

Supplementary Information

Prediction of ternary superconducting YCH_{12} by a novel solid hydrogen source under high pressure

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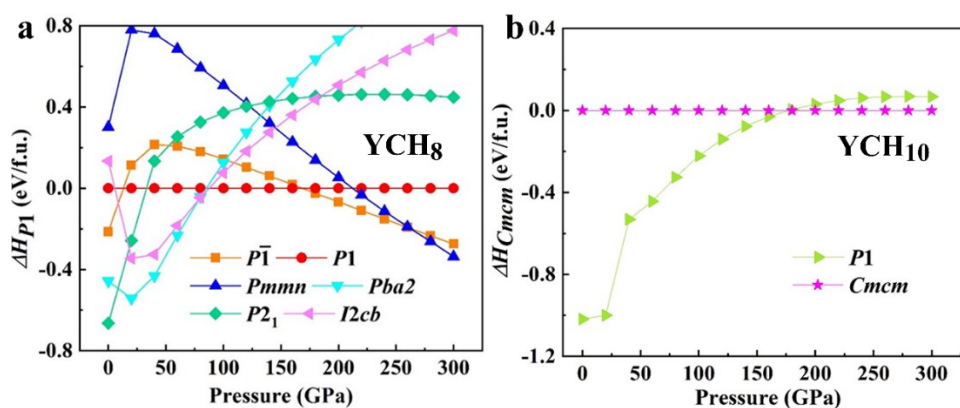


Figure S1: Relative enthalpy per formula unit referenced to the selected phases for YCH_8 (a) and YCH_{10} (b).

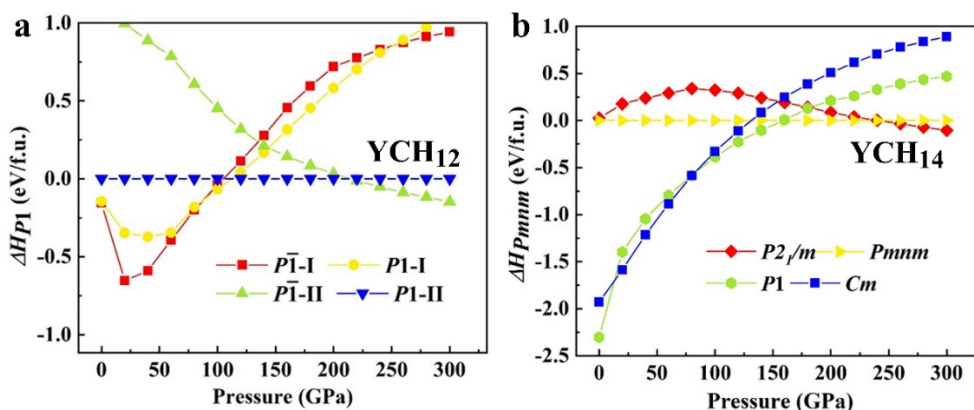


Figure S2: Relative enthalpy per formula unit referenced to the selected phases for YCH_{12} (a) and YCH_{14} (b).

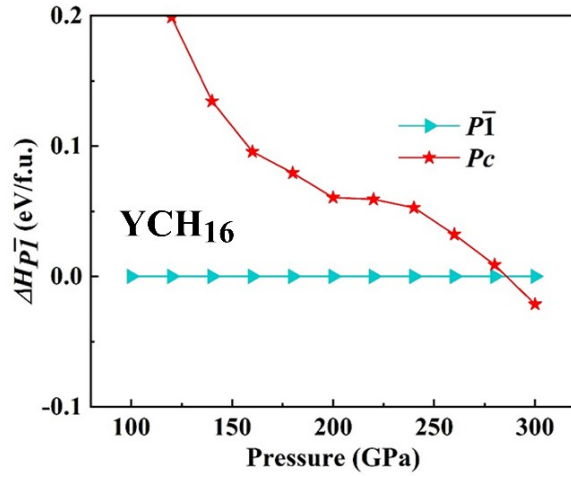


Figure S3: Relative enthalpy per formula unit referenced to the selected phases for YCH_{16} .

