compounds at selected pressures.

Phases	**Pressure (GPa)**	**Lattice parameters (Å)**	**Atomic coordinates (fractional)**			
*R*3*m* YBH	50GPa	a=b=3.179	B(3a)	0.667	0.333	0.079
		c=19.327	B(3a)	1.333	0.667	0.080
		α=β=90.000	Y(3a)	1.000	0.000	-0.014
		γ=120.000	Y(3a)	1.000	1.000	0.171
			H(3a)	1.000	1.000	0.277
			H(3a)	1.333	1.667	0.239
*P*6/*mmm*-YBH	100 GPa	a=b=3.003	H(2d)	-1.667	-0.333	-0.500
		c=6.126	B(2c)	-0.667	-0.333	0.000
		α=β =90.000	Y(2e)	-2.000	0.000	-0.718
		γ=120				
Cmcm-YBH_2	50 GPa	a=3.457	H(4d)	1.000	-0.257	0.250
		b=11.275	H(4d)	0.500	-0.139	0.250
		c=3.139	B(4d)	1.000	-0.530	0.250
		α=β=γ=90.000	Y(4c)	1.000	-0.131	-0.250
*P*3*m*1-YBH_5	50	a= b=3.573	H(3d)	-1.038	-0.519	0.228
		c=3.530	H(1c)	-0.333	0.333	-0.262
		α=β= 90.000	H(1b)	-0.667	0.667	-0.215
		γ=120.000	B(1b)	-0.667	-0.333	0.132
			Y(1a)	0.000	0.000	-0.398
F-43m-YBH_5	50GPa	a=b=c=5.361	H(16e)	0.130	0.630	-0.130
		α=β=γ=90.000	H(4d)	0.250	1.250	-0.250
			B(4b)	0.000	0.500	0.000
			Y(4a)	0.500	1.500	0.000
P_1-YBH_{10}	50 GPa	a=3.541	H(1a)	0.545	-0.470	0.591
		b=3.578	H(1a)	0.207	0.207	0.636
		c=5.043	H(1a)	0.732	0.223	0.323
		α=101.573	H(1a)	0.173	0.324	0.358
		β=92.734	H(1a)	0.332	0.467	0.986
		γ=60.402	H(1a)	0.316	0.025	0.991
			H(1a)	0.872	-0.003	0.237
			H(1a)	0.475	-0.238	0.298
			H(1a)	0.128	0.501	0.282
			H(1a)	0.872	-0.518	0.988
			B(1a)	0.499	-0.316	0.061
			Y(1a)	0.870	-0.106	0.701
P-3*m*1-YB_2H_{10}	50 GPa	a=b=3.649	H(16c)	-0.133	0.133	-0.133
		c=5.338	H(6i)	-0.968	-1.484	0.726
		α=β=90.000	H(2d)	-1.333	-0.667	0.011
		γ=120.000	H(2c)	-1.000	-1.000	0.073
			B(2d)	-1.333	-1.6676	0.796

			Y(1b)	-1.000	-1.000	0.500
*C*2-YB_2H_6	50 GPa	a=8.371	H(4c)	0.168	0.156	-0.175
		b=3.449	H(4c)	0.648	1.285	0.143
		c=3.573	H(4c)	0.207	0.292	0.366
		α=γ=90.000	B(4c)	0.109	0.124	0.083
		β=111.099	Y(2b)	0.500	1.108	0.500
P_1-YB_2H_{12}	50 GPa	a=4.782	H(1a)	0.152	-0.152	0.243
		b=3.538	H(1a)	0.246	0.728	0.306
		c=4.756	H(1a)	0.412	0.863	0.611
		α=73.320	H(1a)	0.975	0.475	0.731
		β=99.695	H(1a)	0.569	0.474	0.137
		γ=73.077	H(1a)	0.390	0.093	0.504
			H(1a)	0.624	0.448	0.533
			H(1a)	0.263	0.895	0.928
			H(1a)	0.370	0.438	0.783
			H(1a)	0.770	0.897	0.429
			H(1a)	0.238	0.307	0.153
			H(1a)	0.991	0.304	0.399
			B(1a)	0.750	0.273	0.379
			B(1a)	0.215	0.269	0.912
			Y(1a)	0.794	0.907	0.957

