Supporting Information

Computational Search for New W–Mo–B Compounds

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Crystal Data

Table S1. Crystal structures, distance to convex hull, and zero-point energy of the predicted W–Mo–B phases.

Phase	Volume of unit, Å^3	Lattice parameters	Coordinates				Δ*H*, meV/atom	ZPE, meV/atom
			Sym.	*x*	*y*	*z*		
Pm-$W_4Mo_4B_{15}$	217.34	*a* = 5.198 Å, *b* = 5.999 Å, *c* = 7.183 Å, β = 76.01°	W1	0.4612	-0.2532	0.2230	0	13.7
			W2	-0.3878	-0.2545	-0.2279		
			Mo1	0.0340	0.0000	0.2246		
			Mo2	-0.0331	0.5000	0.2228		
			Mo3	0.1152	0.0000	-0.2284		
			Mo4	0.1176	0.5000	0.2265		
			B1	-0.2130	0.0000	-0.0037		
			B2	0.2799	0.5000	0.4544		
			B3	0.3582	-0.2599	-0.4577		
			B4	-0.1271	-0.2512	0.0001		
			B5	0.3057	-0.2513	-0.0030		
			B6	0.3704	-0.2533	0.0008		
			B7	0.2224	0.5000	0.4513		
			B8	-0.1453	0.0000	-0.4554		
			B9	0.2205 8	0.0000	0.4536		
			B10	-0.1423	0.5000	-0.4562		
			B11	-0.2942	0.0000	-0.0041		
*P*1-W_5MoB_{14}	182.74	*a* = 8.356 Å, *b* = 5.198 Å, *c* = 5.198 Å, α = 60.04° β = γ = 108.02°	W1	-0.3982	-0.3047	-0.4202	5.1	14.55
			W2	0.3978	0.0375	-0.0914		
			W3	-0.0051	0.1708	0.0440		
			W4	0.0052	-0.1696			
			W5		0.3665			
			Mo1		-0.4996			

	Volume	Lattice	Coordinates				Δ*H*,	ZPE,
			B1	-	0.3026	-		
			B2	0.3981	0.2689	0.2859		
			B3	0.0052	-0.1005	0.2503		
			B4	0.4092	-0.3993	0.3846		
			B5	0.3036	-0.4346	-		
			B6	0.1974	-0.0650	0.1507		
			B7	0.3044	0.1095	0.1456		
			B8	0.1977	0.4339	0.4437		
			B9	0.3036	0.1002	0.4803		
			B10	-	-0.2427	0.1108		
			B11	0.1964	-0.2328	-		
			B12	-	-0.3632	0.1884		
			B13	0.1965	0.2299	-		
			B14	-	-0.0318	0.3535		
				0.1971		-		
				-		0.0301		
				0.1967		0.3131		
				-		0.3229		
				0.1959		-		
				0.4094		0.0198		
				0.1974		0.1816		
				0.4092		-		
						0.2211		
						-		
						0.4850		
$P3m1$-WMo_2B_{11}	124.96	*a* = *b* = 3.008 Å, *c* = 15.942 Å, α = β = 90° γ = 120°	W1	0.3333	0.6667	0.3575	5.2	13.96
			Mo1	0.3333	0.6667	-		
			Mo2	0.6667	0.3333	0.3391		
			B1	0.6667	0.3333	0.0092		
			B2	0.6667	0.3333	0.1512		
			B3	0.6667	0.3333	0.2621		
			B4	0.3333	0.6667	-		
			B5	0.3333	0.6667	0.4393		
			B6	0.3333	0.6667	0.2163		
			B7	0.6667	0.3333	0.1065		
			B8	0.6667	0.3333	-		
			B9	0.3333	0.6667	0.4914		
			B10	0.3333	0.6667	0.4574		
			B11	0.6667	0.3333	-		
						0.2441		

