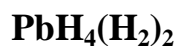


Supplementary information

Pressure-induced superconductivity in H₂-containing hydriden



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Table S1. Lattice parameters and atomic coordinates of $\text{PbH}_4(\text{H}_2)_2$ at difference pressures.

space group	Pressure (GPa)	Lattice parameters (\AA , deg)	atom	x	y	z
<i>Pnmm</i>	20	a=4.820	Pb1(2c)	0.00000	0.50000	-1.00000
		b=13.626	Pb2(2a)	0.00000	0.00000	-1.00000
		c=3.512	H1(4g)	0.48622	0.70157	-1.00000
		$\alpha=\beta=\gamma=90$	H2(4g)	0.51304	0.35404	-1.00000
		H3(4g)	0.76642	0.20436	-1.00000	
		H4(4g)	0.70258	0.85072	-1.00000	
		H5(4g)	0.26227	0.20350	-1.00000	
		H6(4g)	0.00796	0.28016	-1.00000	
		H7(4g)	0.52301	0.16424	-1.00000	
H8(4g)	0.22661	0.34951	-1.00000			
<i>P-1</i>	160	a=2.896	Pb1 (2i)	1.16788	0.14745	-0.84911
		b=4.161	H1 (2i)	2.54257	-0.52858	-1.26204
		c=5.629	H2 (2i)	4.86030	-1.30130	-1.75250
		$\alpha=71.0$	H3 (2i)	0.61711	0.29962	-0.55204
		$\beta=88.2$	H4 (2i)	0.64295	0.30721	-0.41449
		$\gamma=70.8$	H5 (2i)	3.04141	-0.54666	-1.37609
		H6 (2i)	0.55130	0.42805	-0.11390	
		H7 (2i)	1.26202	-0.00233	-0.41815	
		H8 (2i)	1.18245	0.19620	-0.51149	
<i>C2/m</i>	200	a=7.184	Pb1(2a)	0.00000	0.00000	0.00000
		b=2.807	H1(4i)	-0.77734	0.00000	2.30255
		c=2.973	H2(4i)	-0.79226	0.50000	2.42086
		$\alpha=\gamma=90$	H3(4i)	-0.78633	-0.50000	0.97864
		$\beta=68.1$	H4(4i)	-0.90858	-0.50000	1.43768

Table S2. Lattice parameters and atomic coordinates of PbH₃ at special pressures.

space group	Pressure (GPa)	Lattice parameters (Å, deg)	atom	x	y	z
<i>P4/mmm</i> (<45 GPa)	30	a=4.015	Pb1(1a)	0.00000	0.00000	0.00000
		b=4.015	Pb2(1c)	0.50000	0.50000	0.00000
		c=4.422	H1(2h)	0.50000	0.50000	0.41369
		$\alpha=\beta=\gamma=90$	H2(4m)	0.40154	0.00000	0.50000
<i>C2/c</i> (45-110 GPa)	80	a=4.416	Pb1 (4a)	0.00000	0.00000	0.00000
		b=8.505	Pb2 (4e)	0.00000	0.32201	0.25000
		c=5.543	H1 (4c)	0.25000	0.25000	0.00000
		$\alpha=90$ $\beta=91.4$ $\gamma=90$	H2 (4b)	0.00000	0.50000	0.00000
			H3 (4d)	0.25000	0.25000	0.50000
		H4 (4e)	0.00000	0.68690	0.25000	
<i>I4/mmm</i> (>110 GPa)	150	a=3.366	Pb1(2b)	0.00000	0.00000	0.50000
		b=3.366	H1(2a)	0.00000	0.00000	0.00000
		c=3.772 $\alpha=\beta=\gamma=90$	H2(4d)	0.00000	0.50000	0.25000

Table S3. Lattice parameters and atomic coordinates of PbH₂ at special pressures.

space group	Pressure (GPa)	Lattice parameters (Å, deg)	atom	x	y	z	
<i>I4/mcm</i> (<68 GPa)	30	a=4.070	Pb1(8g)	0.00000	0.50000	0.84400	
		b=4.070	H1(32m)	0.29940	0.20060	0.97530	
		c=15.041					
		$\alpha=\beta=\gamma=90$					
<i>Cm</i> (68-140 GPa)	100	a=3.724	Pb1 (2a)	0.00025	0.00000	0.03751	
		b=9.530	Pb2 (4b)	0.50005	0.14877	0.49025	
		c=3.936	H1 (2a)	0.00030	0.00000	0.56036	
		$\alpha=90$	H2 (4b)	0.50002	0.24996	0.98796	
		$\beta=93.9$	H3 (4b)	0.74994	0.75004	0.97751	
		$\gamma=90$	H4 (2a)	0.49945	0.00000	0.87817	
<i>Cmmm</i> (>140 GPa)	150	a=3.937	Pb1(2c)	0.00000	0.50000	0.50000	
		b=3.638	H1(4g)	0.39948	0.50000	0.00000	
		c=2.725					
		$\alpha=\beta=\gamma=90$					