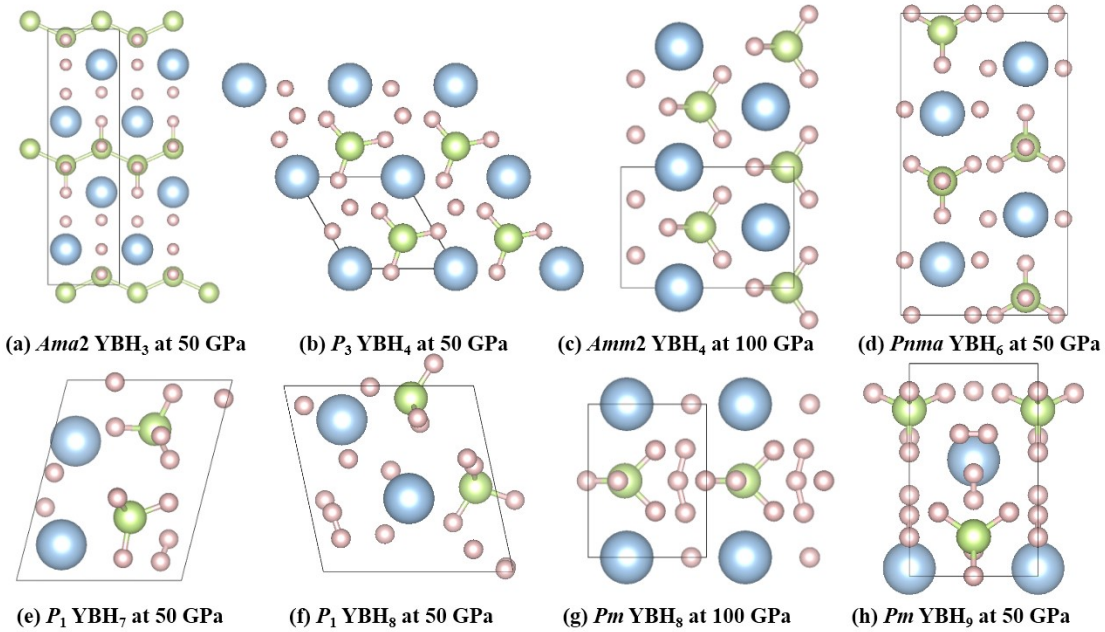

Fig. S1. Structures of the metastable phases of ternary Y-B-H compounds at high pressure. The blue, green and pink spheres represent the Y, B and H atoms, respectively.

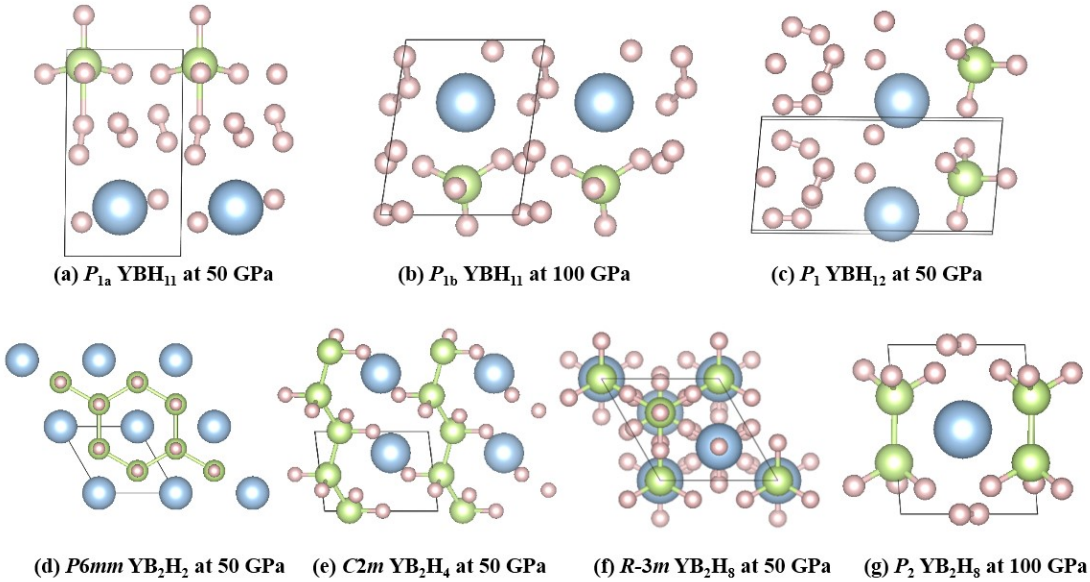

Fig. S2. Structures of the metastable phases of ternary Y-B-H compounds at high pressure. The blue, green and pink spheres represent the Y, B and H atoms, respectively.

