

Supporting information for: Unexpected Stable Phases of Tungsten Borides

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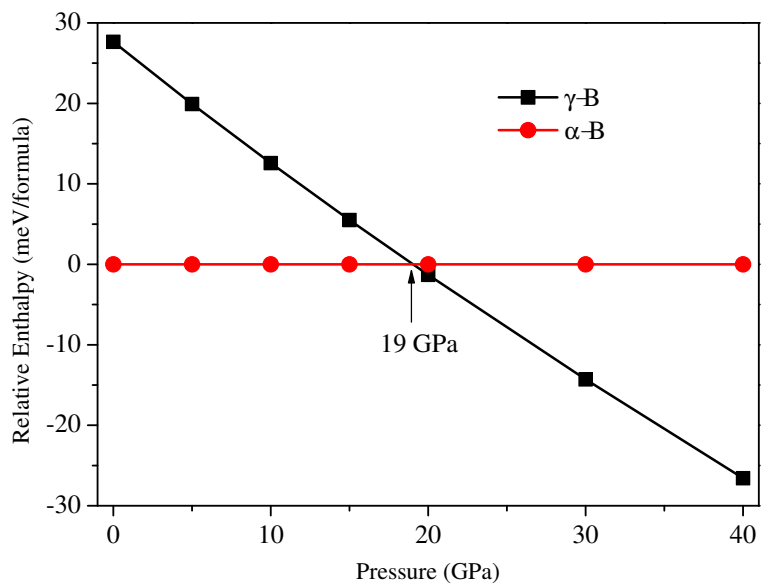


Fig. S1: Enthalpy curves (relative to α phase) for γ phase of B as a function of pressure.

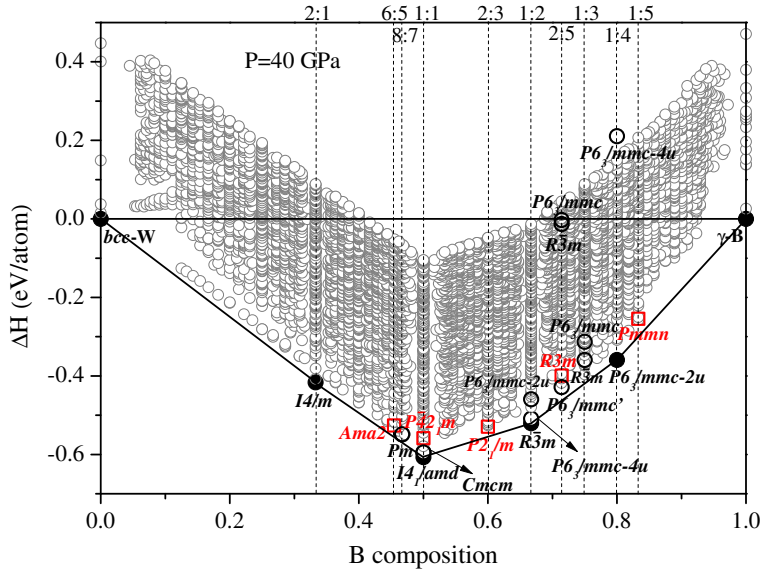


Fig. S2: Thermodynamic convex hull of the W-B system predicted by our structure search at 40 GPa.