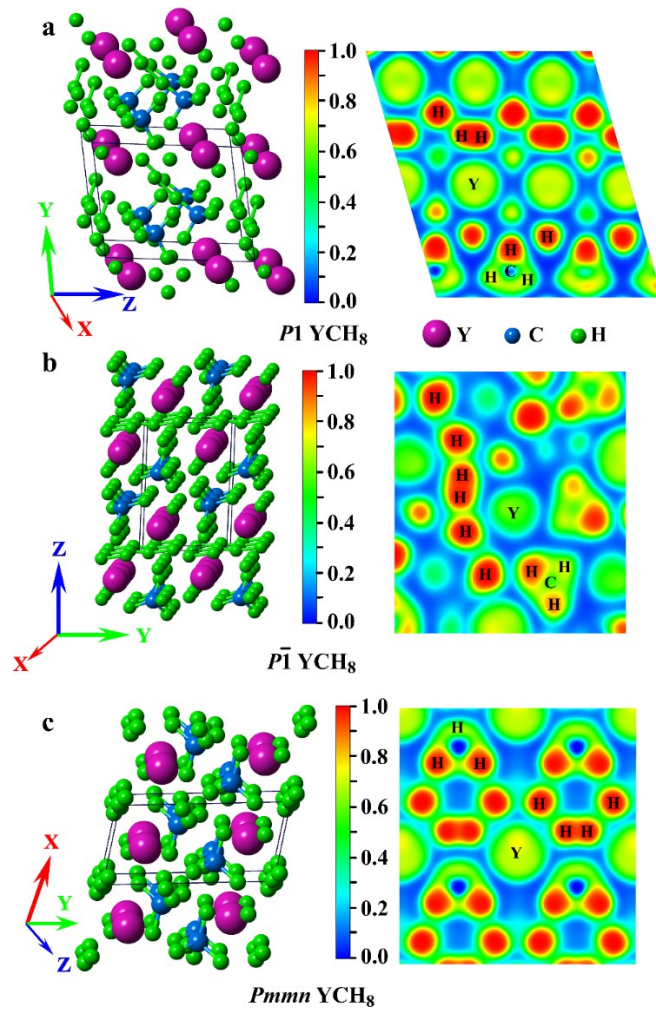


Figure S4: The predicted crystal features and the corresponding the electronic localization function (ELF) of YCH_8 : $P1$ -I at 100 GPa (a), $P\bar{I}$ -I at 200 GPa (b), $Pmmn$ at 280 GPa (c) The Y (pink), C (blue), H (green) atoms are represented by the colored spheres.

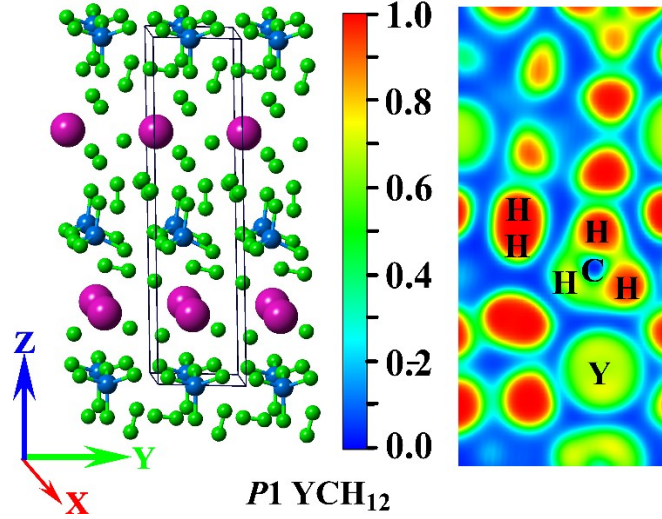


Figure S5: The predicted crystal features and the corresponding the electronic localization function (ELF) of YCH₁₂ P1-I at 100 GPa. The pink, blue, and green spheres represent Y, C, and H atoms, respectively.