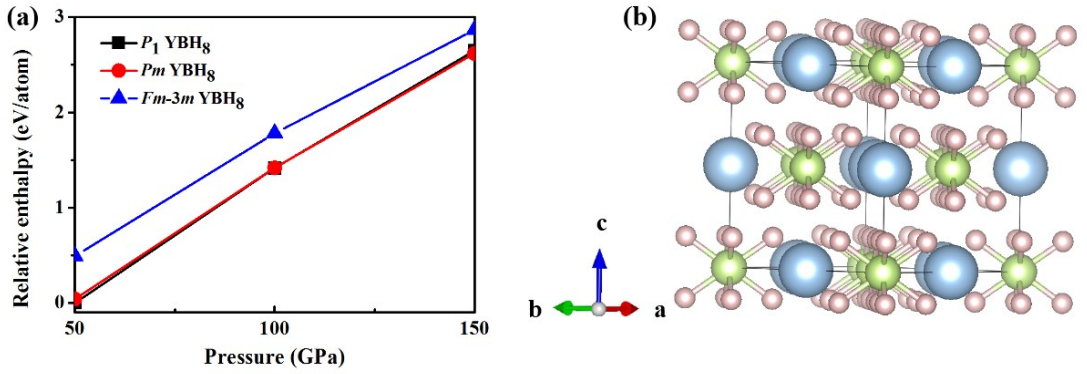

Fig. S3. (a) Calculated relative formation enthalpy per atom of YBH_8 at the different pressures. (b) Structure of *Fm*-3*m* YBH_8 at 50 GPa. The blue, green and pink spheres represent the Y, B and H atoms, respectively.

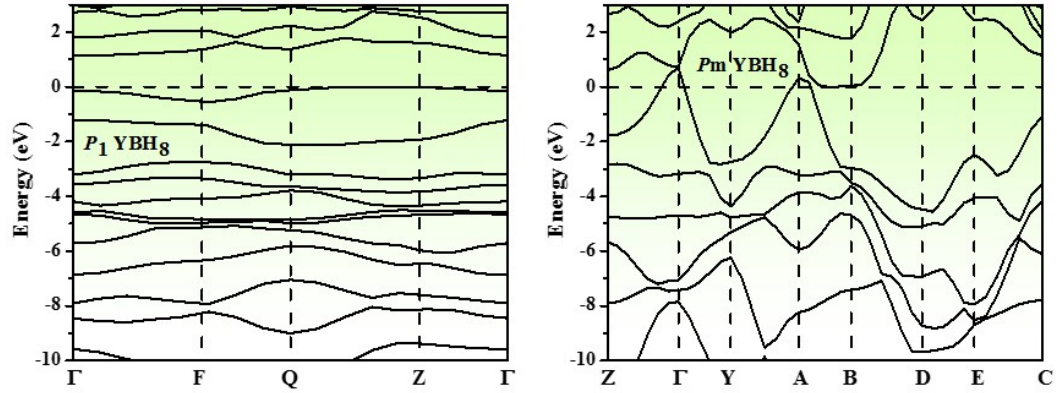

Fig. S4. Electronic band structures of P_1 YBH_8 at 50 GPa and *Pm* YBH_8 at 100 GPa.