	Volume	Lattice	Coordinates	Δ*H*,	ZPE,
			- 0.0886 - 0.1980 - 0.1333		

Phase	Volume of unit, Å^3	Lattice parameters	Coordinates				Δ*H*, meV/atom	ZPE, meV/atom
			Sym.	*x*	*y*	*z*		
$P\bar{1}$-WMo_2B_3	62.77	*a* = b =5.505 Å, *c* = 4.429 Å, α = 79.20° β = 100.78° γ = 78.37°	W1 Mo1 Mo2 B1 B2 B3	0.4385 0.1047 0.2270 - 0.4768 0.1912 0.1446	-0.2287 0.1075 -0.4376 -0.1436 0.1902 0.4767	-0.0831 0.2497 0.4166 0.4169 -0.2498 -0.0831	4.1	10.76
Pm- WMo_5B_6	125.55	*a* = 4.558 Å, *b* = 3.094 Å, *c* = 8.992 Å, β = 81.93°	W1 Mo1 Mo2 Mo3 Mo4 Mo5 B1 B2 B3 B4 B5 B6	0.4049 0.0716 - 0.1126 0.2204 - 0.4471 - 0.2611 - 0.2874 - 0.0885 - 0.4229 0.3790 0.2450 0.0472	0.5000 0.5000 0.0000 0.0000 0.0000 0.5000 0.0000 0.5000 0.5000 0.0000 0.5000 0.0000	0.4117 -0.2547 -0.4919 0.1757 -0.1586 0.0782 0.2733 0.3133 -0.3536 -0.3934 -0.0204 -0.0598	2.5	11.02

Crystal Structure Details

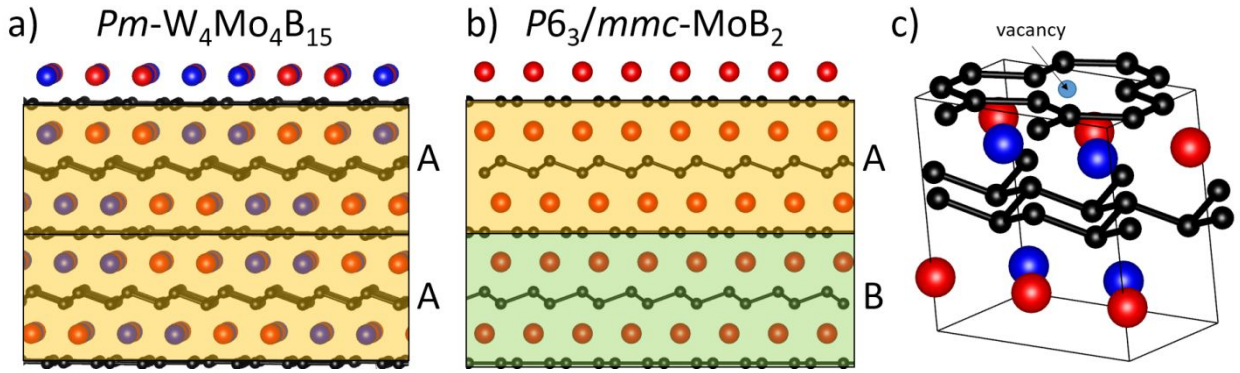

Figure S1. Crystal structures of (a) *Pm*-$W_4Mo_4B_{15}$ and (b) *P*6$_3$/*mmc*-MoB_2. (c) Boron vacancy in the hexagonal B layer of *Pm*-$W_4Mo_4B_{15}$.