Table S4. Lattice parameters and atomic coordinates of PbH at special pressures.

space group	Pressure (GPa)	Lattice parameters (Å, deg)	atom	x	y	z
<i>C2</i> (<32 GPa)	20	a=5.590	Pb1(4c)	0.75459	0.91455	0.64315
		b=9.214	Pb2(2a)	0.00000	0.16874	0.00000
		c=3.092	H1(2b)	0.00000	0.66666	0.50000
		$\alpha=\gamma=90$ $\beta=93.3$	H2(4c)	0.00303	0.66775	0.16443
<i>P4/nmm</i> (32-97 GPa)	60	a=2.901	Pb (2c)	0.00000	0.50000	0.72817
		b=2.901	H (2c)	0.00000	0.50000	0.12580
		c=4.952 $\alpha=\beta=\gamma=90$				
<i>Cmcm</i> (>97 GPa)	150	a=4.235	Pb(4c)	0.00000	0.77521	0.75000
		b=4.281 c=3.925 $\alpha=\beta=\gamma=90$	H(4c)	0.00000	0.30866	0.75000

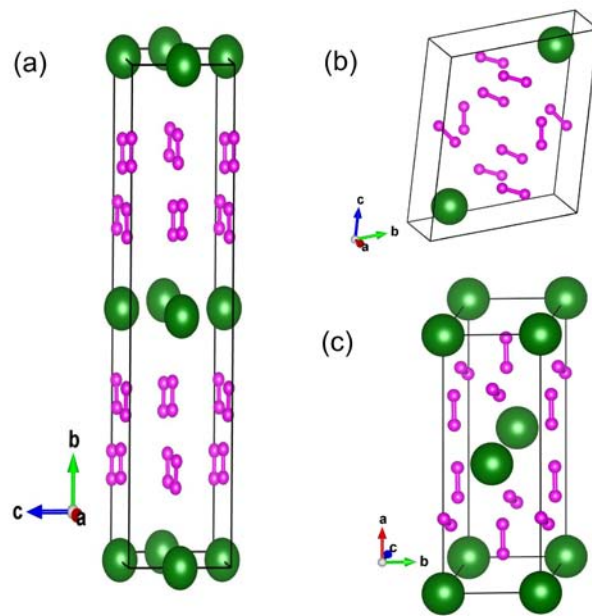


Fig. S1 Structures of $PbH_4(H_2)_2$. (a) $Pnnm$ structure at 20 GPa, (b) $P-1$ structure at 100 GPa, (c) $C2/m$ structure at 200 GPa. Large and small spheres represent Pb and H atoms, respectively.

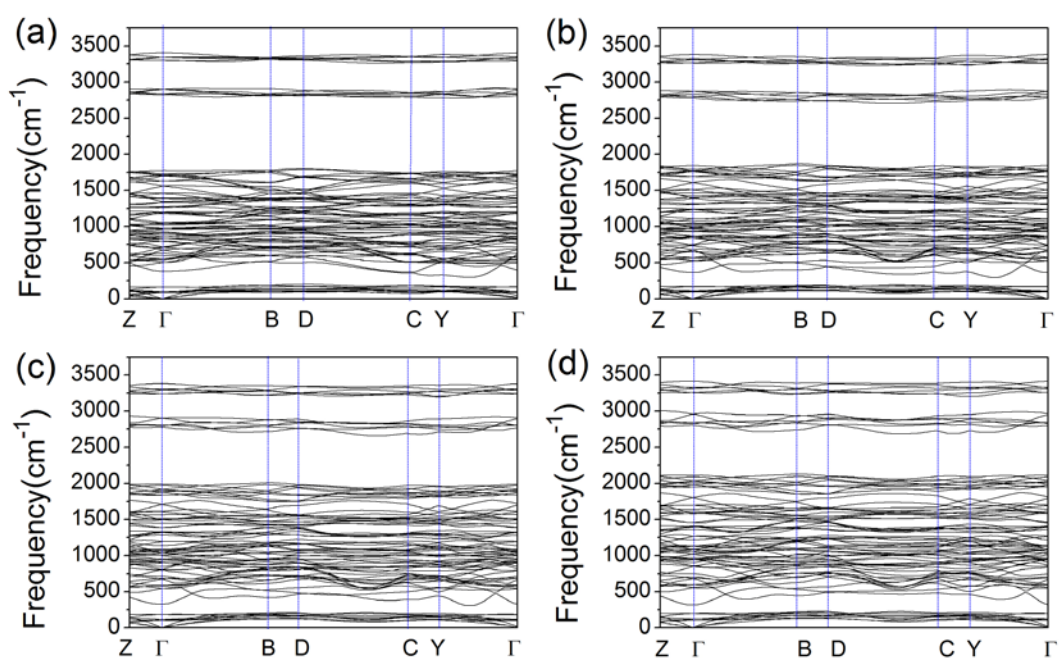


Fig. S2 Phonon spectra. Calculated phonon frequencies of $C2/m$ at 180 GPa (a), 200 GPa (b), 250 GPa (c), and 300 GPa (d), respectively.