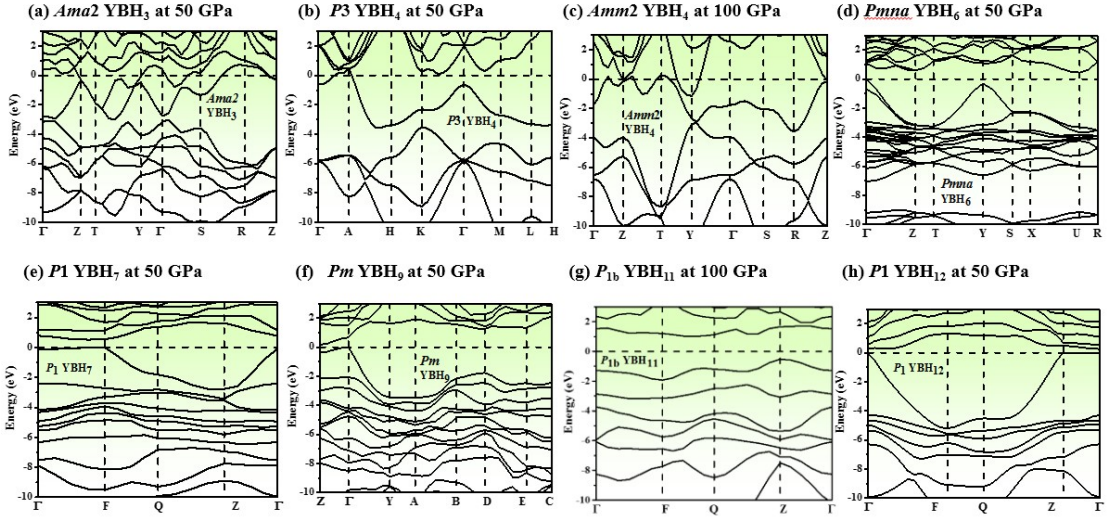

Fig. S5. Electronic band structures of some metastable phases of ternary Y-B-H compounds under specified pressure.

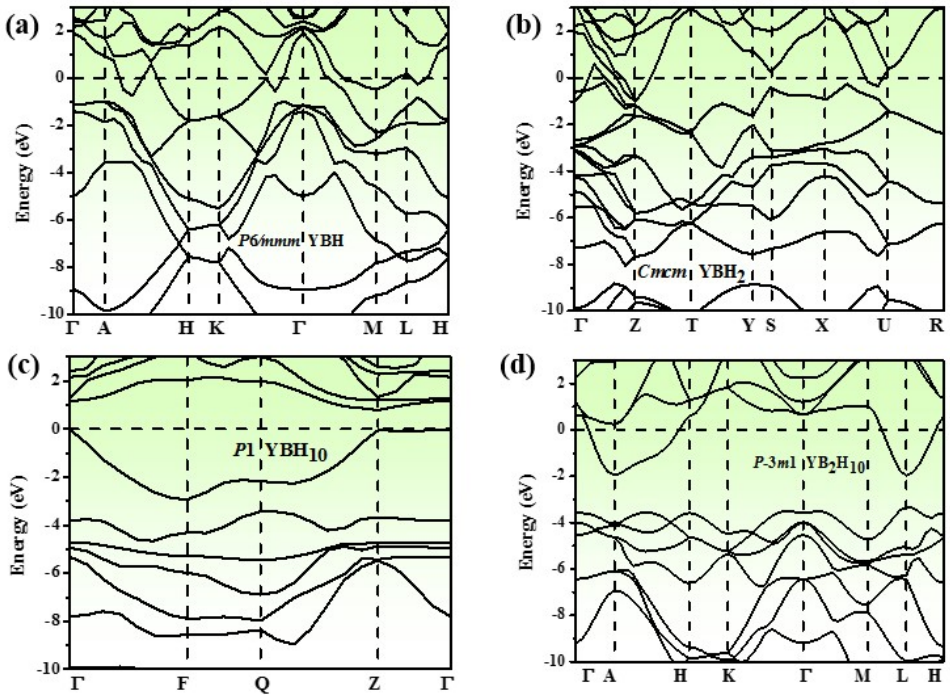

Fig. S6. Electronic band structures of some stable phases of ternary Y-B-H compounds at 50 GPa.