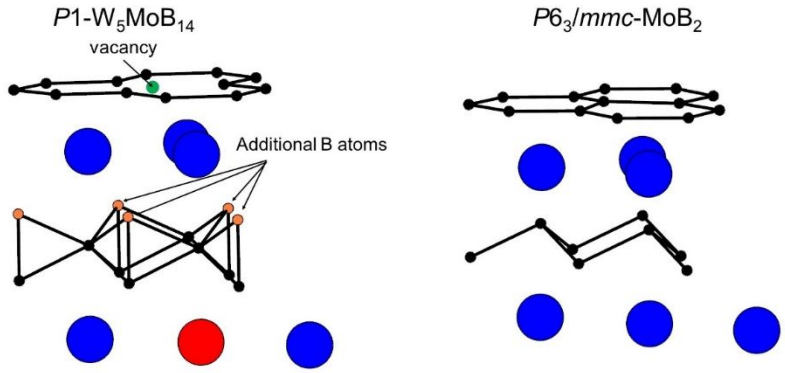

Figure S2. Crystal structures of *P*1-W_5MoB_{14} and *P*6$_3$/*mmc*-MoB_2. The atoms of molybdenum, tungsten, and boron are shown by red, blue, and black circles, respectively. Orange circles indicate additional boron atoms with respect to the *P*6$_3$/*mmc*-MoB_2 structure.

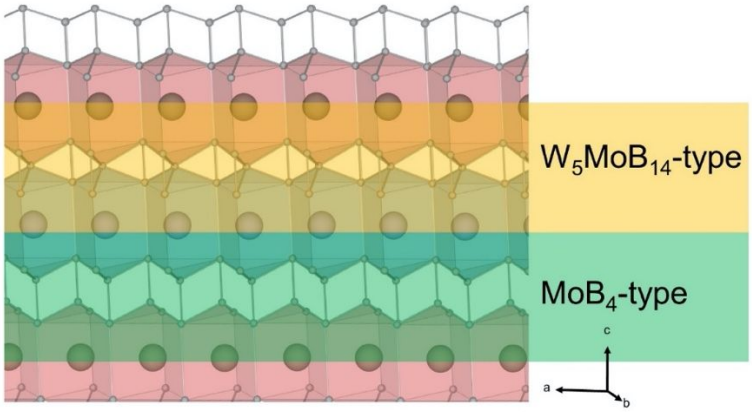

Figure S3. Crystal structure of $P\bar{3}m1$-WMo_2B_{11}.