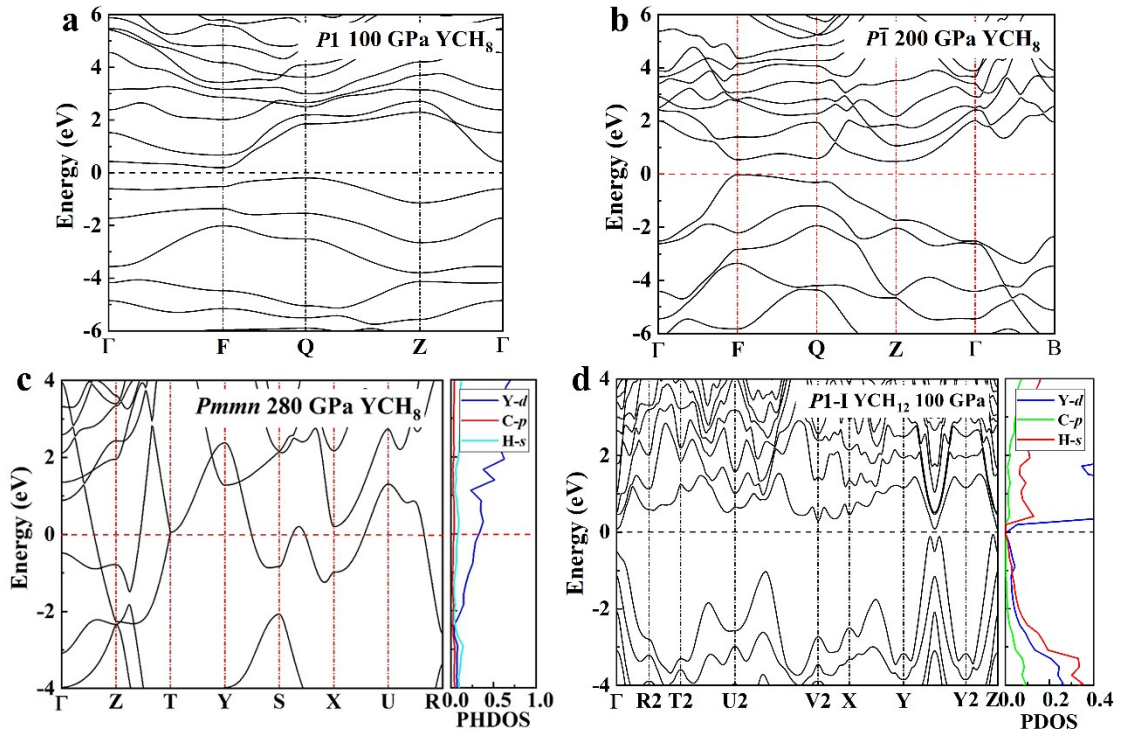


Figure S6: Calculated electronic band structure and projected density of states (PDOS) of YCH₈ P1-I at 100 GPa (a), P1-I at 200 GPa (b), Pmmn at 280 GPa (c) and YCH₁₂ P1-I at 100 GPa (d).