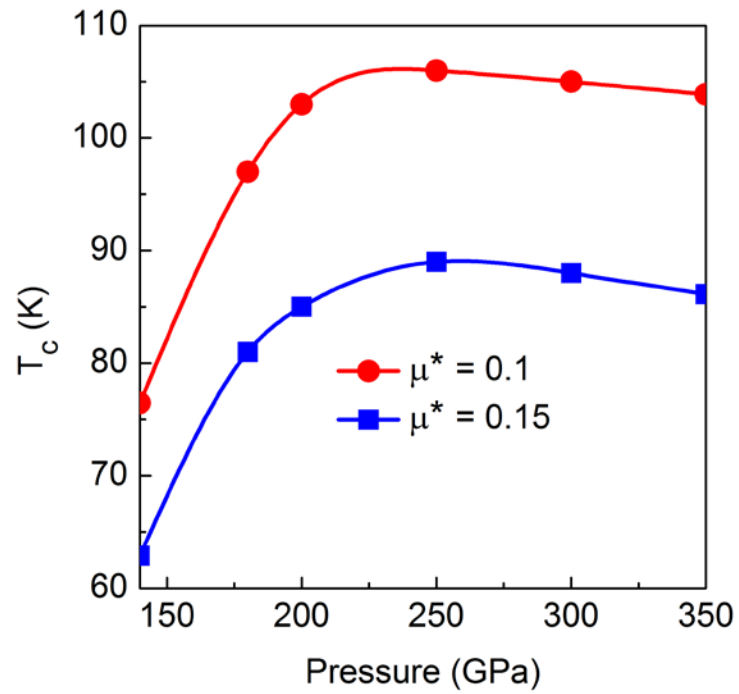


Fig. S3 Pressure effect of T_c . Calculated T_c dependence on pressure for $C2/m$ phase in the range of 133-350 GPa.

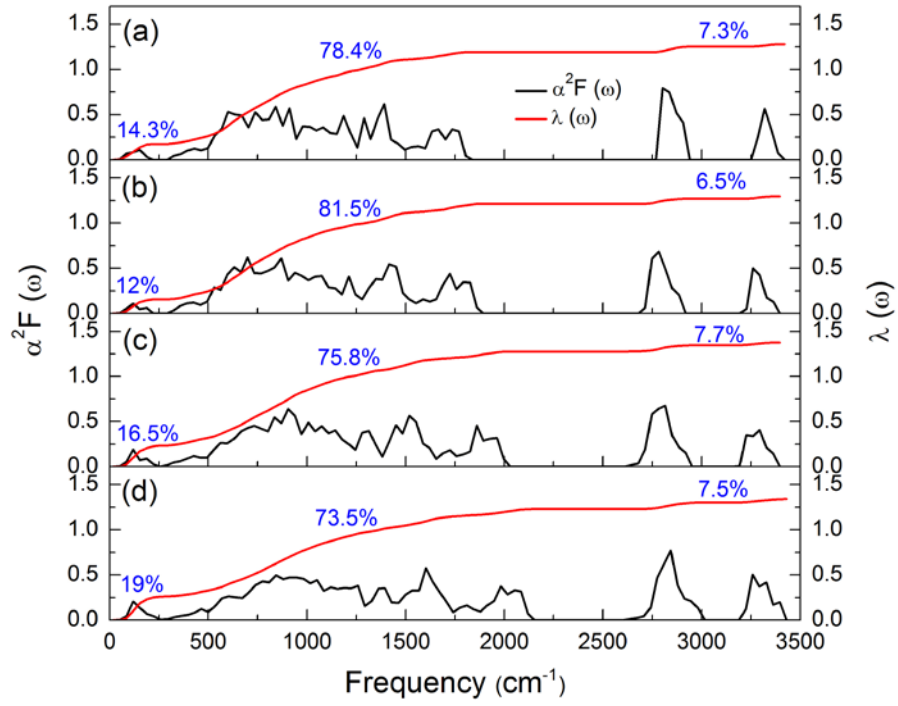


Fig. S4 Phonon properties and Eliashberg spectral function. Calculated Eliashberg phonon spectral function $\alpha^2F(\omega)$ and electron-phonon integral $\lambda(\omega)$ for the $C2/m$ structure. (a) at 180 GPa, $\lambda=1.280$, (b) at 200 GPa, $\lambda=1.296$, (c) at 250 GPa, $\lambda=1.379$, (d) at 300 GPa, $\lambda=1.341$.