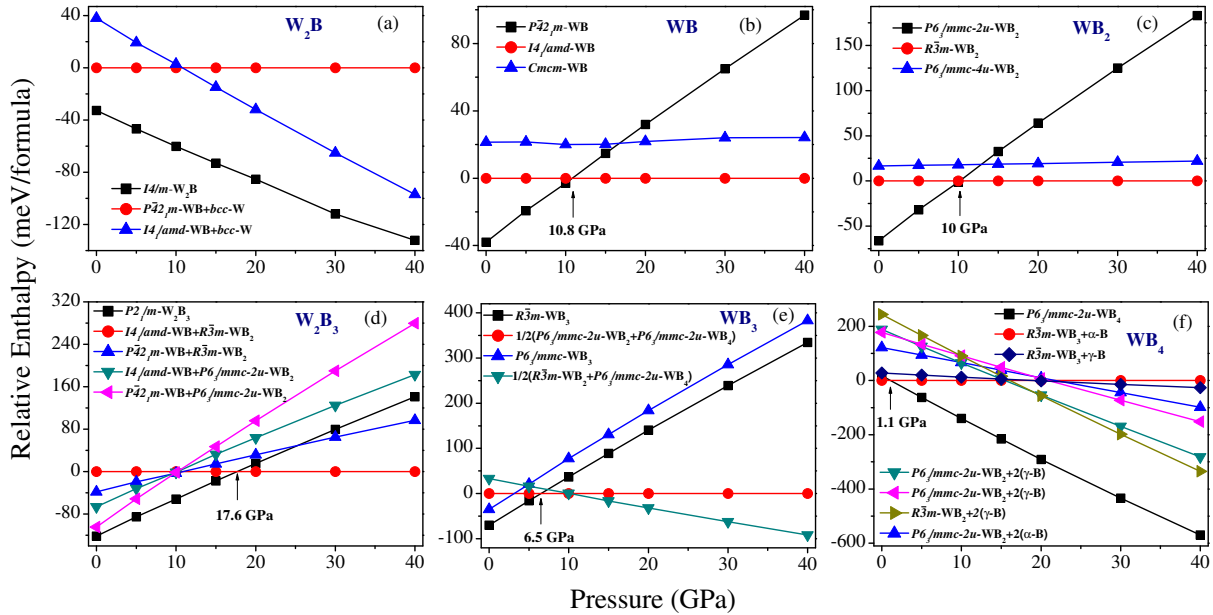


Fig. S3: Calculated enthalpies as the function of pressure for the thermodynamic stable $W_{1-x}B_x$. (a) $14/m$ - W_2B . (b) $P4_2m$ - WB . (c) $P2_1/m$ - W_2B_3 . (d) $P6_3/mmc-4u$ - WB_2 . (e) $R3m$ - WB_3 . (f) $P6_3/mmc-2u$ - WB_4 .

TABLE S1: Crystal structures of the reported tungsten borides at ambient pressure.