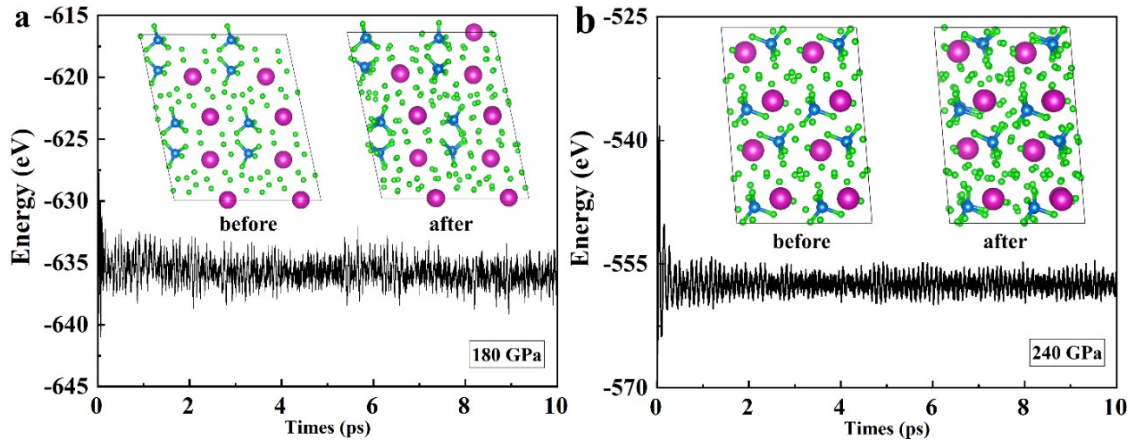


Figure S7: The variation of the free energy in the AIMD simulations over a timescale of 10 ps at 500 K in YCH_{12} $P1\text{-II}$ (a) and $P1$ (b). The snapshots represent the structures at 0 and 10 ps.

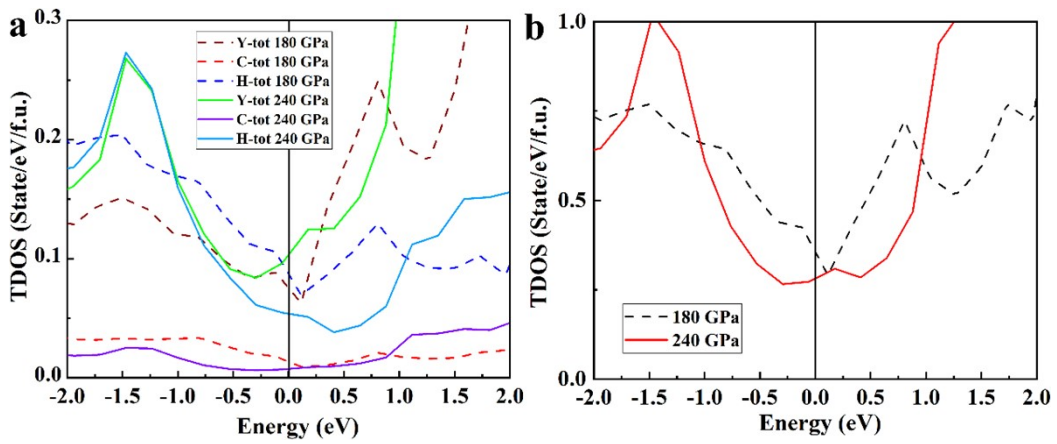


Figure S8: The total DOS of YCH_{12} $P1\text{-II}$ at 180 GPa and $P1$ at 240 GPa.

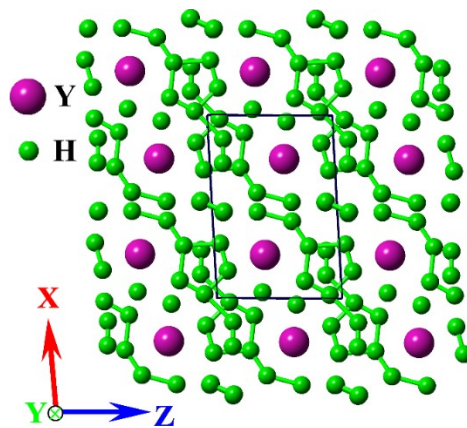


Figure S9: The crystal structure of YH_{12} $P2_1/m$ (remove the C from YCH_{12} $P1\text{-III}$ at 200 GPa) at 200 GPa.