Phonons

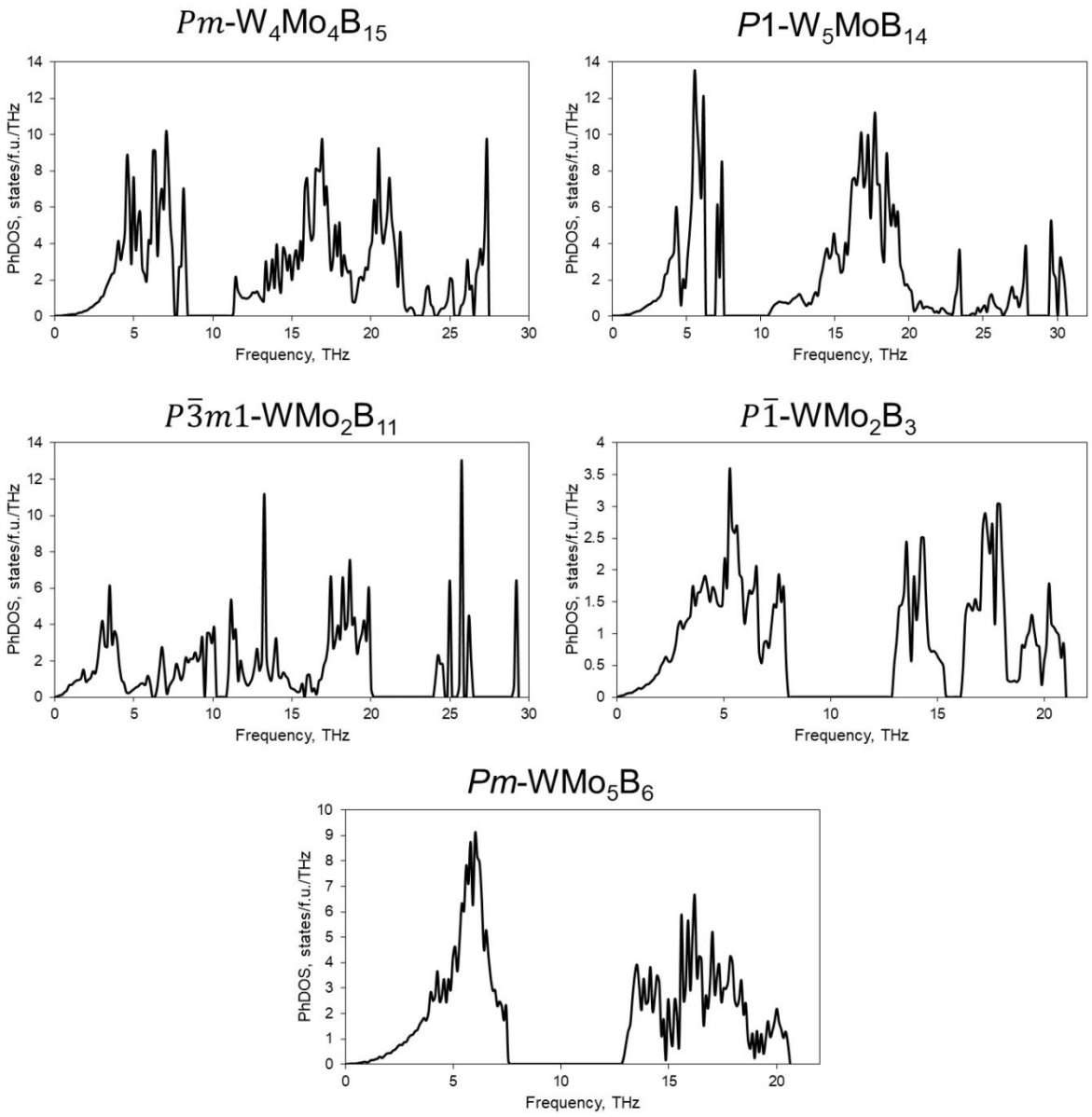

Figure S4. Phonon densities of states for the predicted W–Mo–B compounds.

Electronic Properties

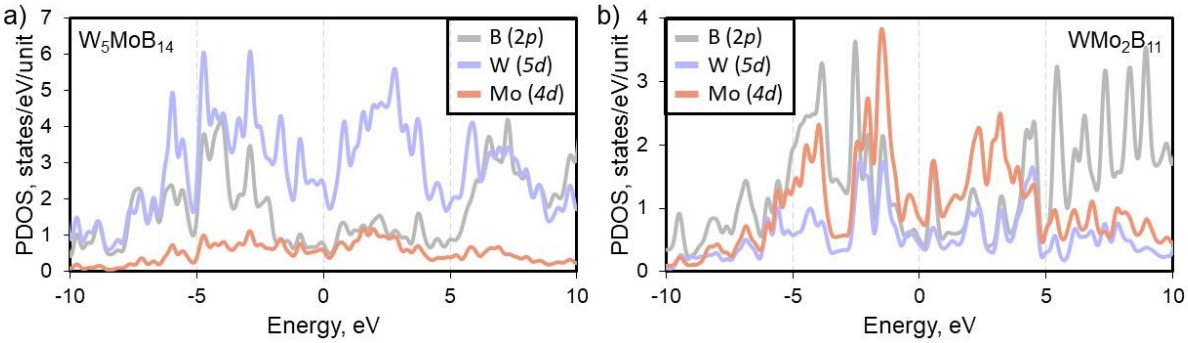

Figure S5. Projected densities of states of (c) W_5MoB_{14}, and (d) WMo_2B_{11}: gray, boron; red, molybdenum; blue, tungsten.

Configurational Entropy

Table S2. Configurational entropy contribution to Gibbs free energy (TS_{conf}) of each ternary compound calculated using Boltzmann's entropy formula.

	TS_{conf}, meV/atom					
	0 K	300 K	500 K	1000 K	1500 K	2000 K
$W_4Mo_4B_{15}$	0.043	12.998	21.664	43.328	64.992	86.656
W_5MoB_{14}	0.023	7.020	11.700	23.400	35.100	46.800
WMo_2B_{11}	0.016	4.871	8.119	16.237	24.356	32.475
WMo_2B_3	0.055	16.572	27.620	55.240	82.860	110.480
WMo_5B_6	0.039	11.786	19.643	39.285	58.928	78.570