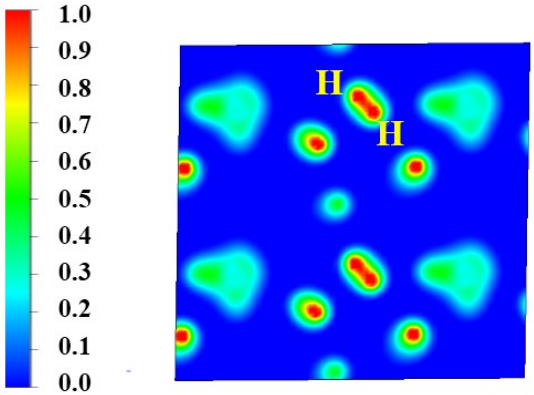

Fig.S7. 2D-ELF of P_1-YB_2H_{12} on the (1-10) plane.

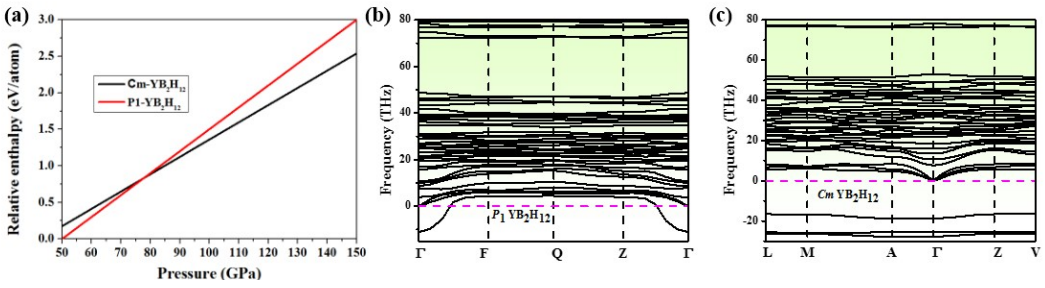

Fig. S8 (a) Calculated relative formation enthalpy per atom of YB_2H_{12} at the different pressures. (b) and (c) The phonon dispersion curves for $P1$-YB_2H_{12} and Cm-YB_2H_{12} at 100 GPa.

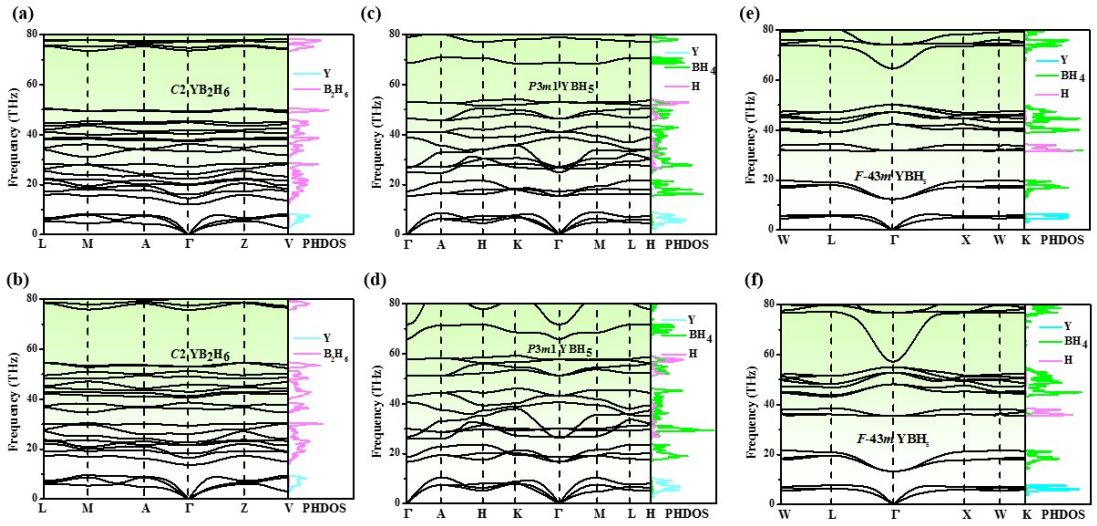

Fig. S9. Calculated phonon band structures and phonon density of states of Y-B-H compounds. (a) and (b) for $C2$ YB_2H_6 at 100 GPa and 150 GPa, (c) and (d) for $P3m1YBH_5$ at 100 GPa and 150 GPa, (e) and (f) for F-43m YBH_5 at 100 GPa and 150 GPa.