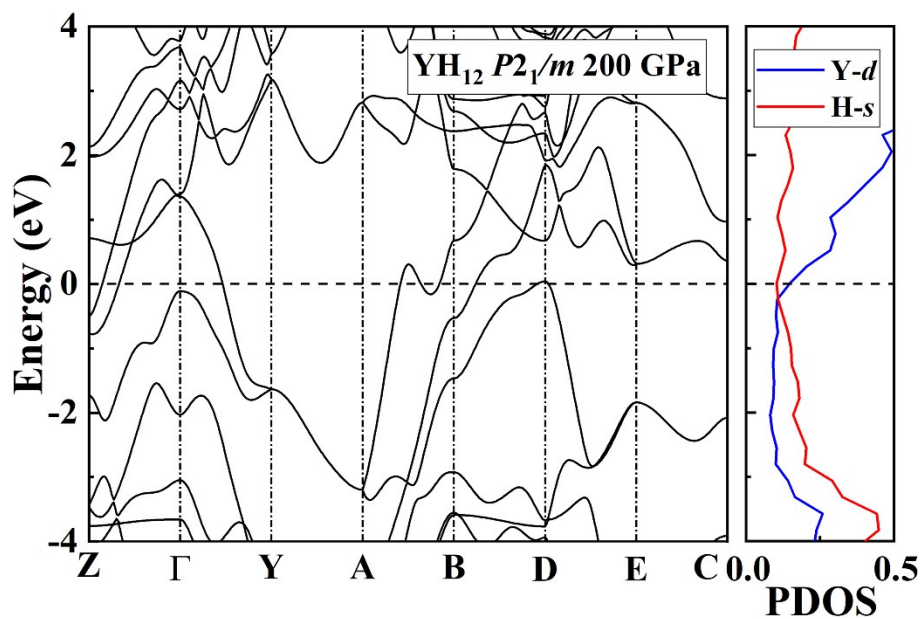


Figure S10: The calculated band structures and projected density of states (PDOS) of YH_{12} $P2_1/m$ (remove C atoms from YCH_{12} $P1$ -III) at 200 GPa.

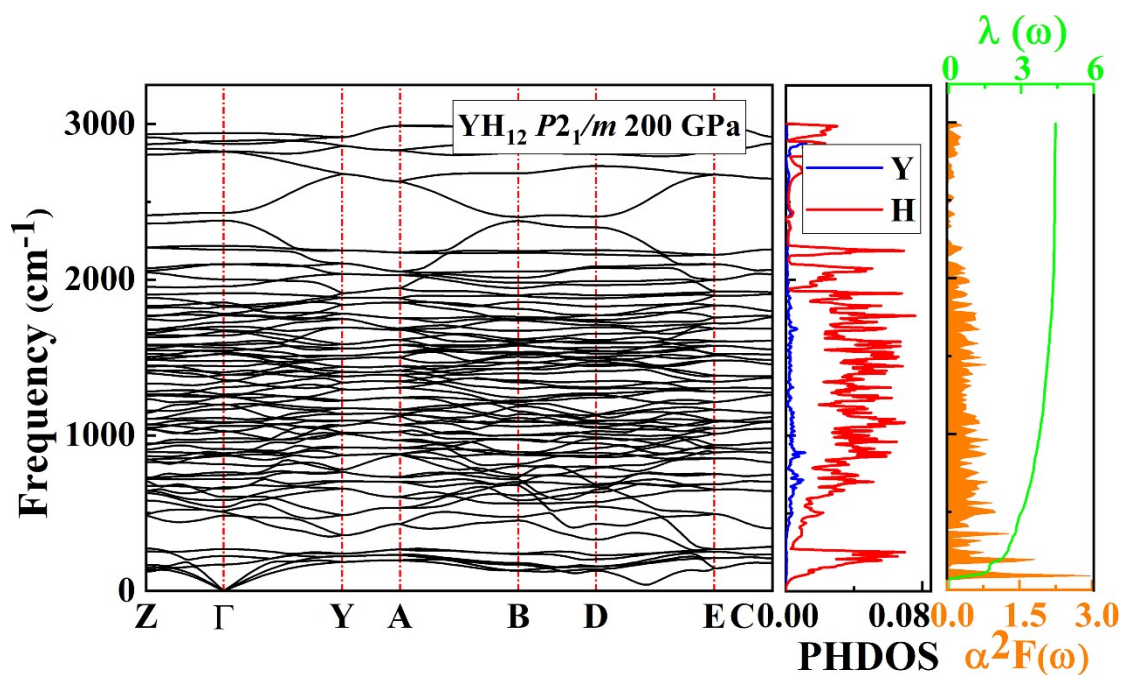


Figure S11: The calculated phonon dispersions, phonon density of states and Eliashberg phonon spectral function $\alpha^2F(\omega)$ (b) of YH_{12} $P2_1/m$ (remove C atoms from YCH_{12} $P1$ -III) at 200 GPa.