	Structure	Parameters (°,)	Atom	x	y	z	
W ₂ B	<i>I4/m</i>	a=b=5.5810 c=4.7542	W(8h)	0.32395	0.16472	0.0	
			B(4e)	0.0	0.0	0.27675	
W ₈ B ₇	<i>Pm</i>	a=6.2796 b=6.1312 c=4.5433 $\beta = 110.19$	W(2c)	0.16179	0.25277	0.93483	
			W(2c)	0.65334	0.25333	0.93508	
			W(1a)	0.01136	0.0	0.34838	
			W(1a)	0.51135	0.0	0.35259	
			W(1b)	0.01545	0.5	0.35658	
			W(1b)	0.51045	0.5	0.35630	
			B(2c)	0.80559	0.25007	0.52579	
			B(2c)	0.30529	0.25508	0.52660	
			B(1a)	0.86725	0.0	0.77425	
			B(1a)	0.36548	0.0	0.76486	
			B(1b)	0.86664	0.5	0.76746	
WB	<i>I4₁/amd(α)</i>	a=b=3.1398 c=16.9522	W(8e)	0.5	0.0	0.0531	
			B(8e)	0.5	0.5	0.65614	
	<i>Cmcm(β)</i>	a=3.1761 b=8.4824 c=3.1019	W(4c)	0.0	0.14519	0.75	
			B(4c)	0.0	0.43882	0.75	
WB ₂	<i>R$\bar{3}m$</i>	a=b=3.0151 c=21.0663	W(6c)	0.66667	0.33333	0.75698	
			B(6c)	0.66667	0.33333	0.65162	
			B(6c)	0.0	0.0	0.83205	
	<i>P6₃/mmc-2u</i>	a=b=2.9274 c=7.7479	W(2c)	0.33333	0.66667	0.25	
			B(4f)	0.33333	0.66667	0.54064	
	<i>P6₃/mmc-4u</i>	a=b=3.0188 c=14.0220	W(4f)	0.33333	0.66667	0.36451	
			B(4f)	0.33333	0.66667	0.97689	
				B(2d)	0.33333	0.66667	0.75
				B(2b)	0.0	0.0	0.25
	W ₂ B ₅	<i>R$\bar{3}m$</i>	a=b=3.0937 c=21.3685	W(6c)	0.0	0.0	0.07642
B(6c)				0.0	0.0	0.33119	
B(6c)				0.0	0.0	0.18537	
B(3b)				0.0	0.0	0.5	
<i>P6₃/mmc</i>		a=b=3.0956 c=14.2372	W(4f)	0.33333	0.66667	0.13525	
			B(2b)	0.0	0.0	0.25	
			B(4f)	0.33333	0.66667	0.97278	
			B(2d)	0.33333	0.66667	0.75	
			B(2a)	0.0	0.0	0.0	
<i>P6₃/mmc'</i>		a=b=3.0169 c=15.7070	W(4e)	0.0	0.0	0.39697	
			B(2b)	0.0	0.0	0.25	
			B(4f)	0.33333	0.66667	0.30270	
			B(4f)	0.33333	0.66667	0.49717	
WB ₃	<i>R$\bar{3}m$</i>	a=b=5.2130 c=9.4050	W(6c)	0.0	0.0	0.16617	
			B(18f)	0.33502	0.0	0.0	
	<i>P6₃/mmc</i>	a=b=5.1975 c=6.3156	W(2b)	0.0	0.0	0.25	
			W(2c)	0.33333	0.66667	0.25	
			B(12i)	0.33481	0.0	0.0	
WB ₄	<i>P6₃/mmc-2u</i>	a=b=2.9524 11.0026	W(2d)	0.33333	0.66667	0.75	
			B(4f)	0.33333	0.66667	0.54552	
			B(4f)	0.33333	0.66667	0.11109	
	<i>P6₃/mmc-4u</i>	a=b=5.3674 c=6.4287	W(2b)	0.0	0.0	0.25	
			W(2c)	0.33333	0.66667	0.25	
			B(12i)	0.33705	0.0	0.0	
			B(4f)	0.33333	0.66667	0.61841	

TABLE S2: Elastic constants C_{ij} of tungsten borides at ambient pressure.

	Structure	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{23}	C_{25}	C_{35}	C_{46}
W ₂ B	<i>I4/m</i>	583		542	165		187	209	236			-27				
W ₆ B ₅	<i>Ama2</i>	578	568	589	236	217	257	224	222				234			
W ₈ B ₇	<i>Pm</i>	567	579	580	211	233	255	226	242		-1		229	0.5	-0.4	0.3
WB	<i>P$\bar{4}$2₁m</i>	737		609	255		211	124	191							
	<i>I4₁/amd(α)</i>	575		600	236		256	237	242							
	<i>Cmcm(β)</i>	524	567	568	220	249	234	270	238				253			
W ₂ B ₃	<i>P2₁/m</i>	749	589	596	258	275	234	163	202		19		176	-11	14	-8
WB ₂	<i>P6₃/mmc-2u</i>	607		988	288		223	161	99							
	<i>R$\bar{3}$m</i>	621		780	242		236	149	168	21						
W ₂ B ₅	<i>R3m</i>	560		918	280		197	166	121	26						
WB ₃	<i>R$\bar{3}$m</i>	656		475	277		284	88	178	0.1						
	<i>P6₃/mmc</i>	644		481	264		270	104	167							
WB ₄	<i>P6₃/mmc-2u</i>	588		1003	230		239	111	97							
	<i>P6₃/mmc-4u</i>	401		439	150		71	259	230							
WB ₅	<i>Pmmn</i>	591	631	637	279	277	284	142	131				93			