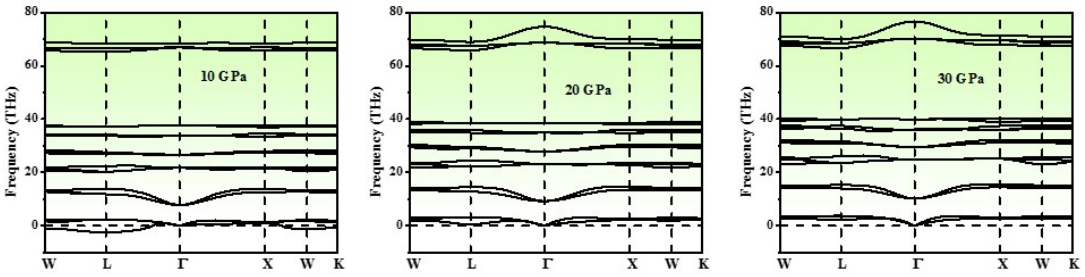

Fig. S10 Phonon spectrum of F-43m YBH_5 at 10, 20 and 30 GPa.

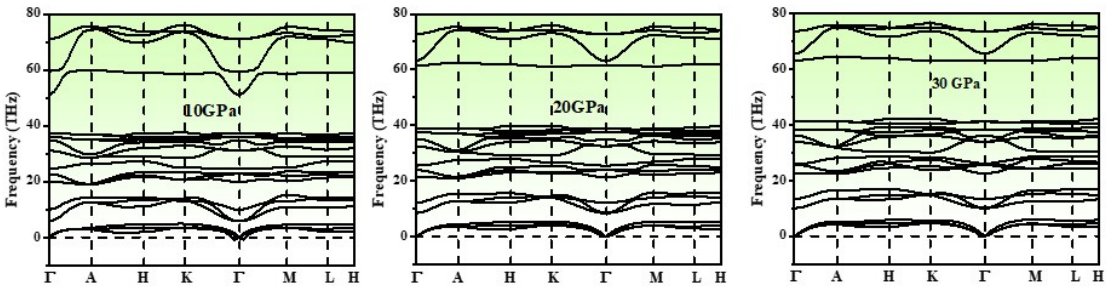

Fig. S11. Phonon spectrum of $P3m1$ YBH_5 at 10, 20 and 30 GPa.

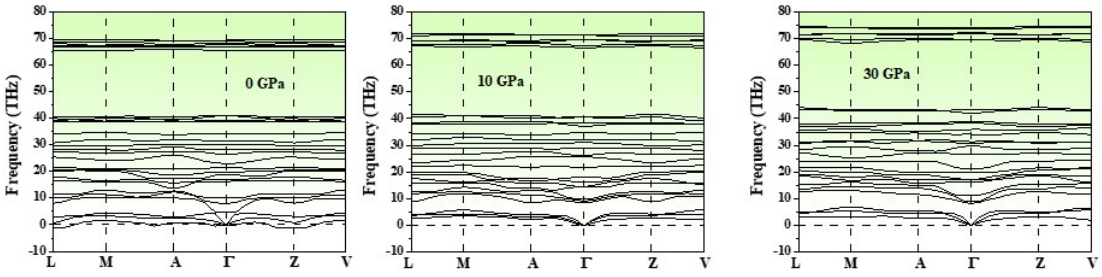

Fig. S12. Phonon spectrum of *C*2 YB_2H_6 at 0, 10 and 30 GPa.

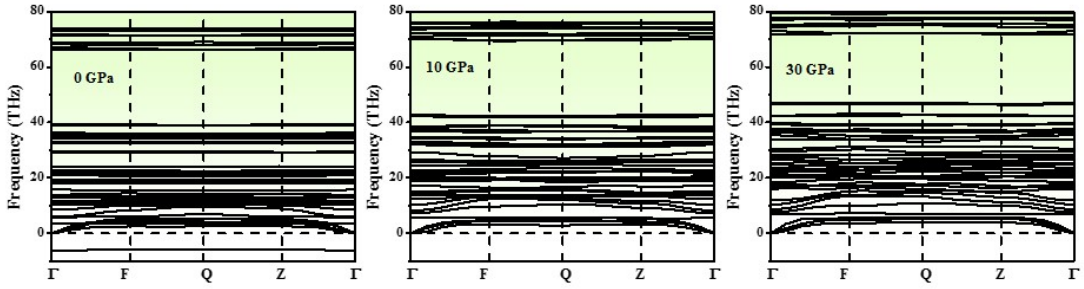

Fig. S13. Phonon spectrum of P_1 YB_2H_{12} at 0, 10 and 30 GPa.