Table S1. Structural information of the predicted stable phases.

Compound	Phase	Pressure (GPa)	Lattice Parameters (Å)	Atomic Positions		
				<i>x</i>	<i>y</i>	<i>z</i>
YCH ₈	<i>P1</i>	100	a = 3.0527 b = 4.5188 c = 5.8836	Y 0.9363	0.91455	0.24225
				Y 0.34937	0.74612	0.79524
				C 0.67187	0.34860	0.32096
				C 0.09336	0.23653	0.65501
				H 0.80895	0.25299	0.75341
				H 0.19670	0.43348	0.52215
				H 0.37180	0.25192	0.77086
				H 0.02251	0.41560	0.25283
				H 0.70044	0.49236	0.46041
				H 0.48651	0.41397	0.17815
				H 0.95285	0.31987	0.00232
				H 0.81934	0.68450	0.59423
				H 0.32563	0.68662	0.12404
				H 0.21389	0.30540	0.00596
				H 0.36523	0.77390	0.44623
				H 0.71954	0.48349	0.91653
H 0.98880	0.01248	0.58549				
H 0.53515	0.11824	0.42400				
H 0.51323	0.08293	0.01309				

				H 0.92801	0.90533	0.93688
YCH ₈	$P\bar{1}$	200	a = 2.8629	Y 0.50971	0.76255	0.80226
			b = 3.9675	Y 0.49029	0.23745	0.19774
				C 0.28324	0.19462	0.62533
			c = 5.8469	C 0.71676	0.80538	0.37467
				H 0.98864	0.40479	0.36407
				H 0.01136	0.59520	0.6359
				H 0.66436	0.31018	0.63863
				H 0.33565	0.68982	0.36137
				H 0.62220	0.24863	0.88540
				H 0.37780	0.75137	0.11460
				H 0.19928	0.92580	0.57440
				H 0.80072	0.07420	0.42560
				H 0.18567	0.35288	0.50978
				H 0.81433	0.64712	0.49022
				H 0.96747	0.89005	0.00934
				H 0.03252	0.10994	0.99066
				H 0.14870	0.39489	0.01433
				H 0.85130	0.60511	0.98567
	H 0.97008	0.75803	0.21609			
	H 0.02992	0.24197	0.7839			

			a = 2.7374	Y 0.50000	0.00000	0.19560
YCH ₈	<i>Pmmn</i>	280		Y 0.00000	0.50000	0.80441
			b = 4.0892	C 0.50000	0.50000	0.44942
			c = 4.8453	C 0.00000	0.00000	0.55059
				H 0.00000	0.89977	0.94906
				H 0.00000	0.10023	0.94906
				H 0.50000	0.39977	0.05094
				H 0.50000	0.60023	0.05094
				H 0.00000	0.68689	0.15719
				H 0.00000	0.31311	0.15719
				H 0.50000	0.18689	0.84281
				H 0.50000	0.81311	0.84281
				H 0.00000	0.21037	0.42087
				H 0.00000	0.78963	0.42087
				H 0.50000	0.71037	0.57913
				H 0.50000	0.28963	0.57913
				H 0.21452	0.50000	0.30504
				H 0.78549	0.50000	0.30504
				H 0.28549	0.00000	0.69497
				H 0.71452	0.00000	0.69497
			a = 3.0923	Y 0.72027	0.04357	0.71931
				Y 0.08840	0.39487	0.20541

			b = 3.1393	C 0.04772	0.41686	0.99934
YCH ₁₂	P1-I	100	c = 11.3007	C 0.17792	0.29299	0.43183
				H 0.37808	0.73752	0.84093
				H 0.77358	0.98146	0.90176
				H 0.37571	0.71082	0.67942
				H 0.54672	0.61117	0.56013
				H -0.00142	0.95204	0.55748
				H 0.05520	0.37046	0.63790
				H 0.71070	0.44349	0.03049
				H 0.40412	0.74567	0.14141
				H 0.73699	0.07833	0.13245
				H 0.02271	0.06980	0.40686
				H 0.99316	0.64374	0.38516
				H 0.55857	0.09018	0.41349
				H 0.79934	0.99707	0.29122
				H 0.57614	0.45791	0.32586
				H 0.44450	0.73194	0.30825
				H 0.02916	0.41444	0.90367
				H 0.08683	0.72370	0.02931
				H 0.36774	0.08032	0.03243
				H 0.15538	0.34748	0.52559
				H 0.53051	0.61102	0.49418

				H 0.76813	0.94309	0.54258'
				H 0.59179	0.23940	0.89063
				H 0.05171	0.39198	0.79715
				H 0.34356	0.81183	0.90530
			a = 2.7812	Y 0.53522	0.72728	0.00807
YCH ₁₂	P1-II	180	b = 4.9524	Y 0.03076	0.60316	0.49184
			c = 5.7184	C 0.51812	0.23214	0.93266
				C 0.03245	0.14510	0.56716
				H 0.53129	0.50161	0.25675
				H 0.53343	0.52356	0.69148
				H 0.03709	0.53401	0.82210
				H 0.02733	0.53491	0.14531
				H 0.53061	0.35184	0.34243
				H 0.27601	0.30506	0.64919
				H 0.74966	0.35230	0.84265
				H 0.05369	0.33792	0.18875
				H 0.04863	0.01171	0.12107
				H 0.03997	0.00462	0.97937
				H 0.53495	0.90414	0.55730
				H 0.64248	0.99229	0.30464
				H 0.64335	0.22218	0.10091
				H 0.17089	0.31290	0.94273

				H 0.69334	0.22564	0.53482'
				H 0.16668	0.02095	0.40941
				H 0.51011	0.10954	0.26093
				H 0.51271	0.04272	0.81283
				H 0.00537	0.02859	0.70340
				H 0.04721	0.23237	0.27421
				H 0.52794	0.77135	0.33829
				H 0.53080	0.83177	0.67716
				H 0.02427	0.84072	0.79630
				H 0.04563	0.81940	0.24828
				<hr/>		
			a = 3.6903	Y 0.84186	0.67659	0.25322
YCH ₁₂	$P\bar{1}$	240	b = 4.0333	Y 0.15814	0.32341	0.74678
			c = 5.3018	C 0.51342	0.28150	0.16385
				C 0.48658	0.71850	0.83615
				H 0.70275	0.50057	0.51499
				H 0.29725	0.49943	0.48501
				H 0.00379	0.76159	0.96408
				H 0.99621	0.23841	0.03592
				H 0.62394	0.32083	0.57452
				H 0.37606	0.67917	0.42548
				H 0.33217	0.20490	0.26044
				H 0.66783	0.79510	0.73956

H 0.92306	0.99234	0.54152
H 0.07694	0.00766	0.45848
H 0.90919	0.96446	0.85893
H 0.09081	0.03554	0.14107
H 0.74621	0.26547	0.31573
H 0.25379	0.73453	0.68428
H 0.65021	0.09121	0.01310
H 0.34979	0.90879	0.98690
H 0.34024	0.55146	0.09294
H 0.65976	0.44854	0.90706
H 0.75238	0.14101	0.77226
H 0.24762	0.85899	0.22774
H 0.90229	0.75475	0.60899
H 0.09771	0.24525	0.39101
H 0.45848	0.91596	0.49380
H 0.54152	0.08404	0.50620

Table S2. The calculated superconducting transition temperature T_c with correction factors for YCH_{12} $P1\text{-II}$ and $P\bar{1}$ phases under various μ^*

Pressure (GPa)	μ^*	0.08	0.10	0.13
	160		89	84
180		108	112	101
200		108	104	98
220		41	37	26
240		94	86	74
300		44	37	28