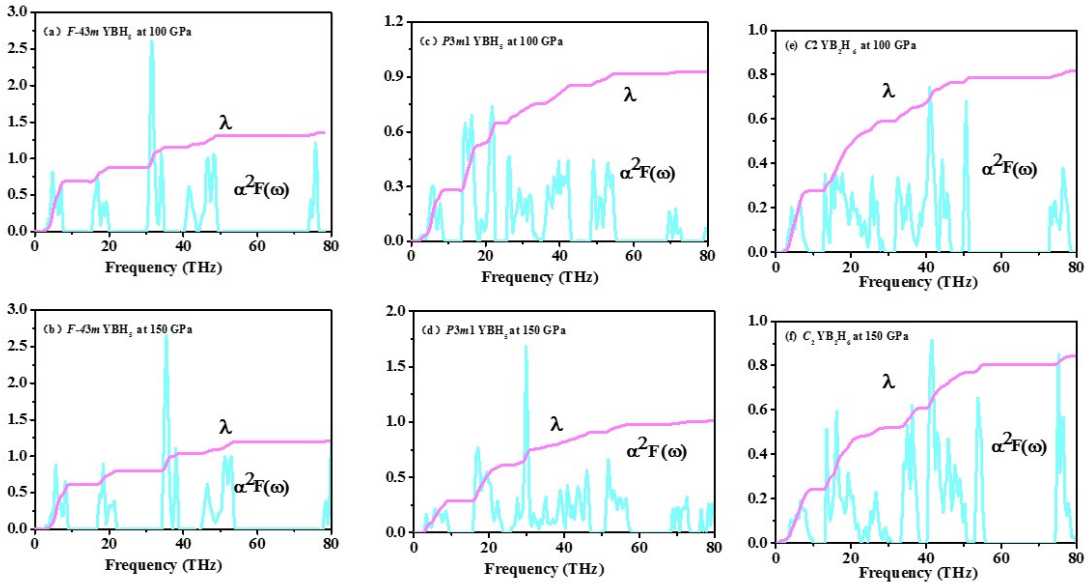

Fig. S14. The Eliashberg phonon spectral function, $\alpha^2F(\omega)$, and the partial electron-phonon intergral, $\lambda(\omega)$, for the Y-B-H system at 150 GPa and 100 GPa. (a) and (b) for *F*-43*m* YBH_5, (c) and (d) *P*3*m*1 YBH_5, (e) and (f) *C*2 YB_2H_6.

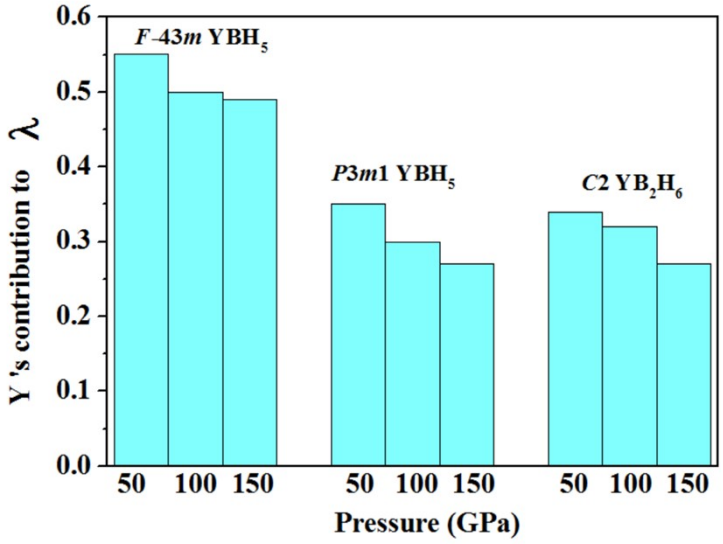

Fig. S15. The contribution of Y to λ for *F*-43*m* YBH_5, *P*3*m*1YBH_5 and *C*2 YB_2H_6 at 50, 100 GPa and 150 GPa.